Summary

September 26, 2022

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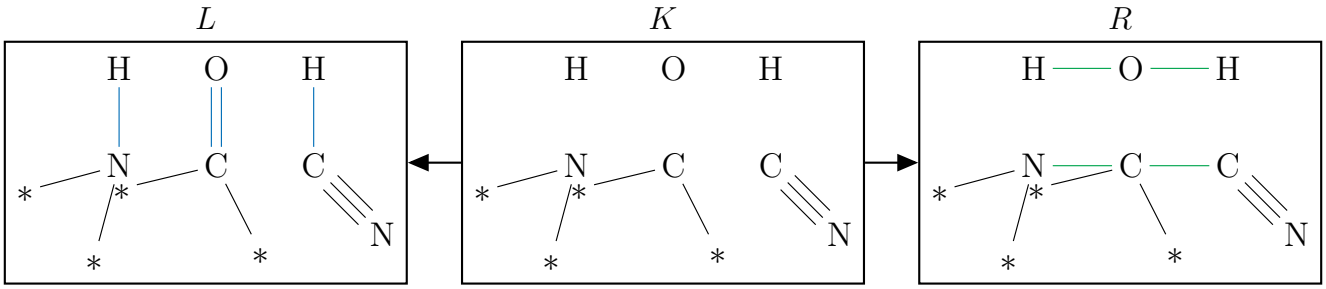
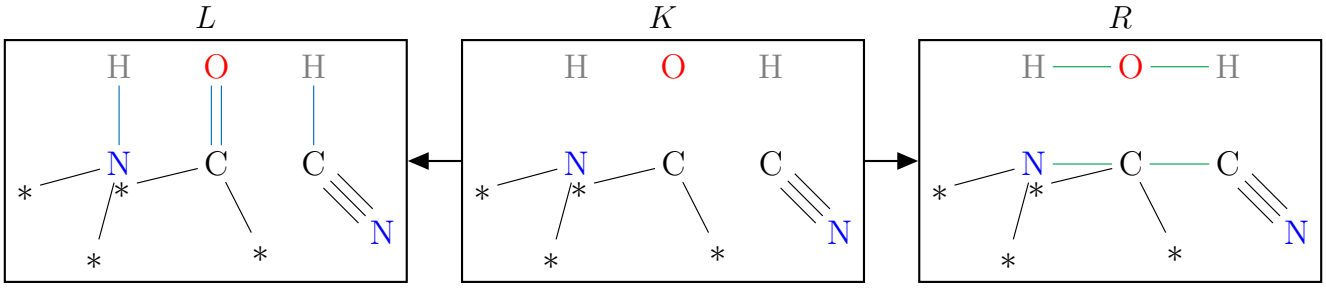
0.0.1 Strecker Synthesis



Files: out/001_r_106_10300000_{L, K, R}



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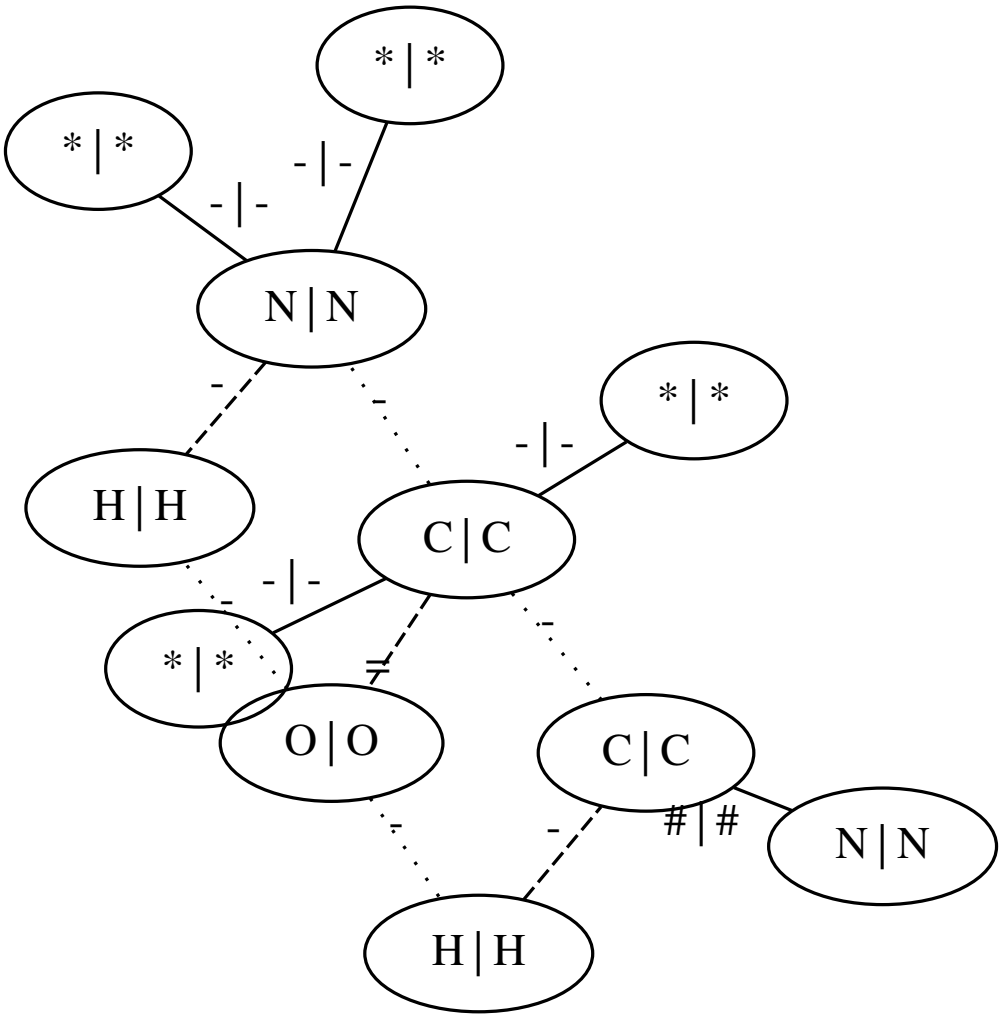


File: out/003_r_106_combined

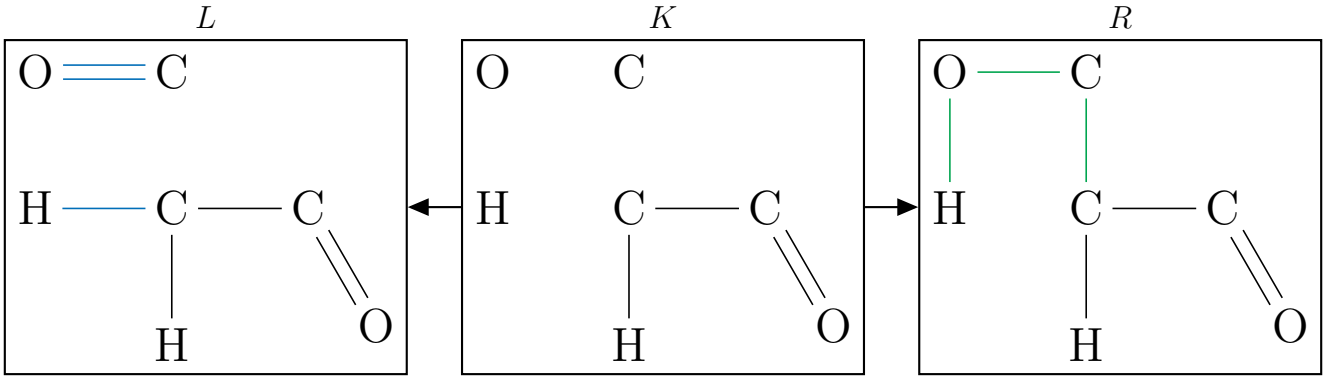
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(4) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

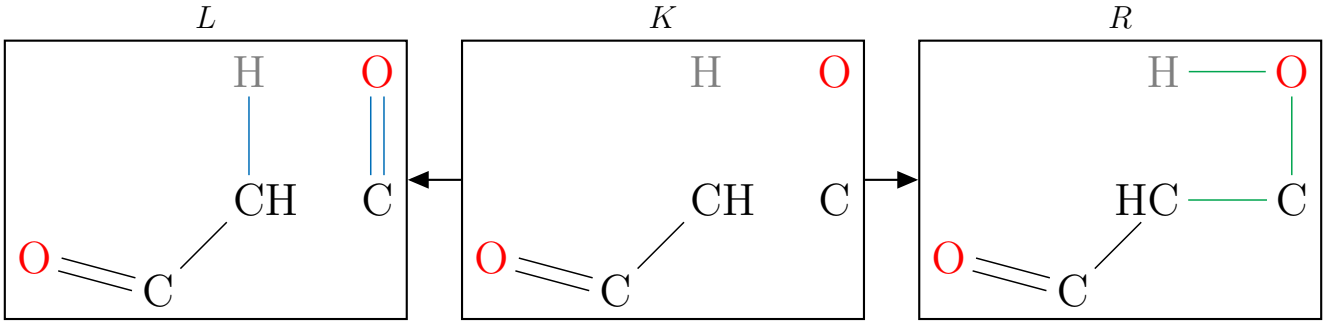
$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

0.0.2 Aldol Condensation



Files: out/006_r_0_10300000_{L, K, R}



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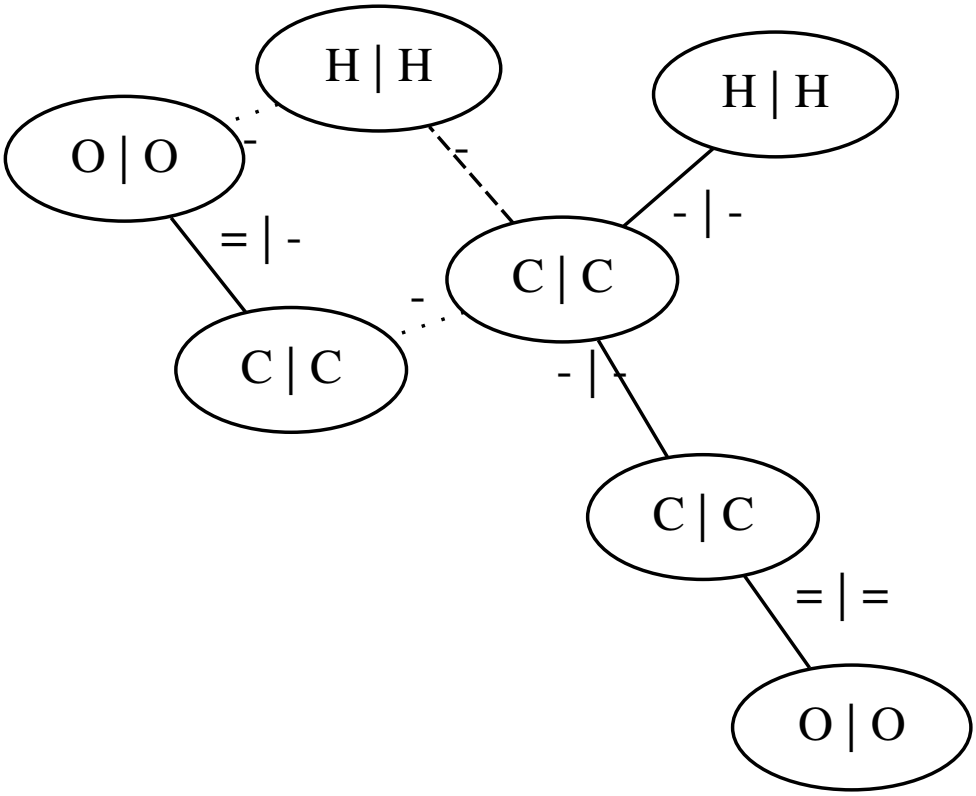

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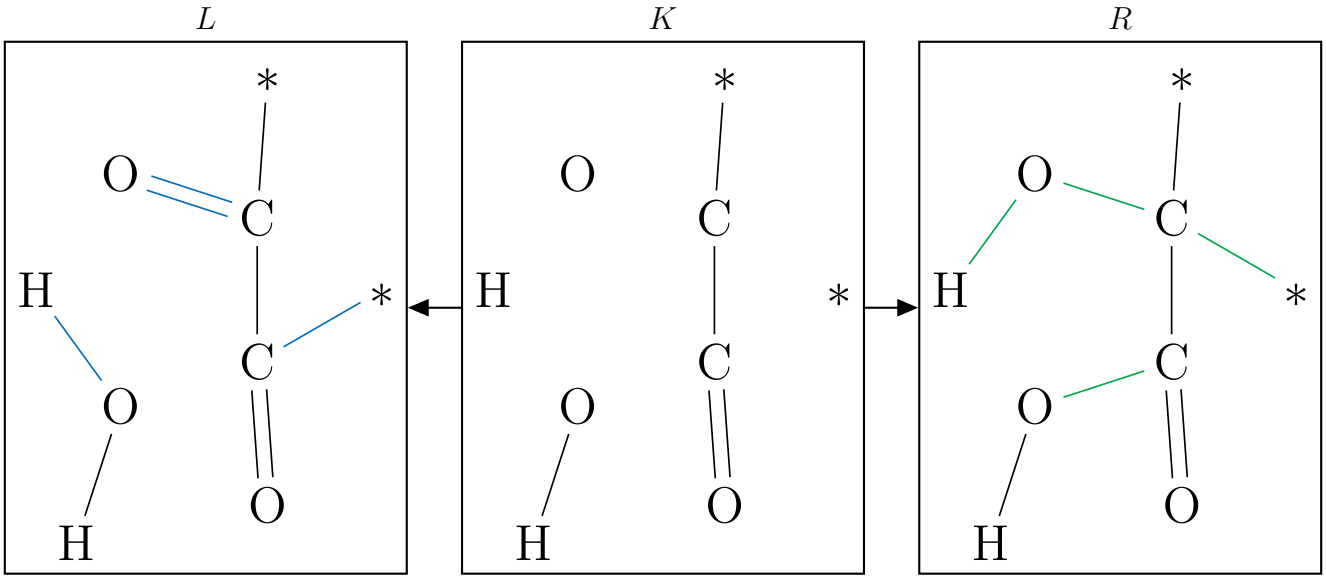
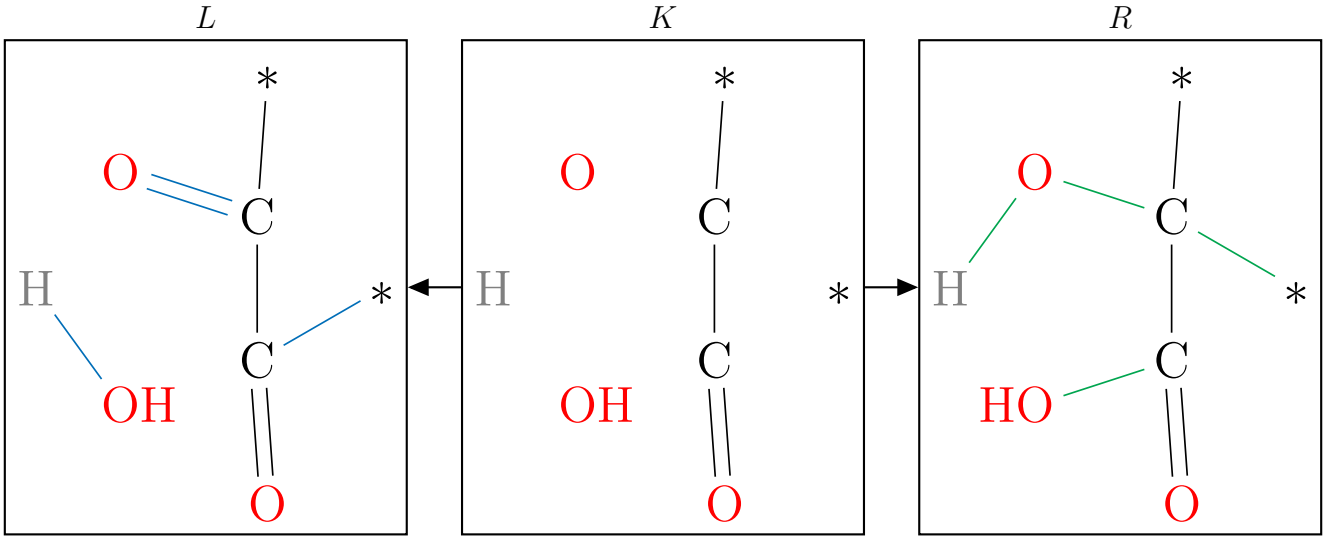
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

0.0.3 Benzilic Acid Rearrangement



Files: out/011_r_1_10300000_{L, K, R}



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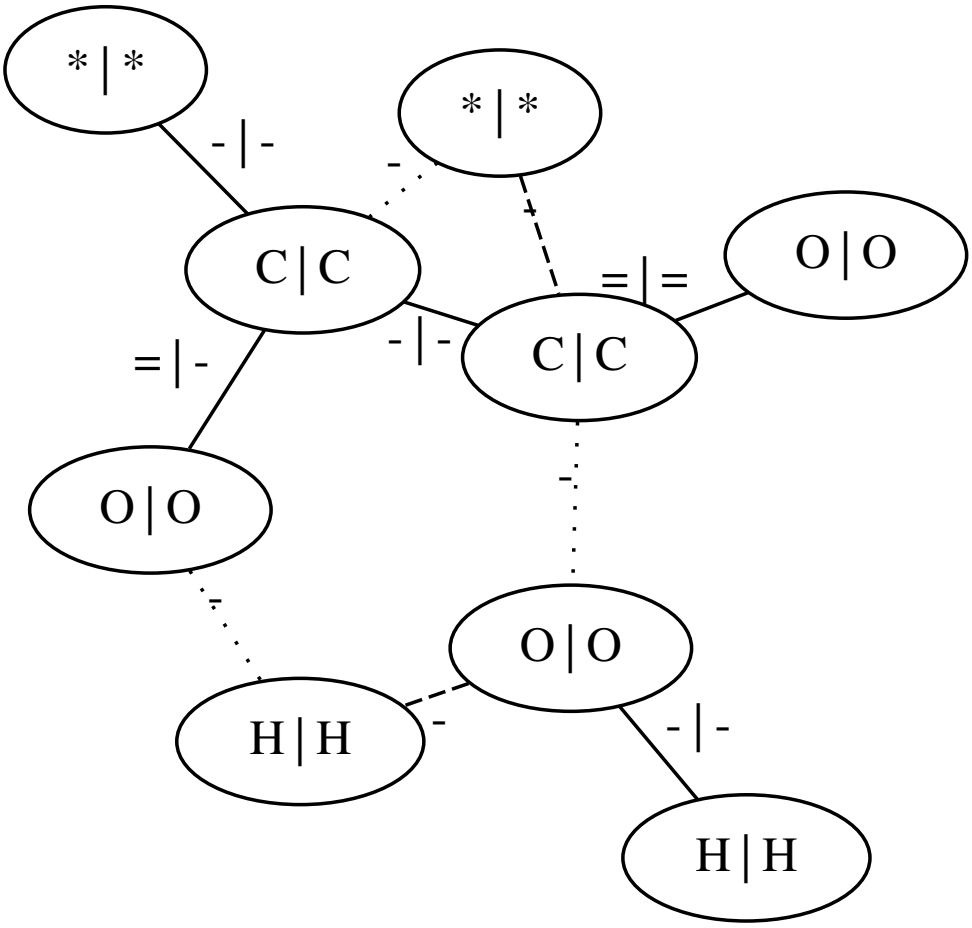

File: out/013_r_1_combined

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\begin{aligned}
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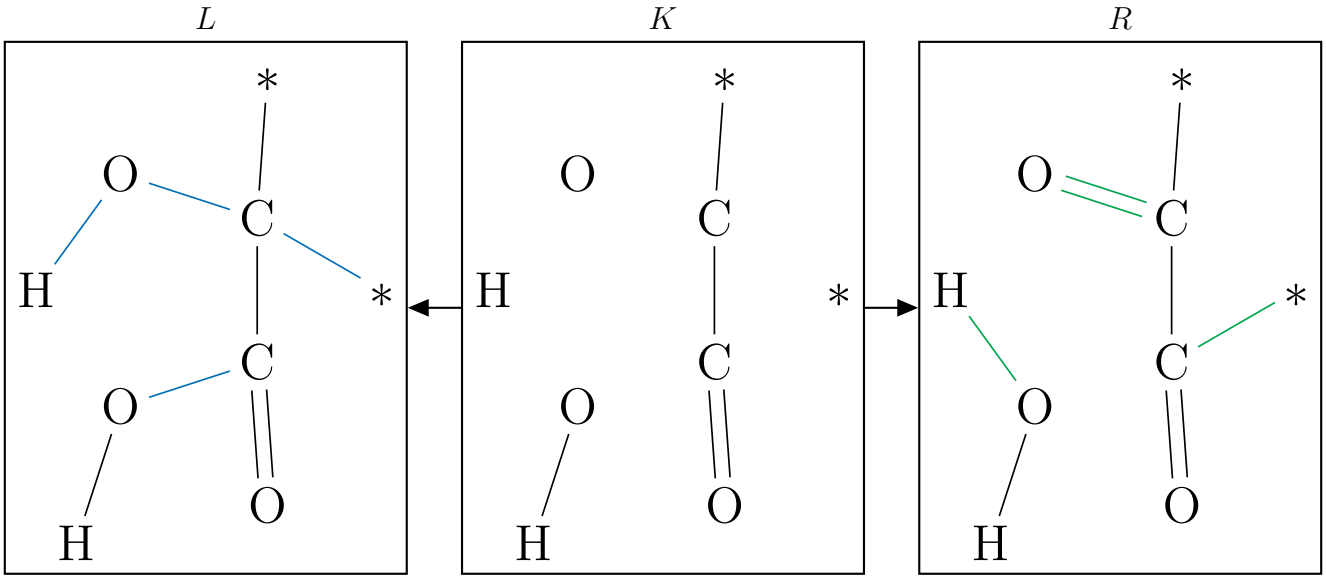
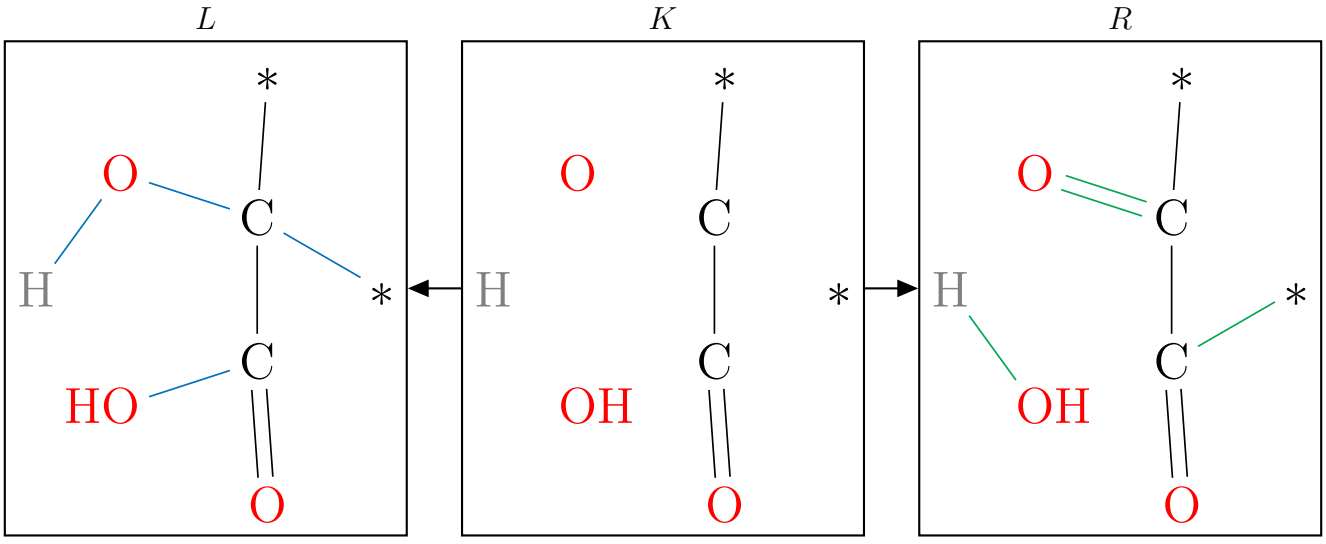
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

0.0.4 Benzilic Acid Rearrangement (inverse)



Files: out/016_r_2_10300000_{L, K, R}



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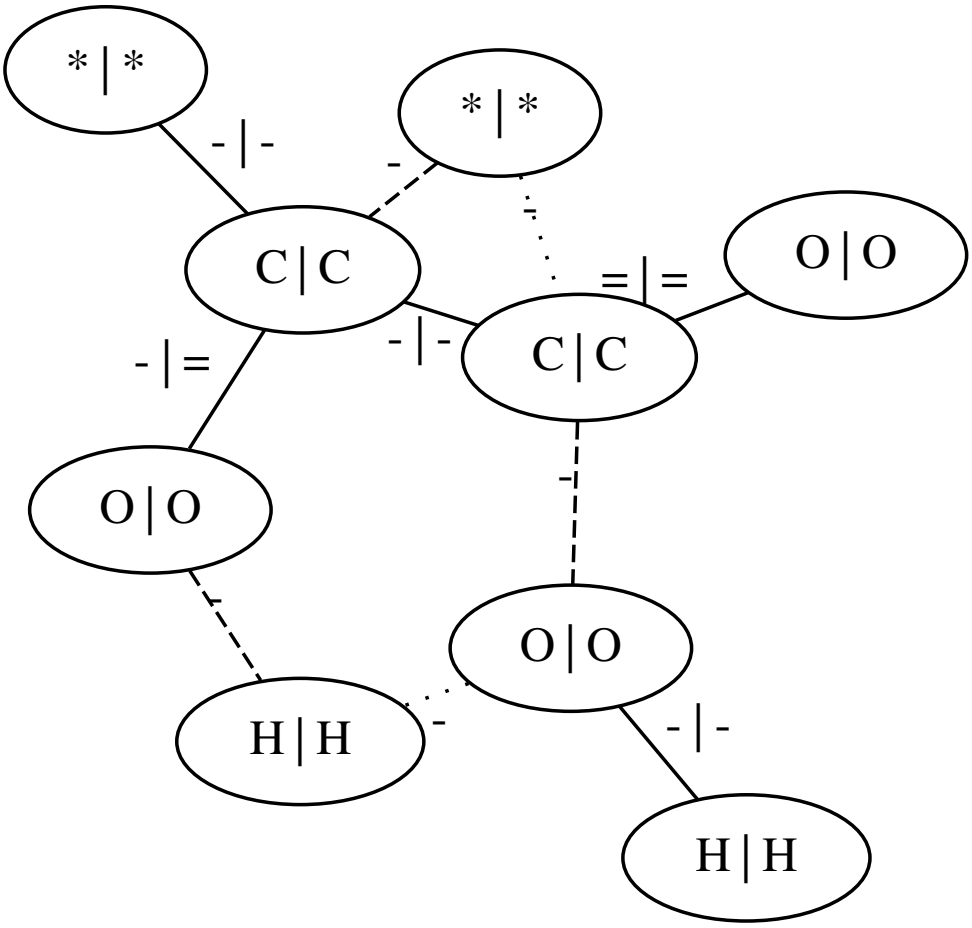

File: out/018_r_2_combined

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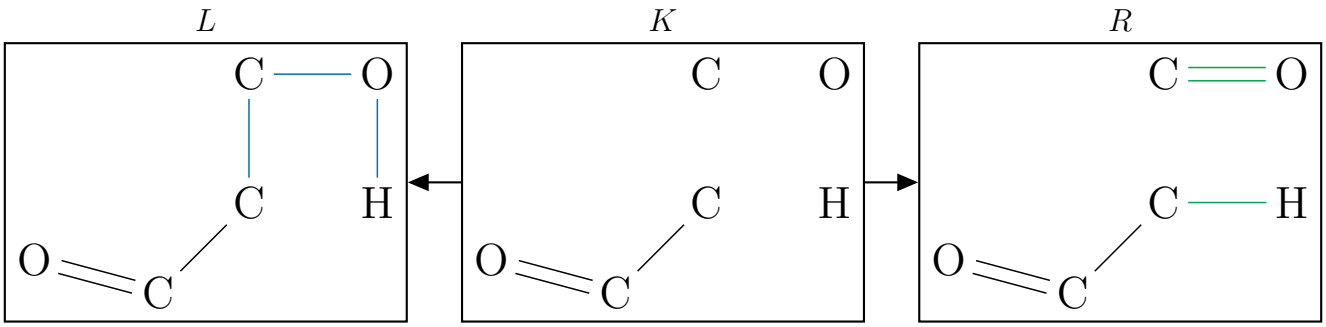
$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

0.0.5 Retro Aldol



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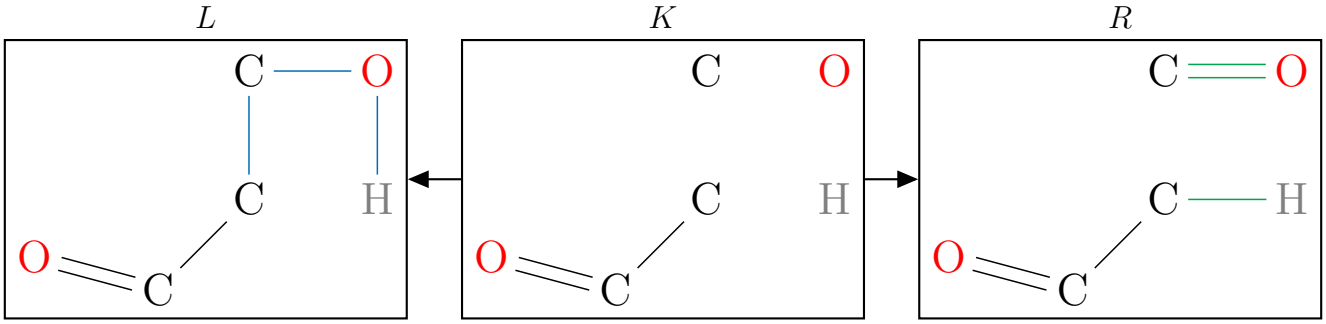

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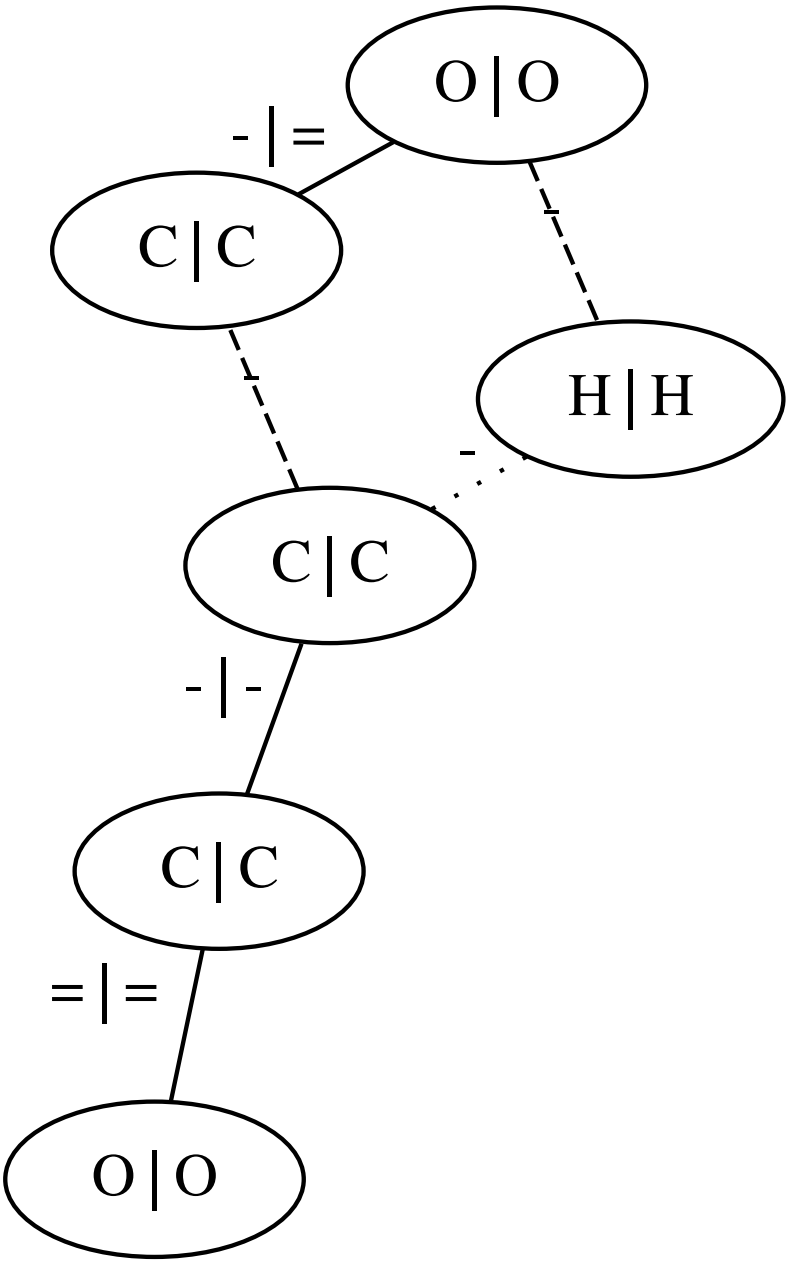

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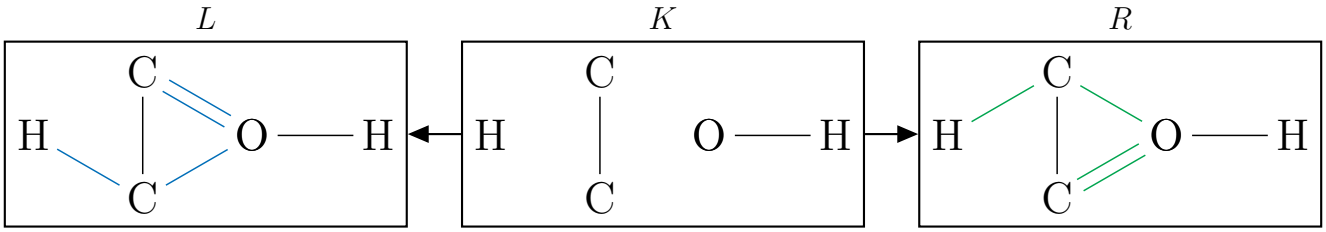
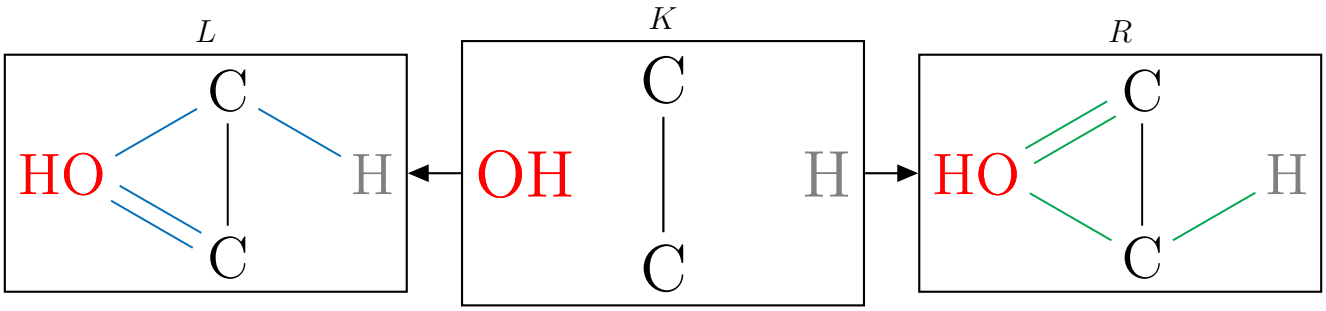
$$
\begin{aligned}
&|\{e \in \text{outEdges}(3) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

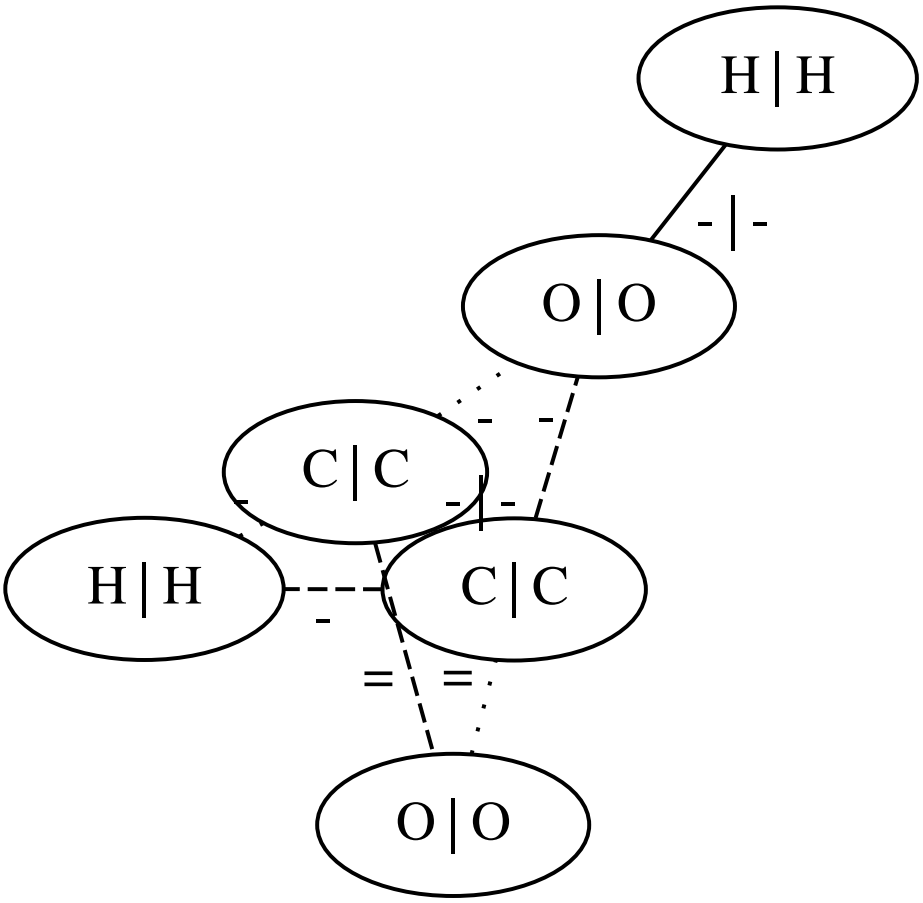
0.0.6 Keto-enol migration twice



Files: out/026_r_4_10300000_{L, K, R}



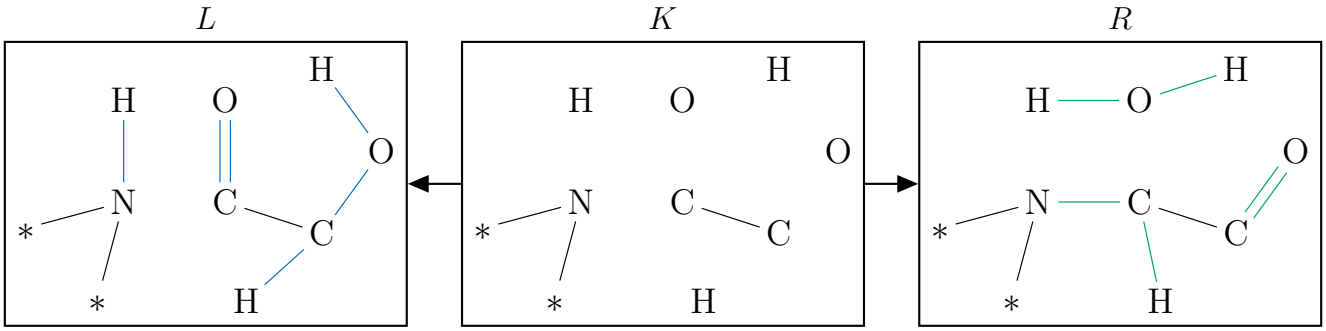
Files: out/027_r_4_11300100_{L, K, R}



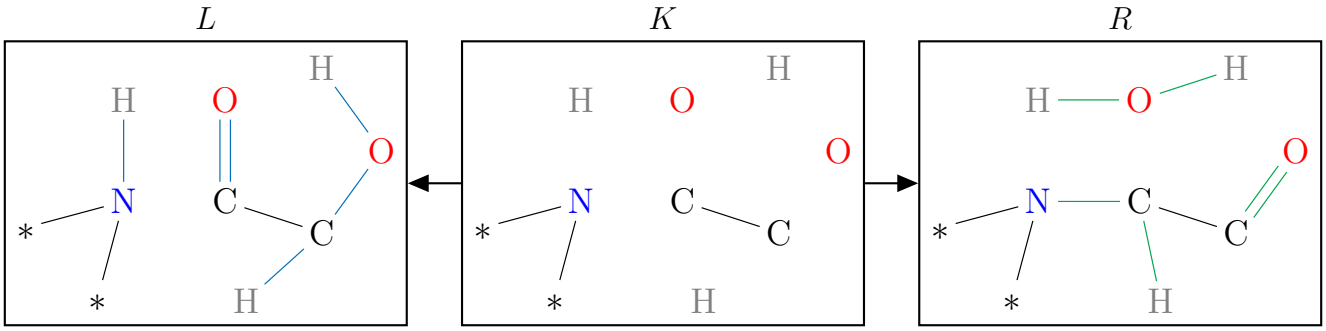
File: out/028_r_4_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

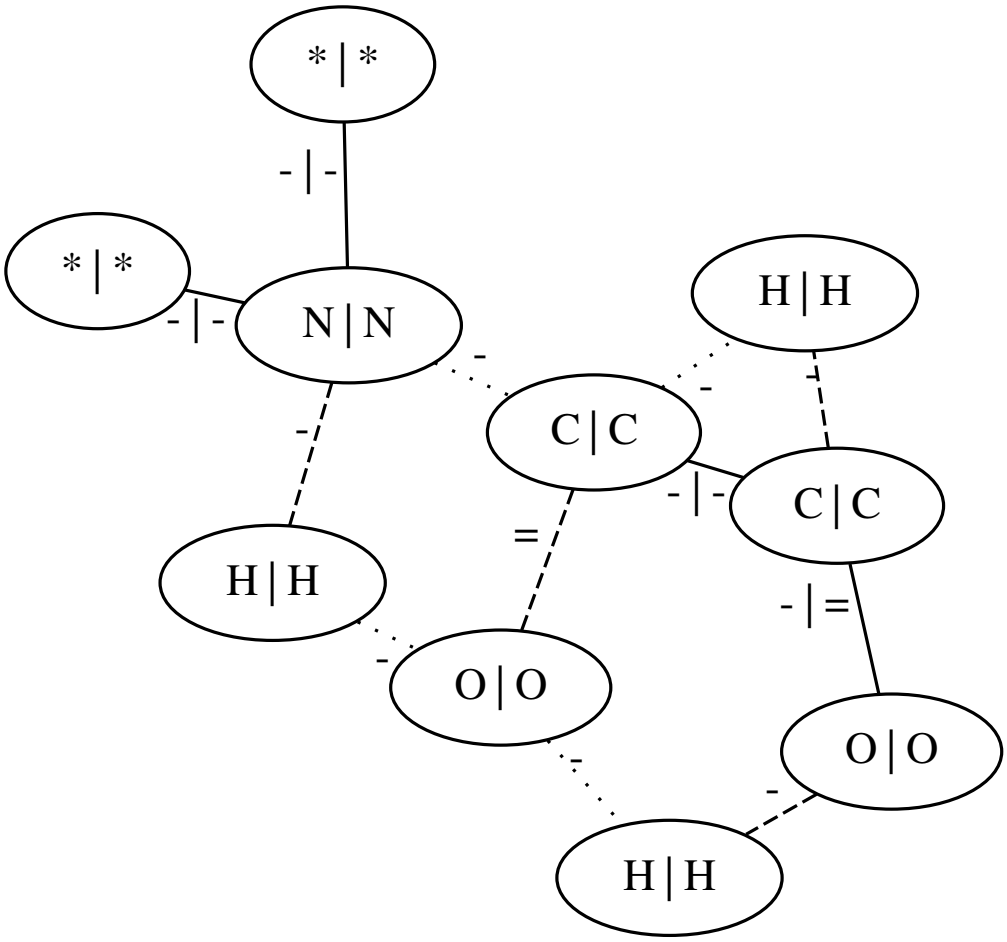
0.0.7 Amadori/Heyns Rearrangement



Files: out/031_r_5_10300000_{L, K, R}



Files: out/032_r_5_11300100_{L, K, R}



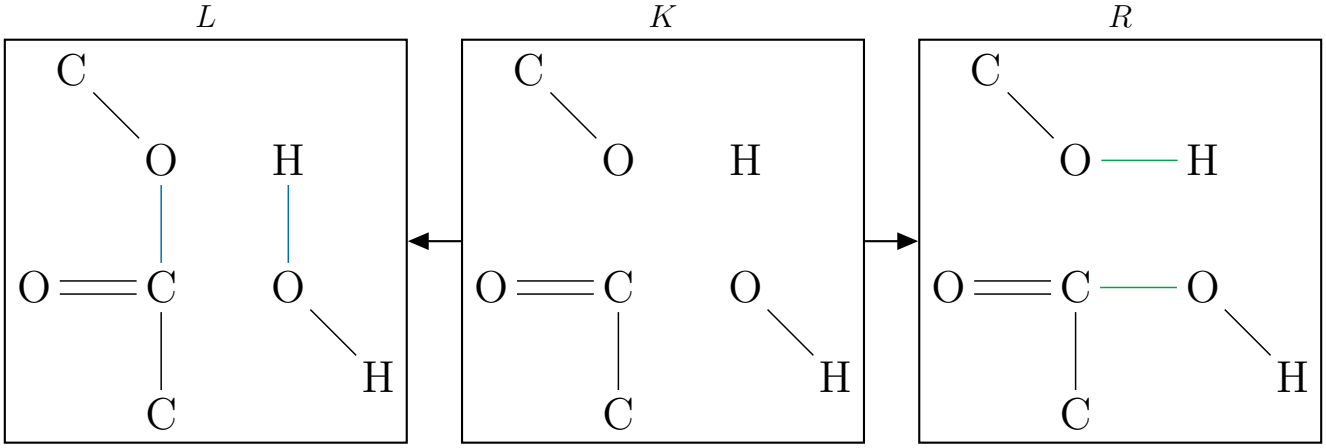
File: out/033_r_5_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

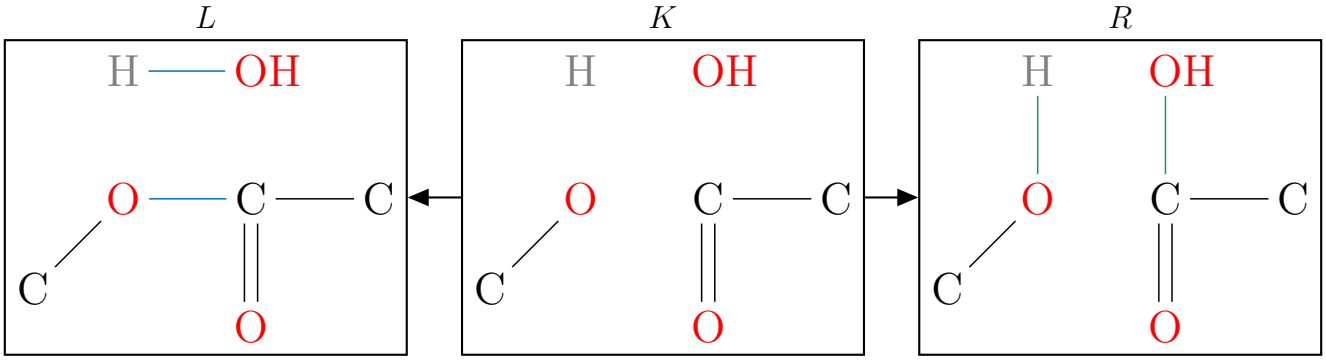
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$|\{e \in \text{outEdges}(4) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

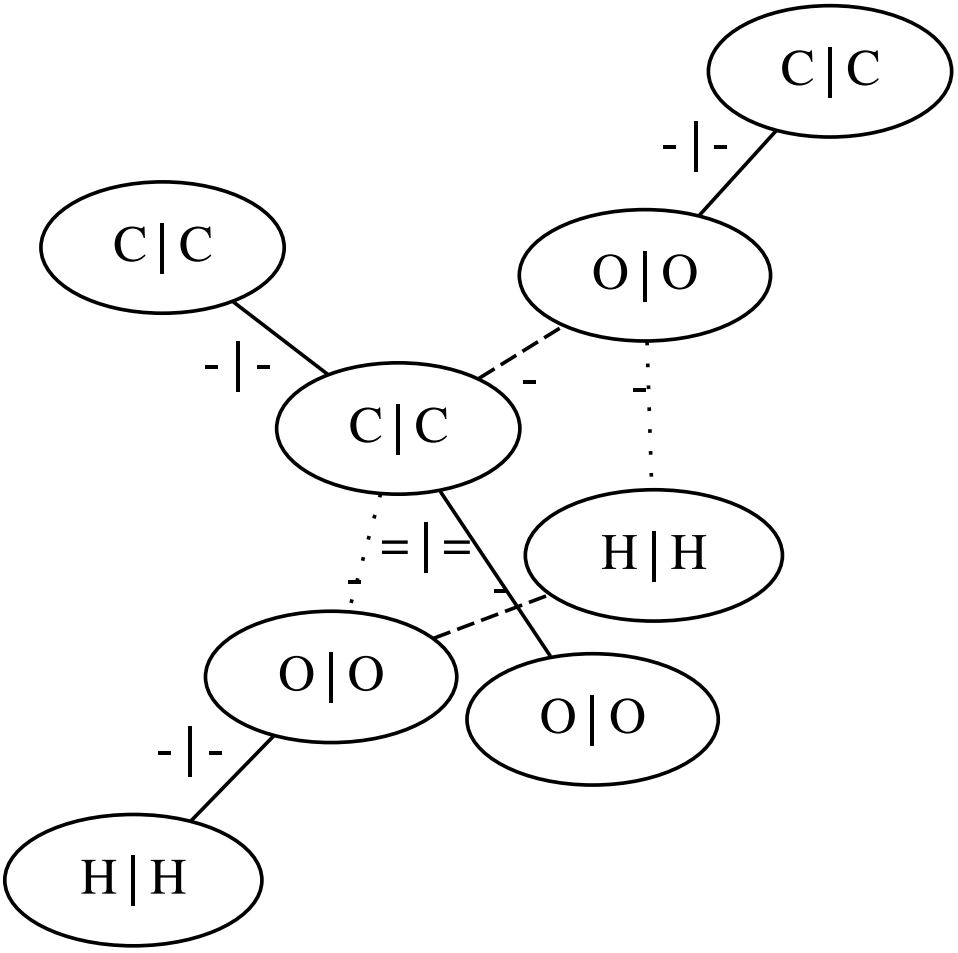
0.0.8 Ester Hydrolysis



Files: out/036_r_6_10300000_{L, K, R}



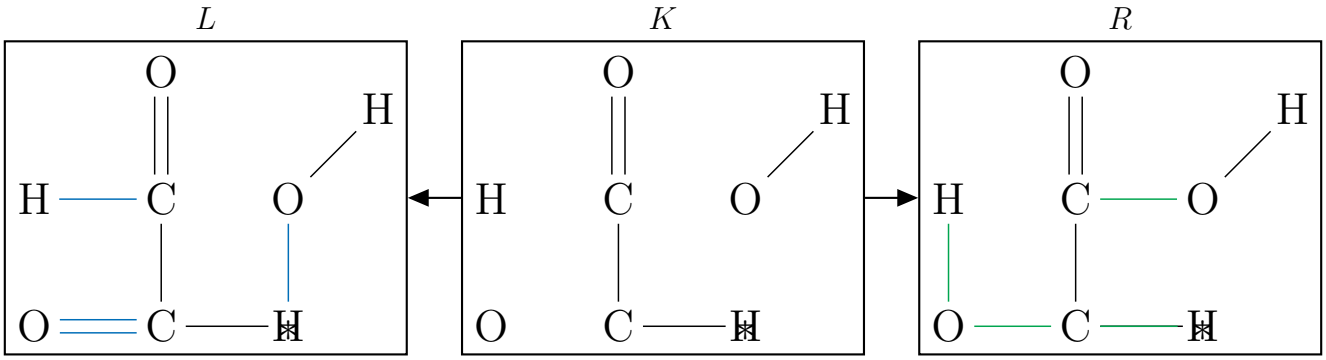
Files: out/037_r_6_11300100_{L, K, R}



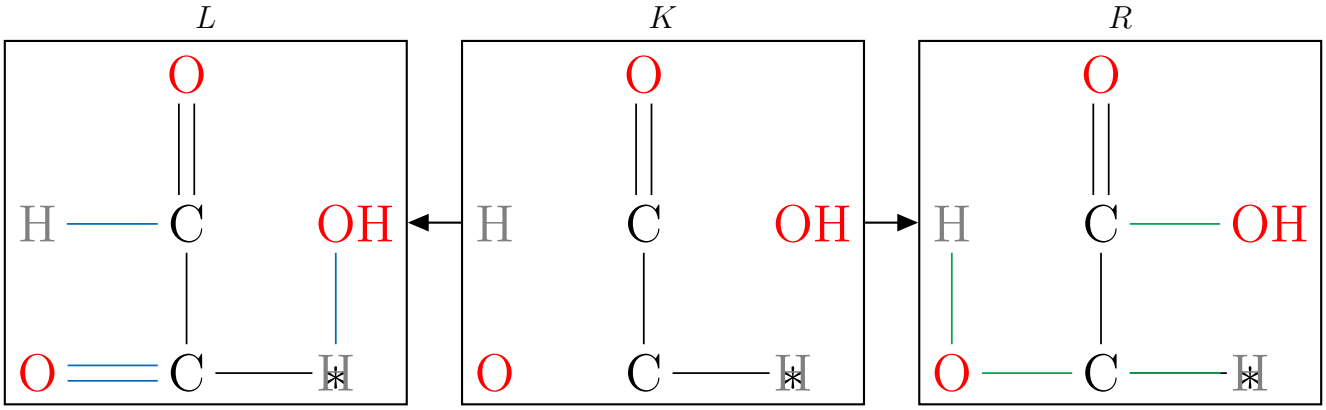
File: out/038_r_6_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

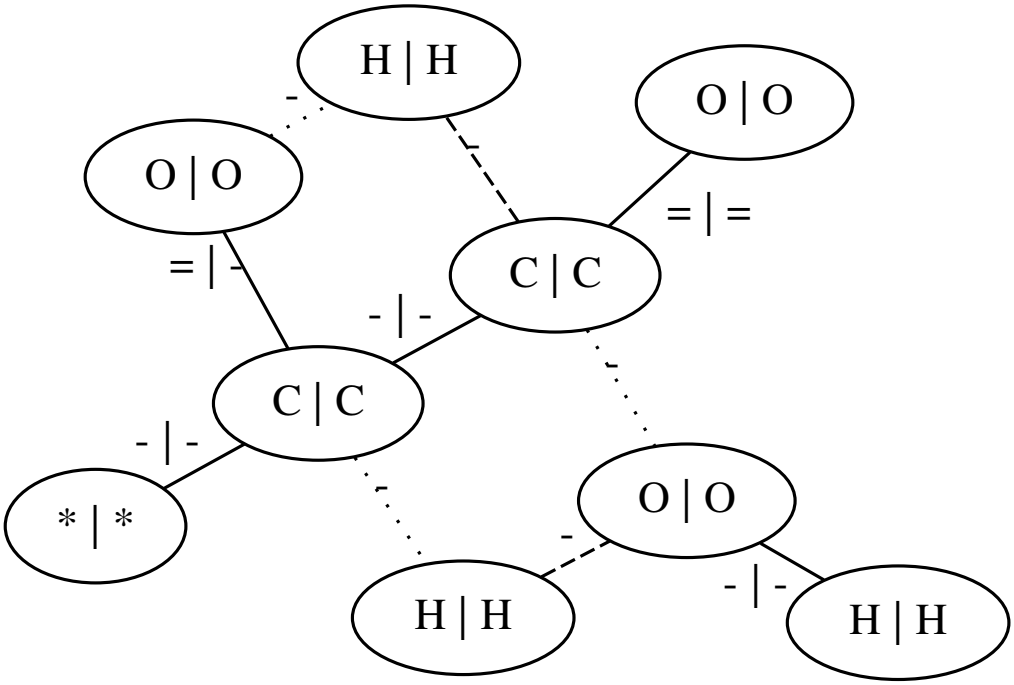
0.0.9 Cannizarro 1



Files: out/041_r_7_10300000_{L, K, R}



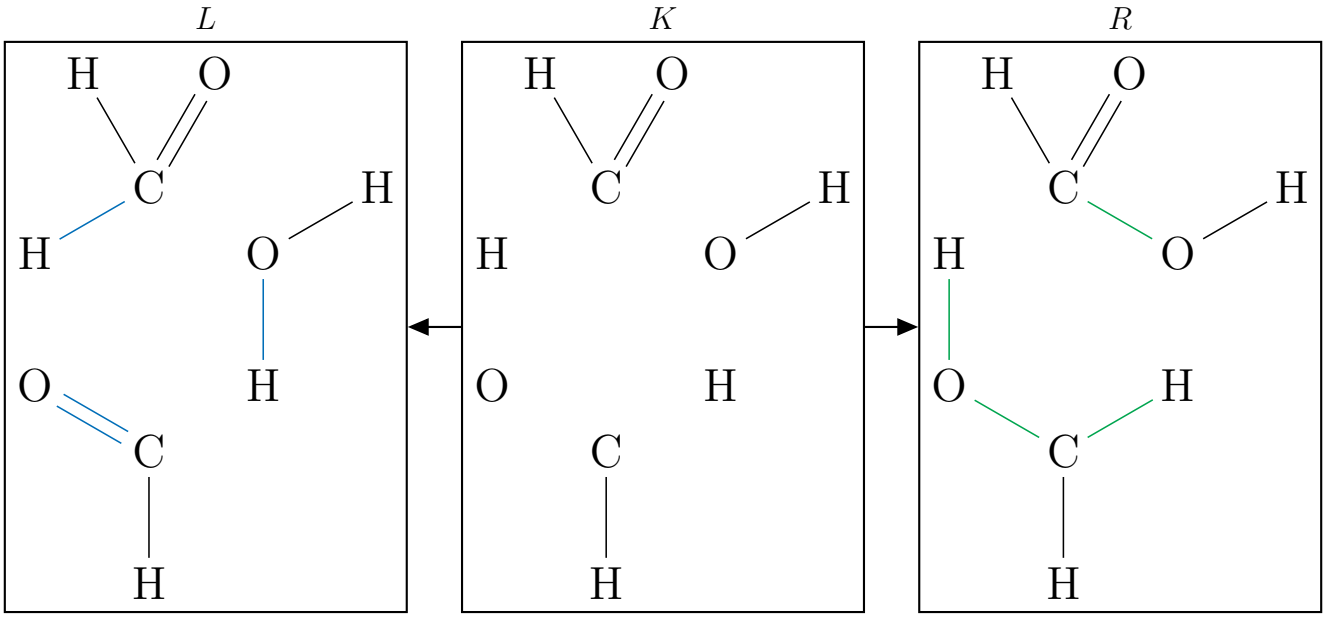
Files: out/042_r_7_11300100_{L, K, R}



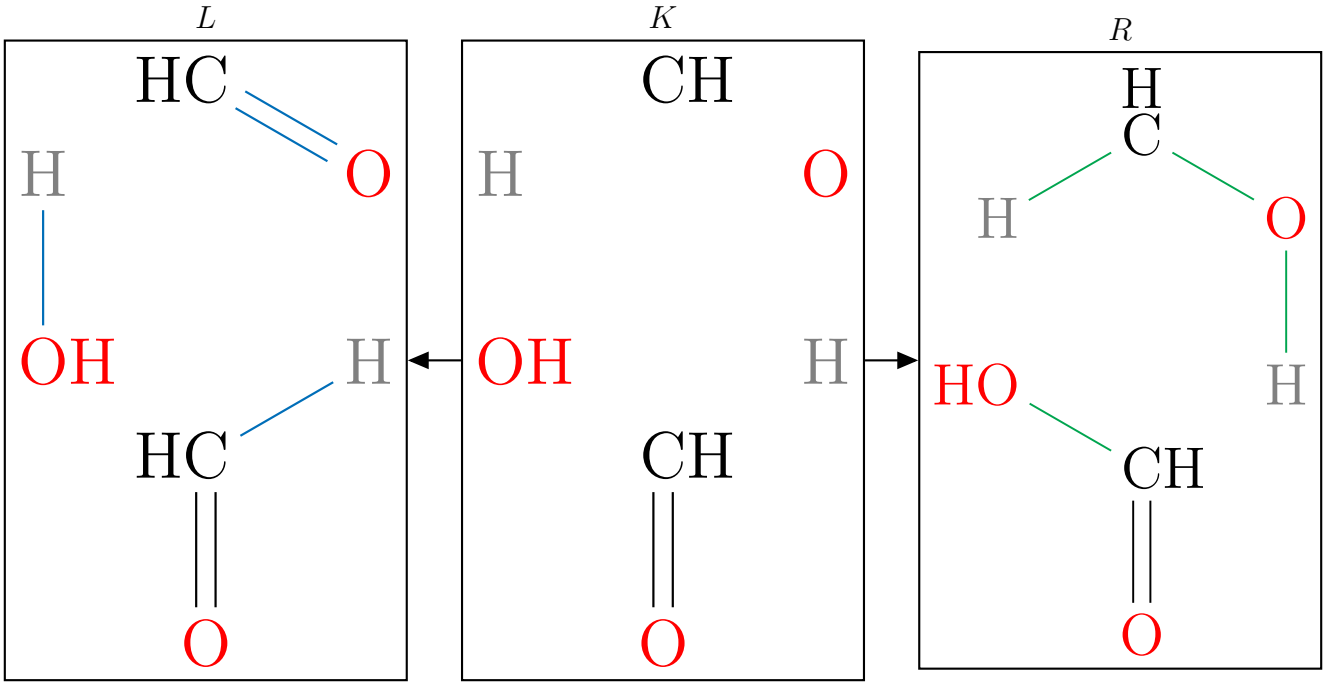
File: out/043_r_7_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`}\texttt{S}\text{'}, \text{`}\texttt{O}\text{'}, \text{`}\texttt{N}\text{'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`}\texttt{-}\text{'}\} \\
&\}| = 0
\end{aligned}
$$

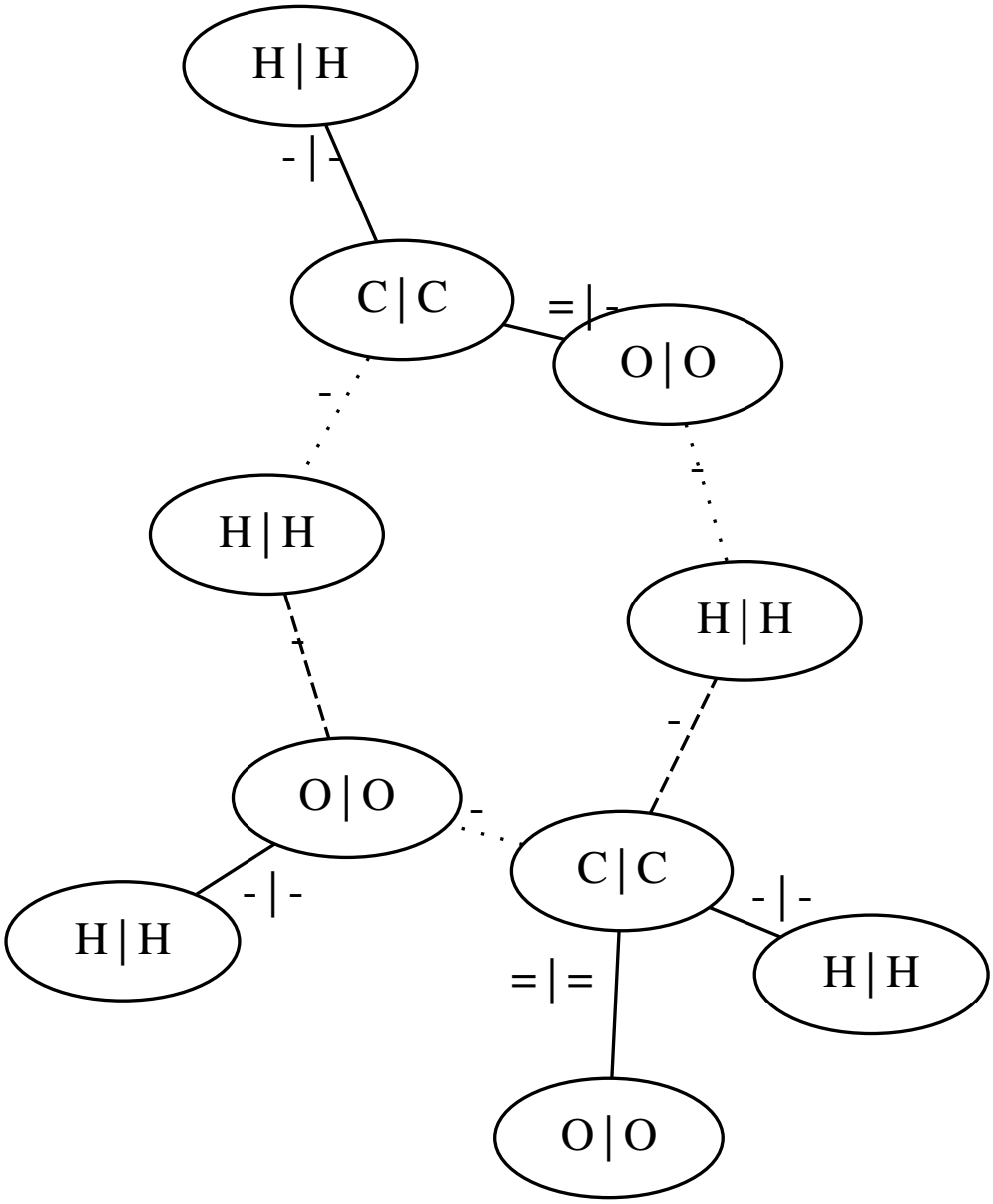
0.0.10 Cannizarro 2, HCHO (oxidation)



Files: out/046_r_8_10300000_{L, K, R}



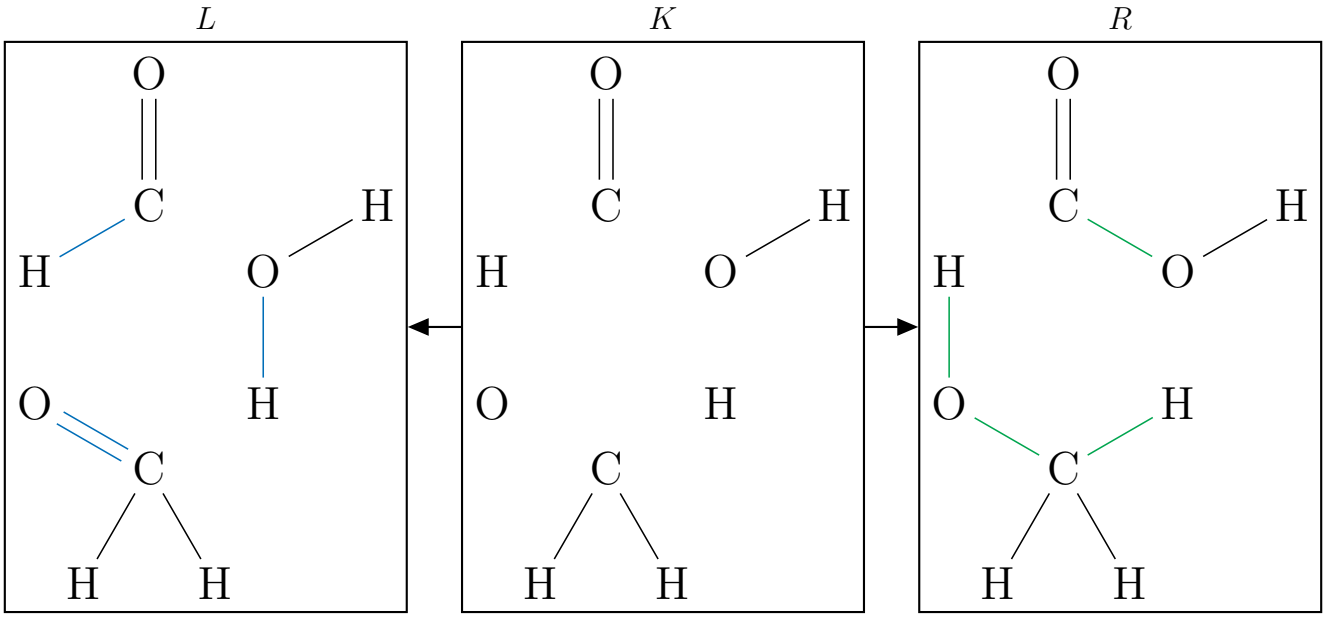
Files: out/047_r_8_11300100_{L, K, R}



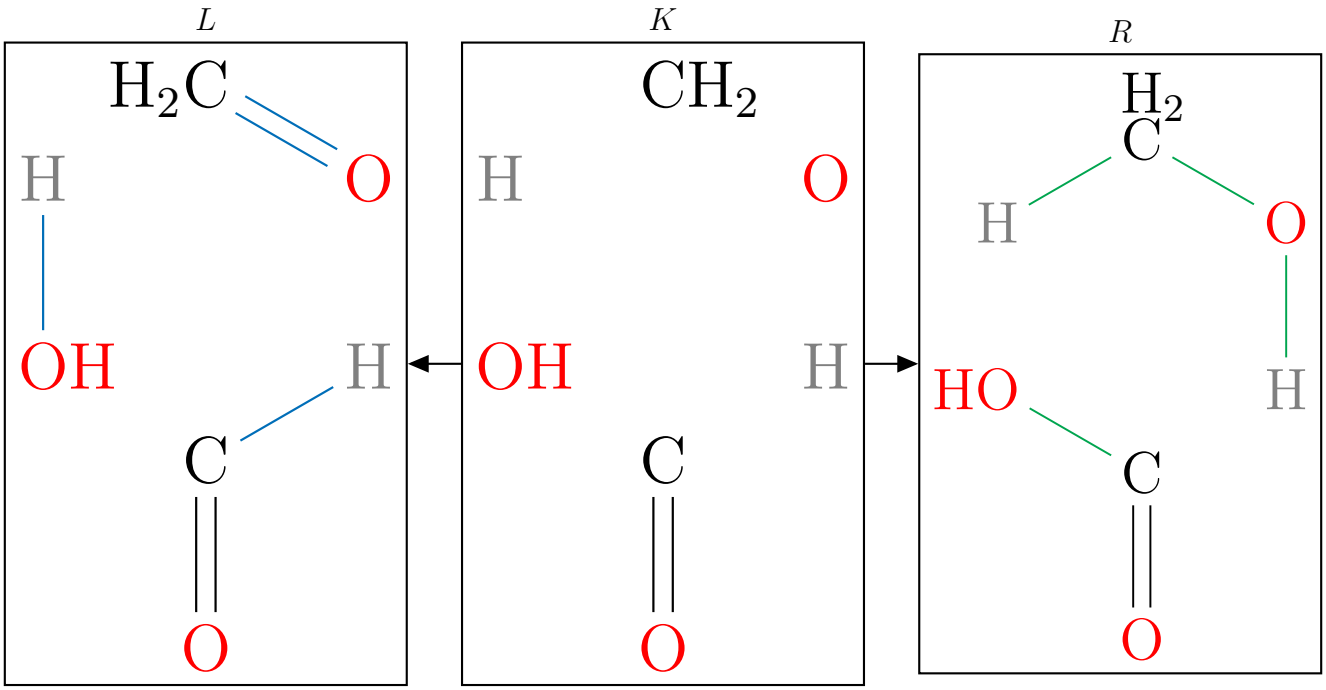
File: out/048_r_8_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

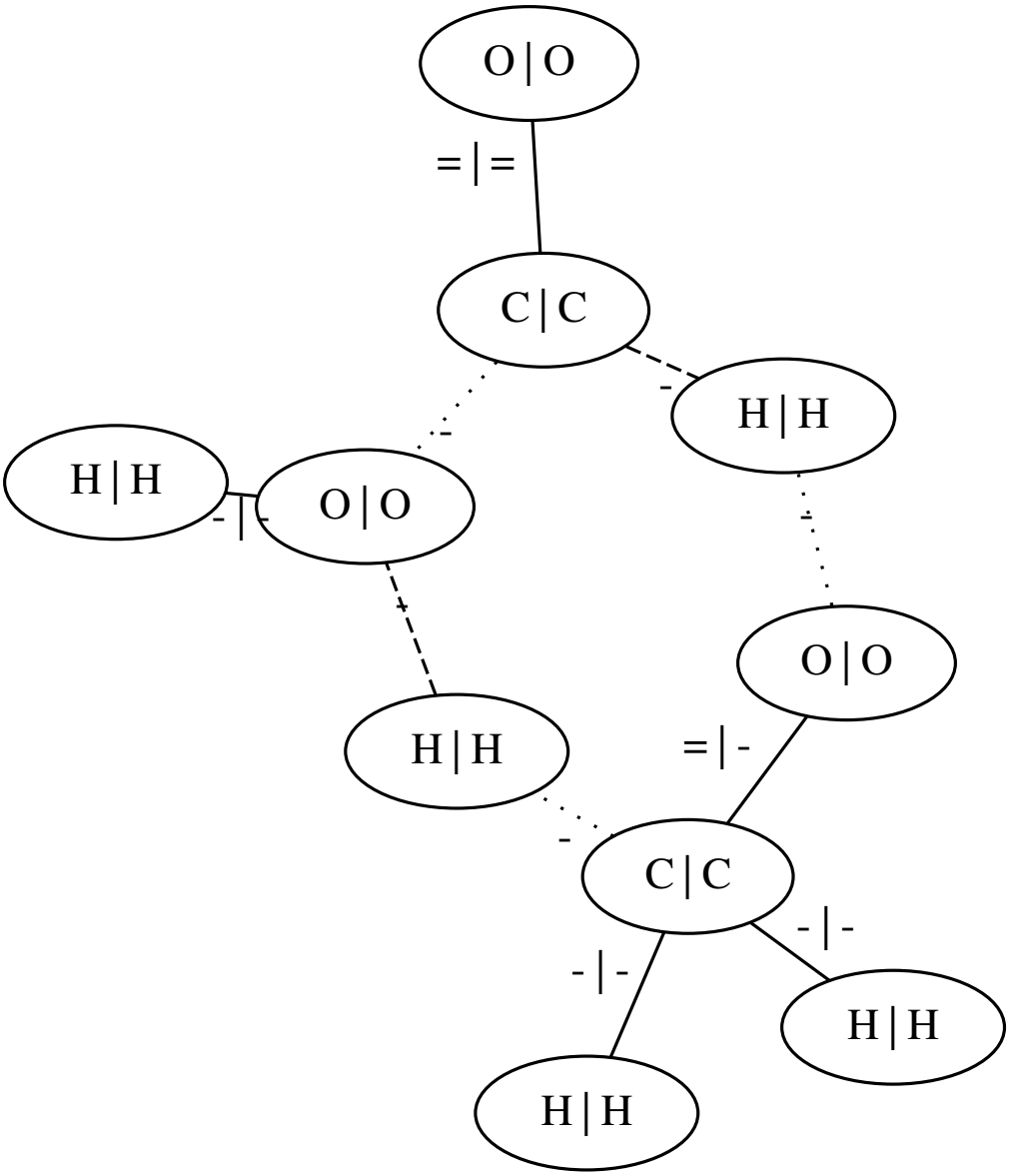
0.0.11 Cannizarro 2, HCHO (reduction)



Files: out/051_r_9_10300000_{L, K, R}



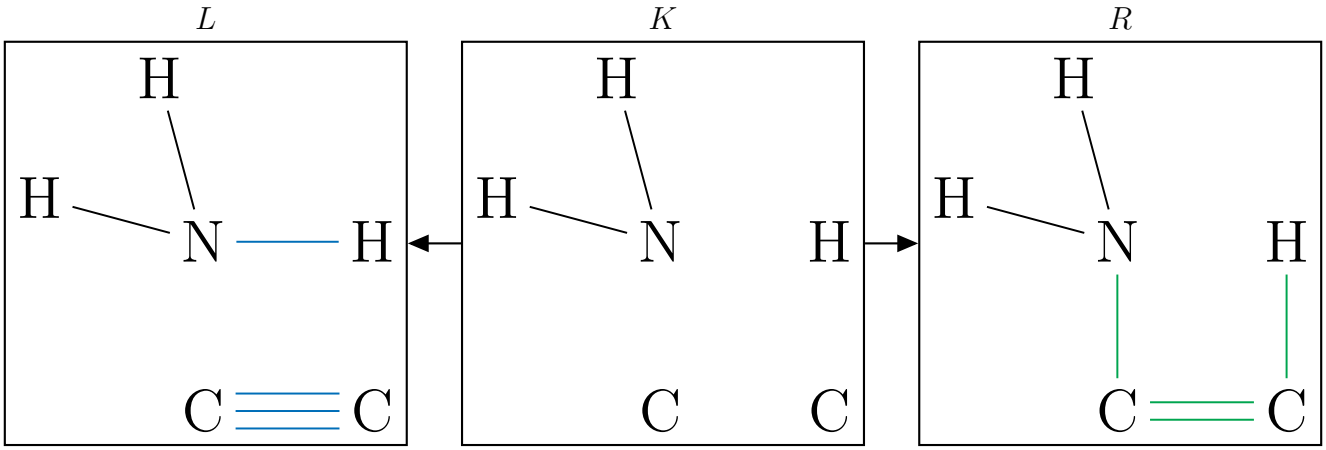
Files: out/052_r_9_11300100_{L, K, R}



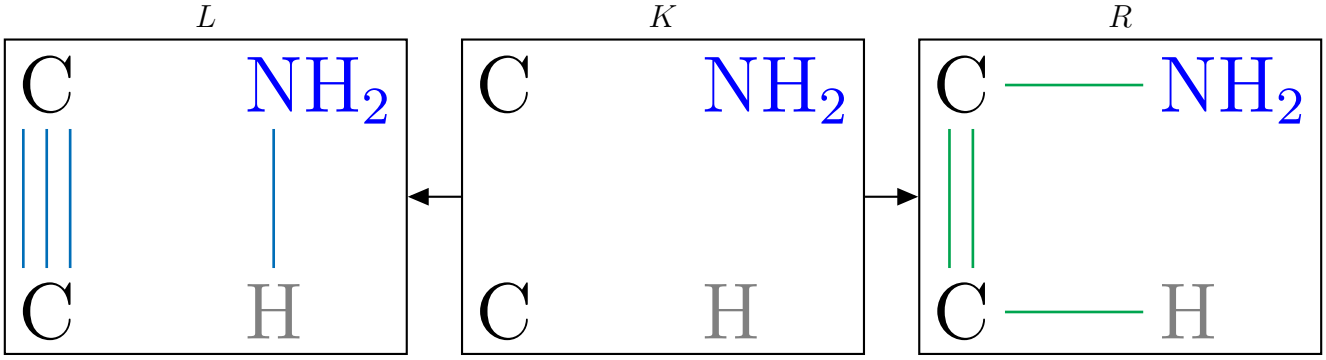
File: out/053_r_9_combined

$$|\{e \in \text{outEdges}(3) \mid \\ \quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\ \quad \wedge \\ \quad \text{label}(e) \in \{\text{`-'}\} \\ \}| = 0$$

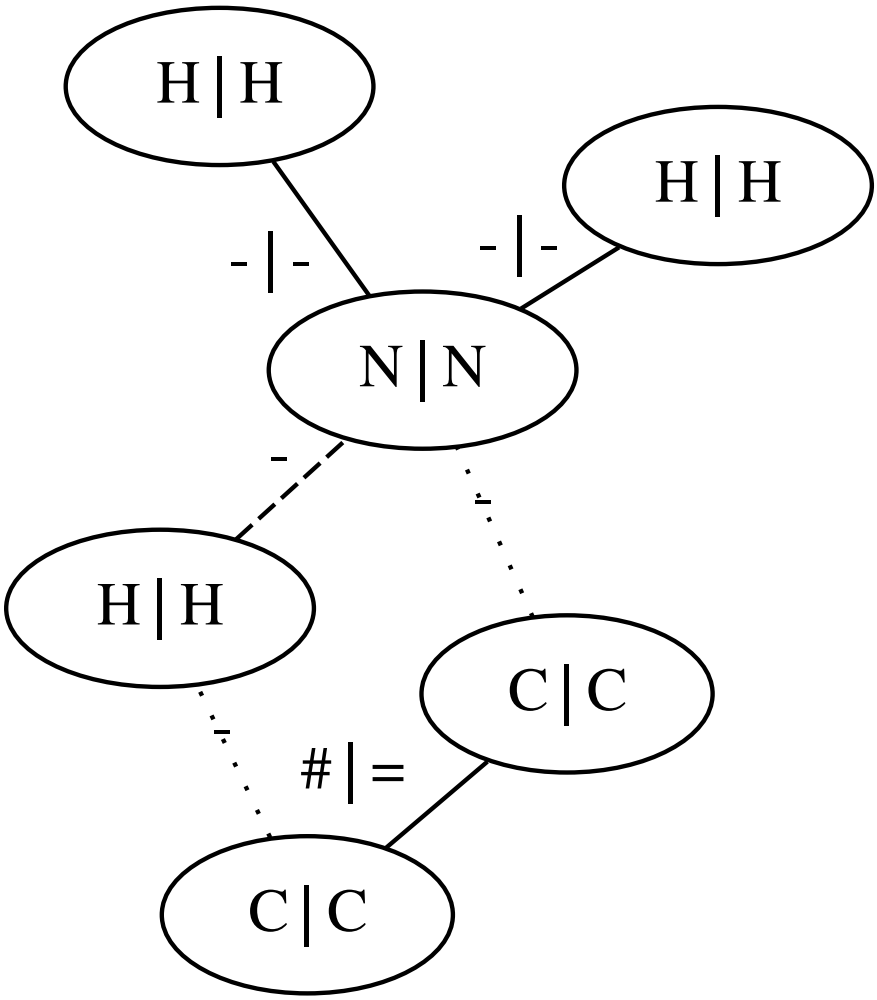
0.0.12 Alkyne Addition, N, HH



Files: out/056_r_10_10300000_{L, K, R}

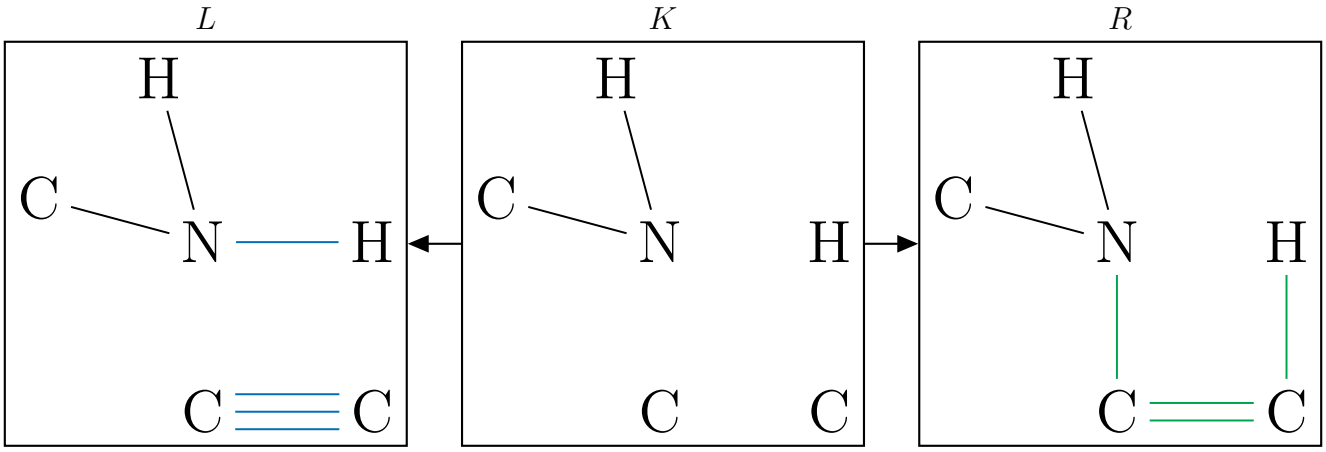


Files: out/057_r_10_11300100_{L, K, R}

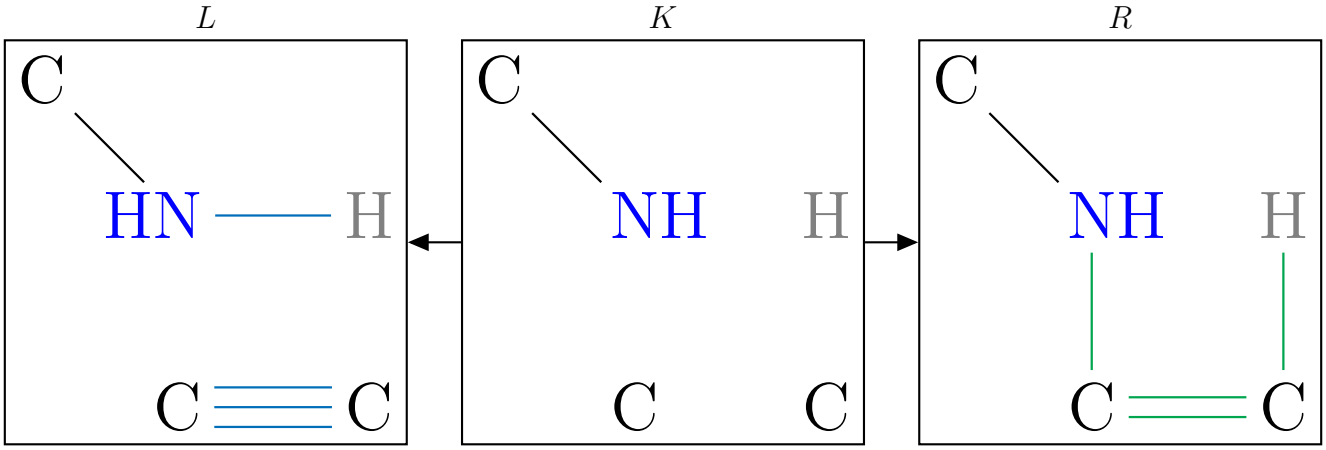


File: out/058_r_10_combined

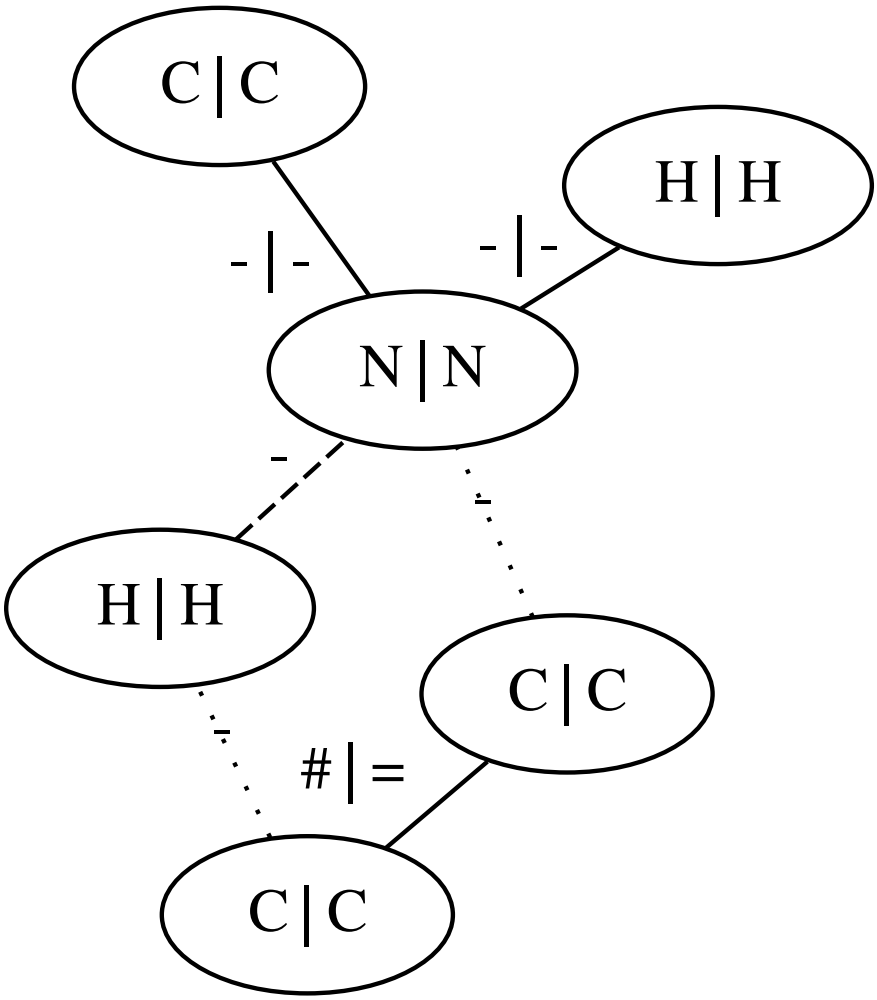
0.0.13 Alkyne Addition, N, HC



Files: out/061_r_11_10300000_{L, K, R}



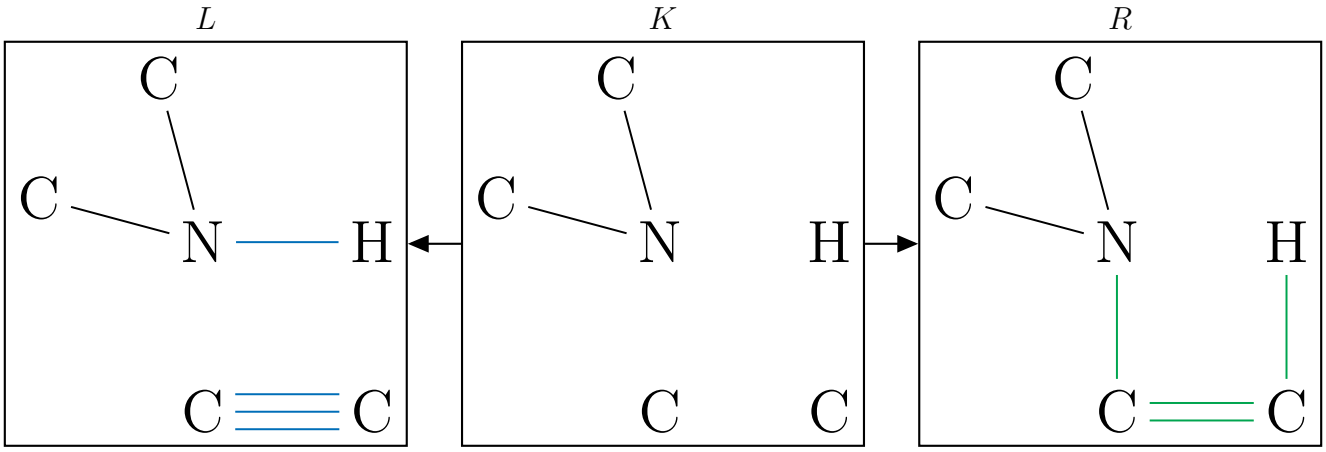
Files: out/062_r_11_11300100_{L, K, R}



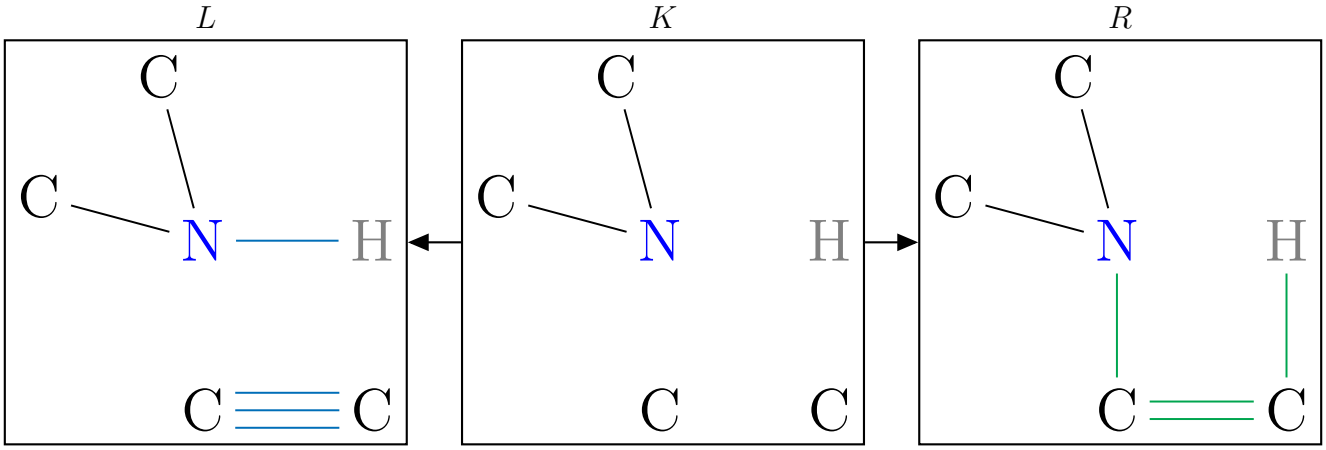
File: out/063_r_11_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

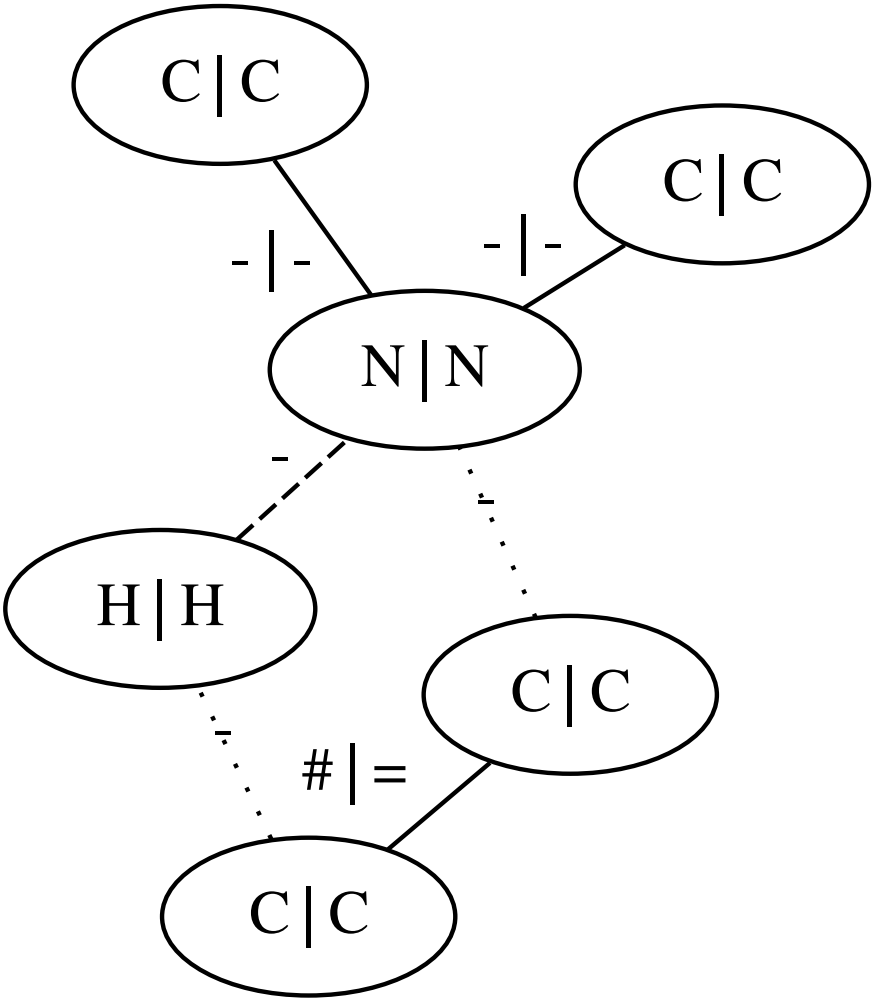
0.0.14 Alkyne Addition, N, CC



Files: out/066_r_12_10300000_{L, K, R}



Files: out/067_r_12_11300100_{L, K, R}

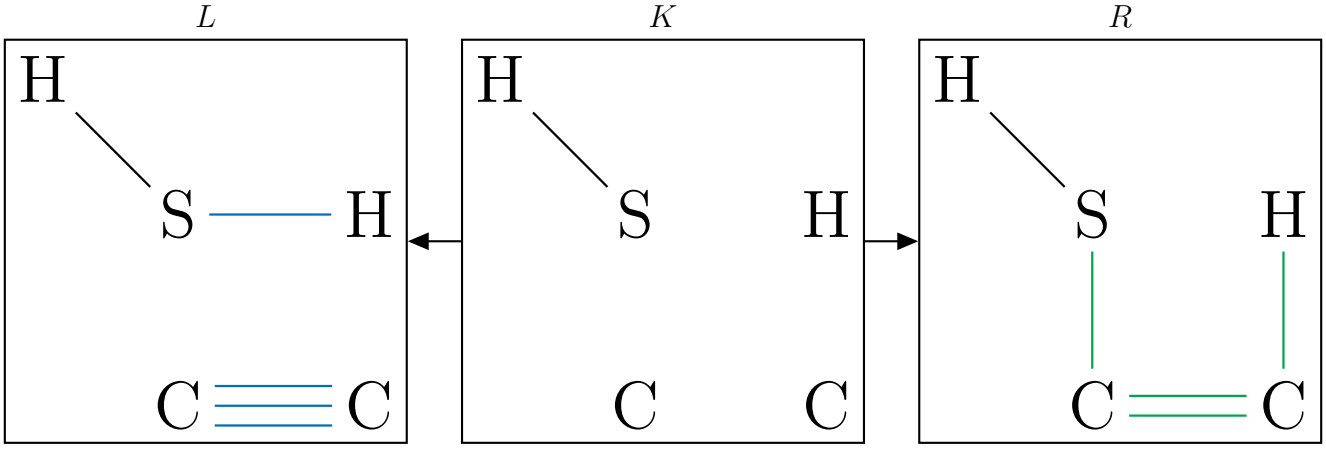


File: out/068_r_12_combined

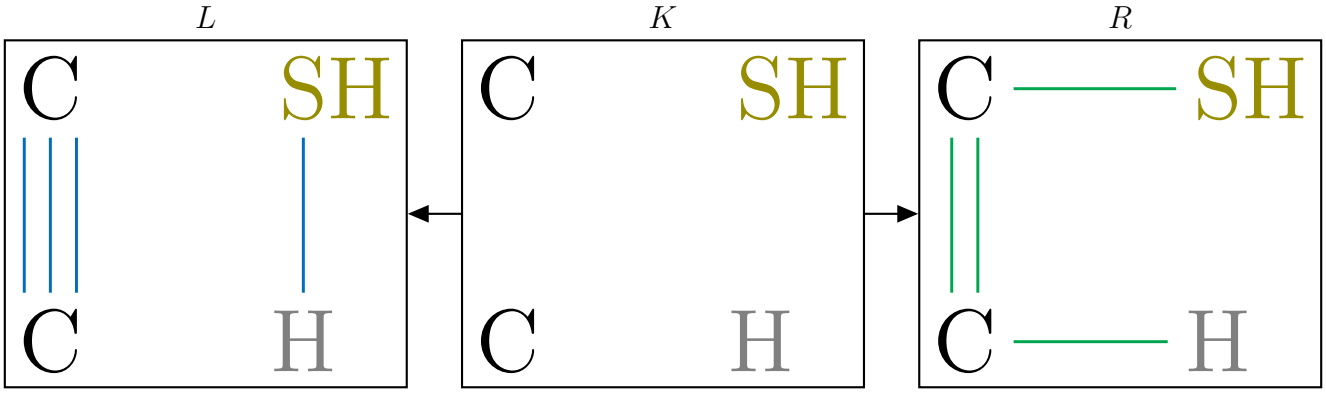
$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

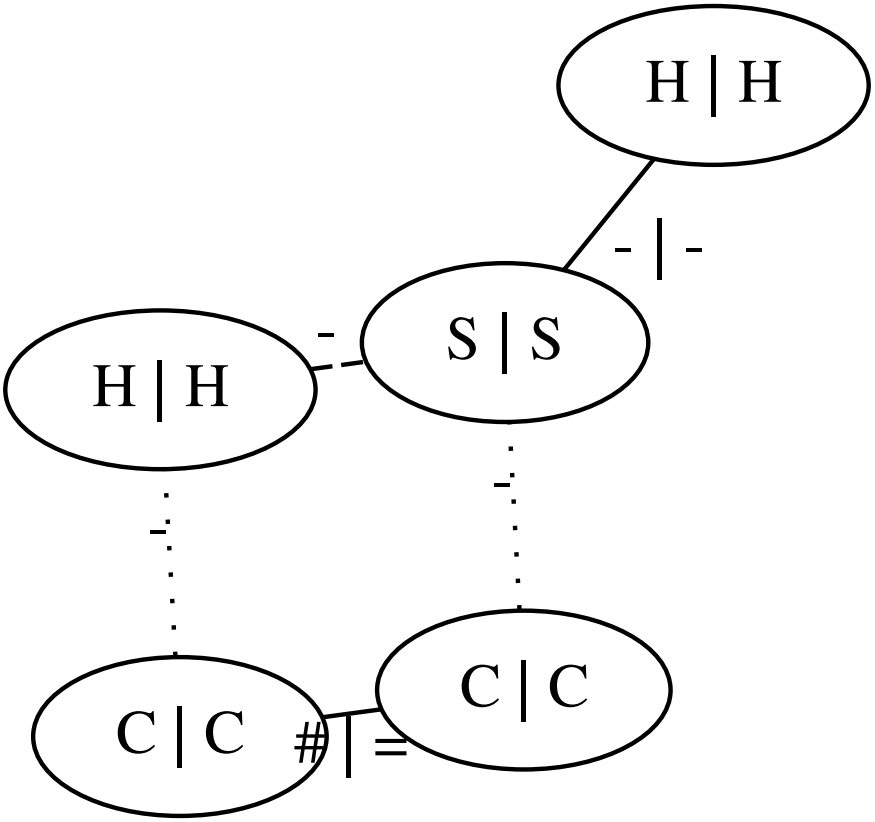
0.0.15 Alkyne Addition, S, H



Files: out/071_r_13_10300000_{L, K, R}

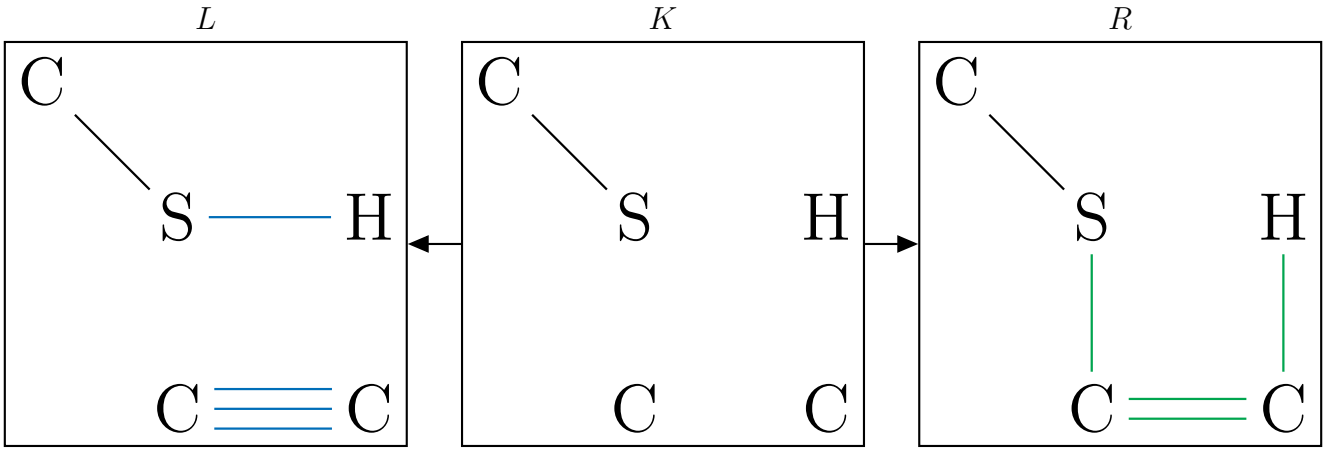


Files: out/072_r_13_11300100_{L, K, R}

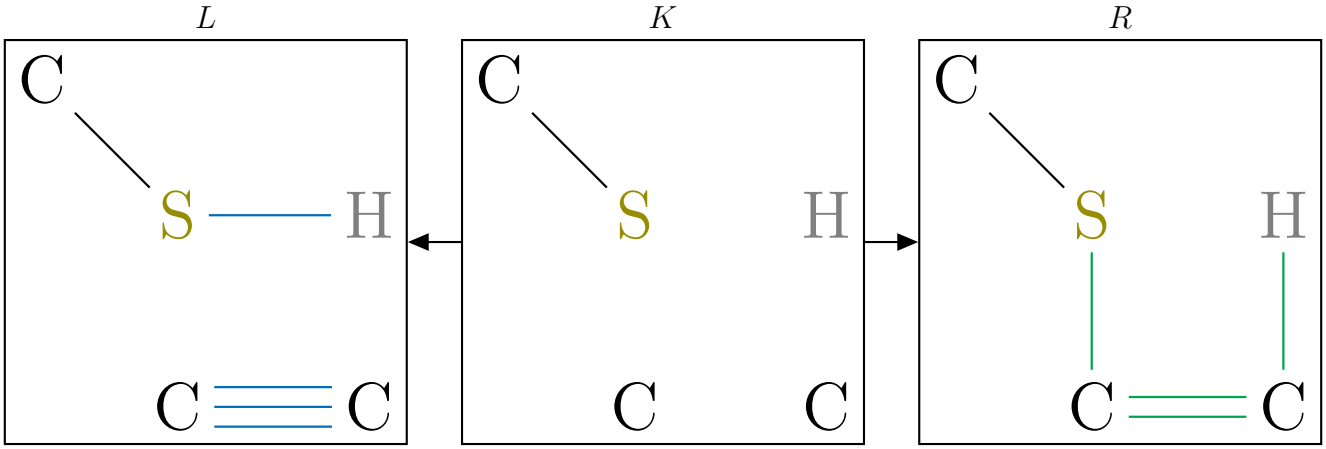


File: out/073_r_13_combined

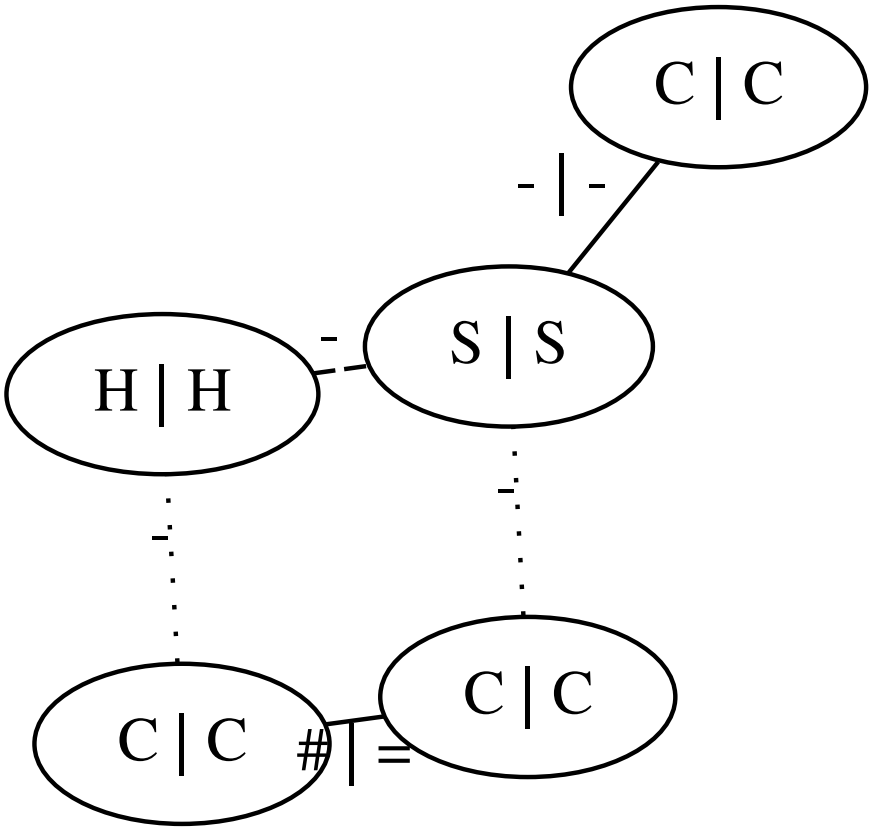
0.0.16 Alkyne Addition, S, C



Files: out/076_r_14_10300000_{L, K, R}

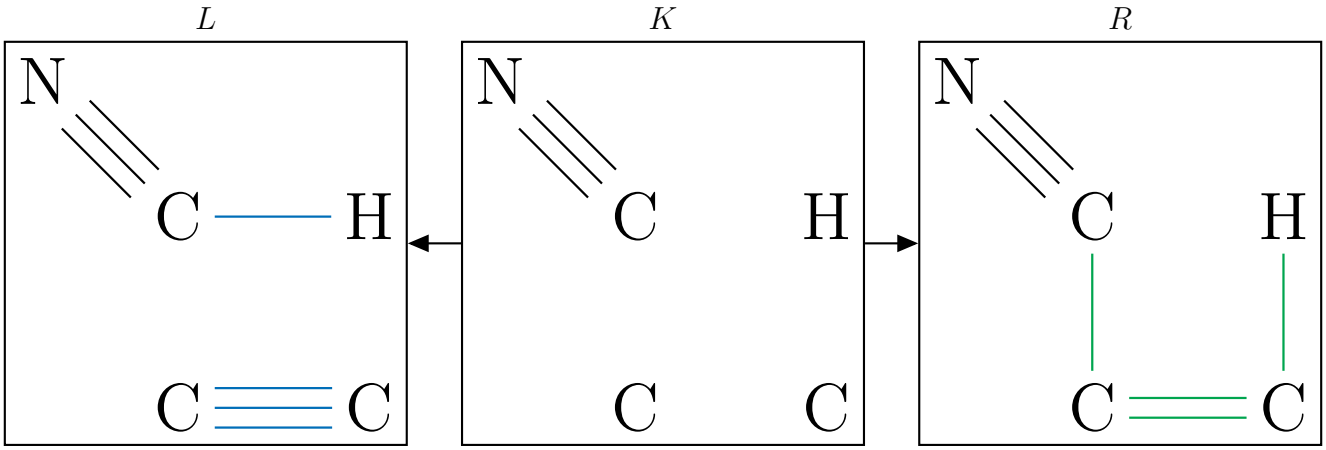


Files: out/077_r_14_11300100_{L, K, R}

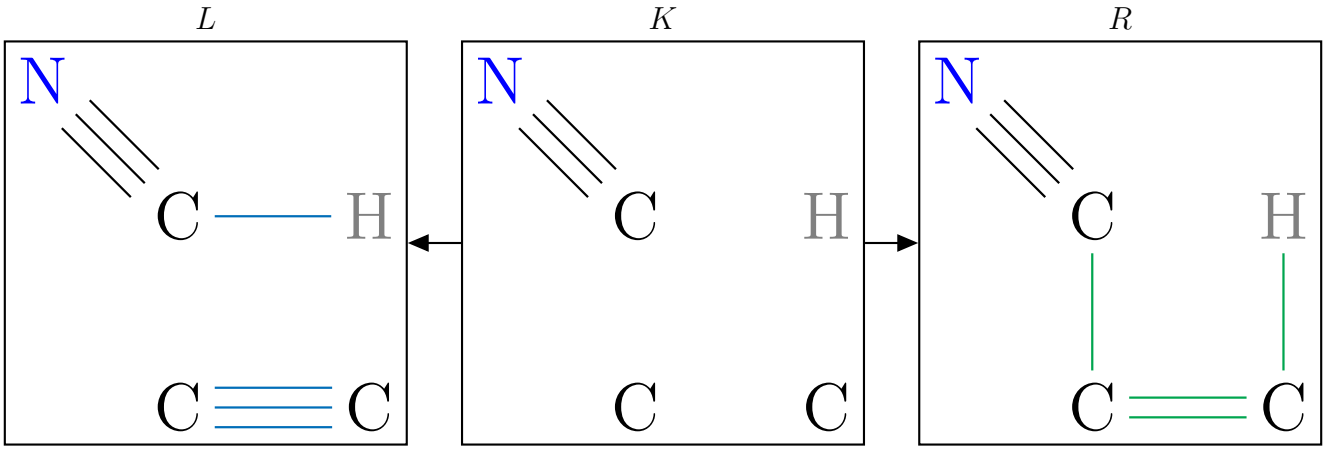


$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

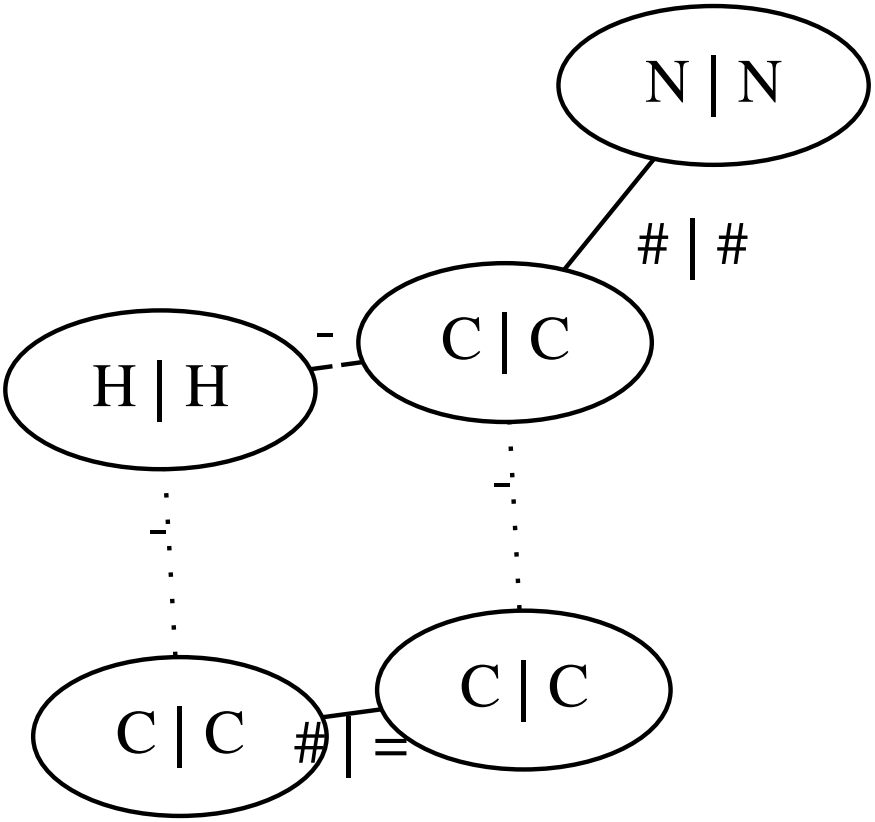
0.0.17 Alkyne Addition, C



Files: out/081_r_15_10300000_{L, K, R}

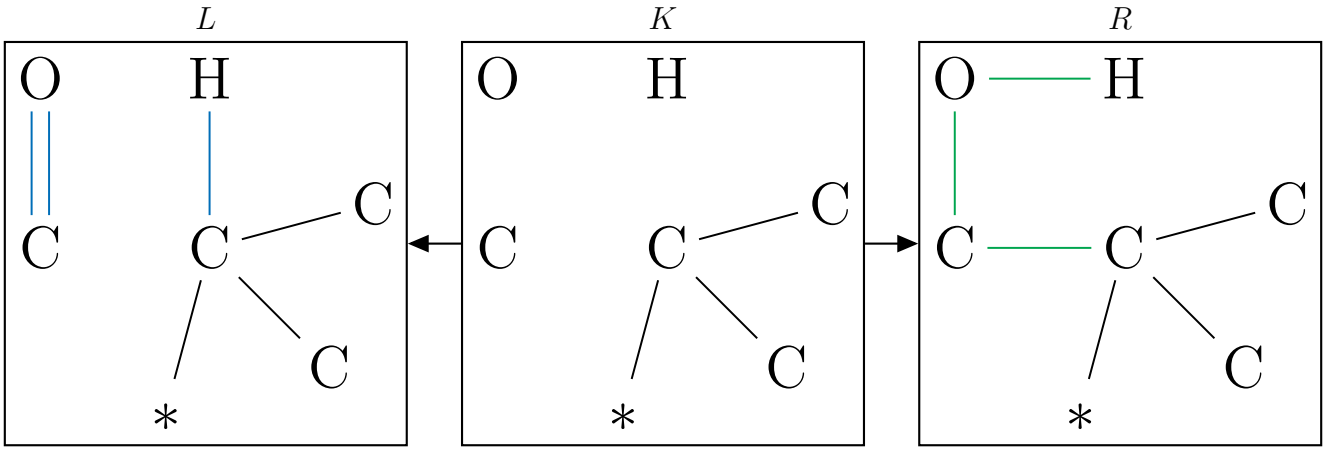


Files: out/082_r_15_11300100_{L, K, R}

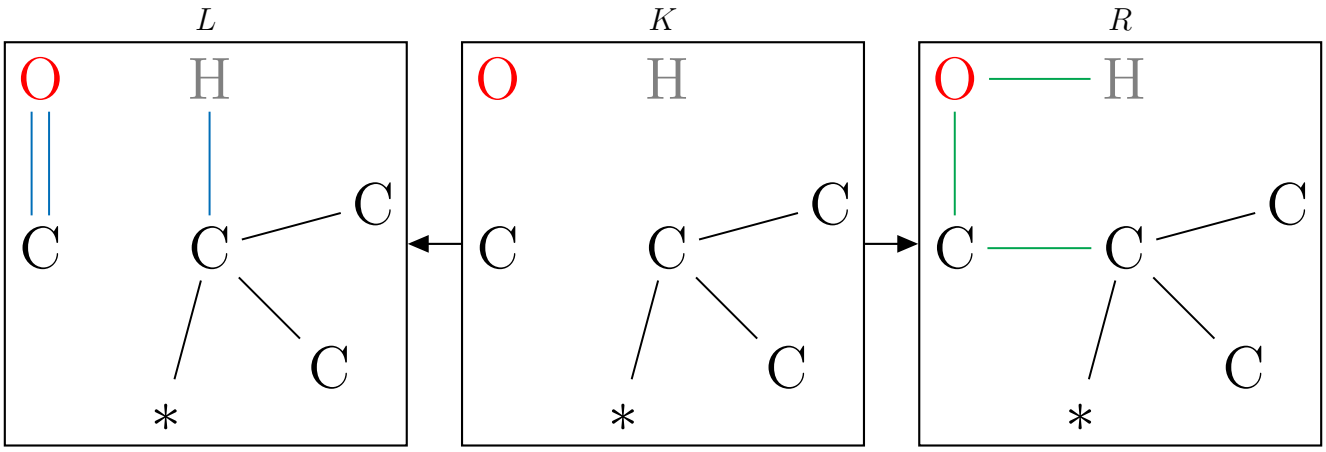


File: out/083_r_15_combined

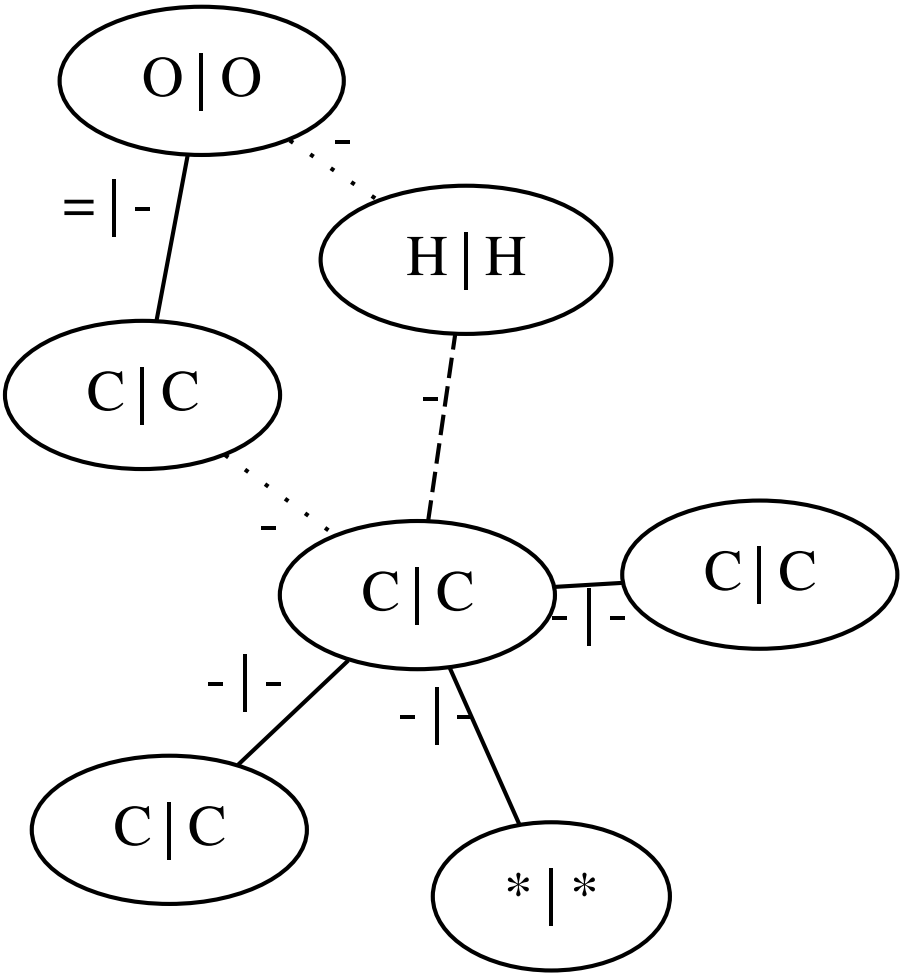
0.0.18 Knoevenagel C



Files: out/086_r_16_10300000_{L, K, R}



Files: out/087_r_16_11300100_{L, K, R}



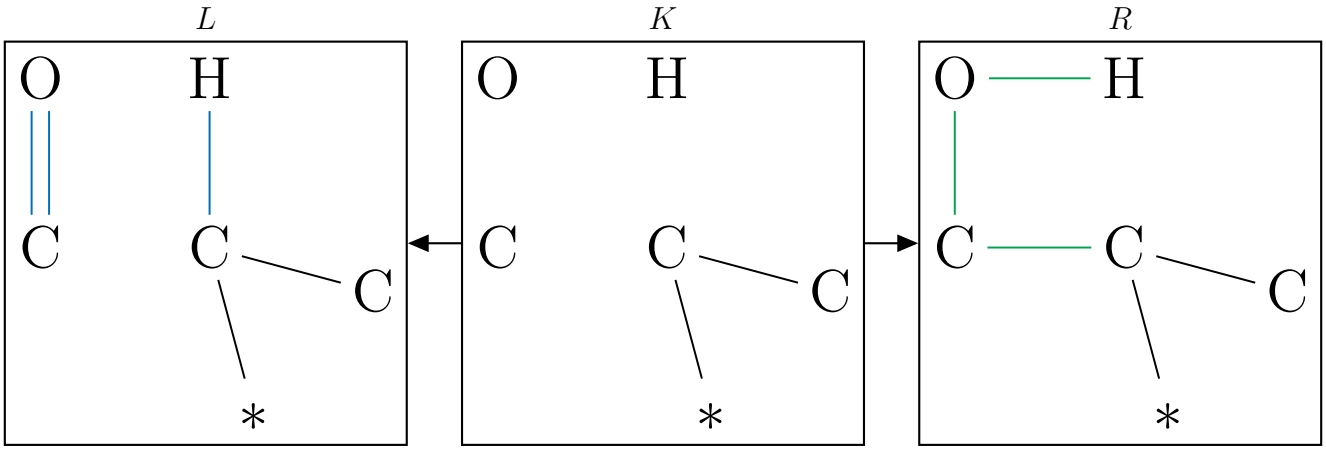
File: out/088_r_16_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

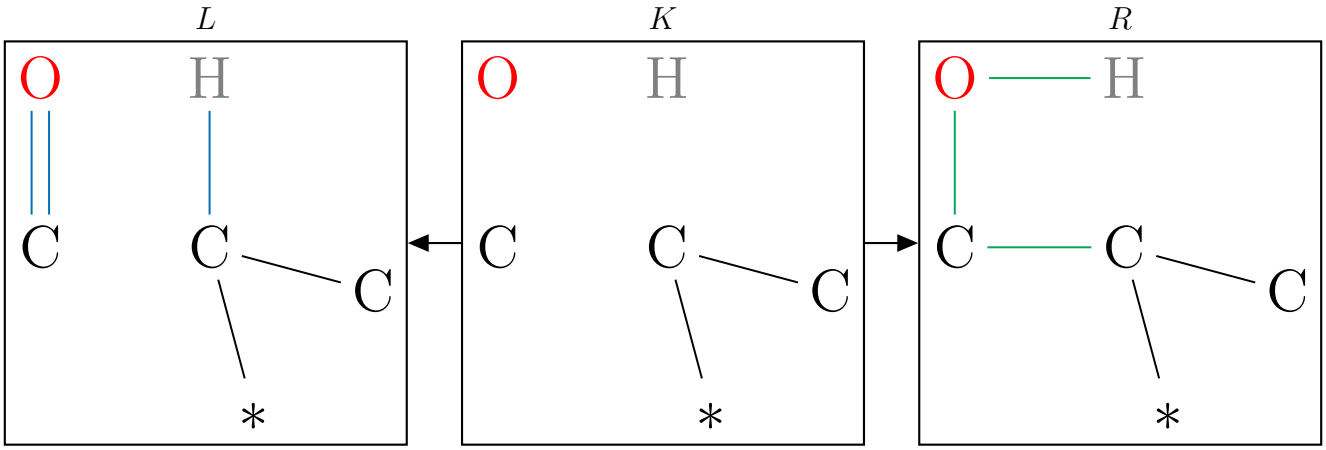
$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`='}\}\}| = 1$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`-'}, \text{`='}\}\}| \geq 1$$

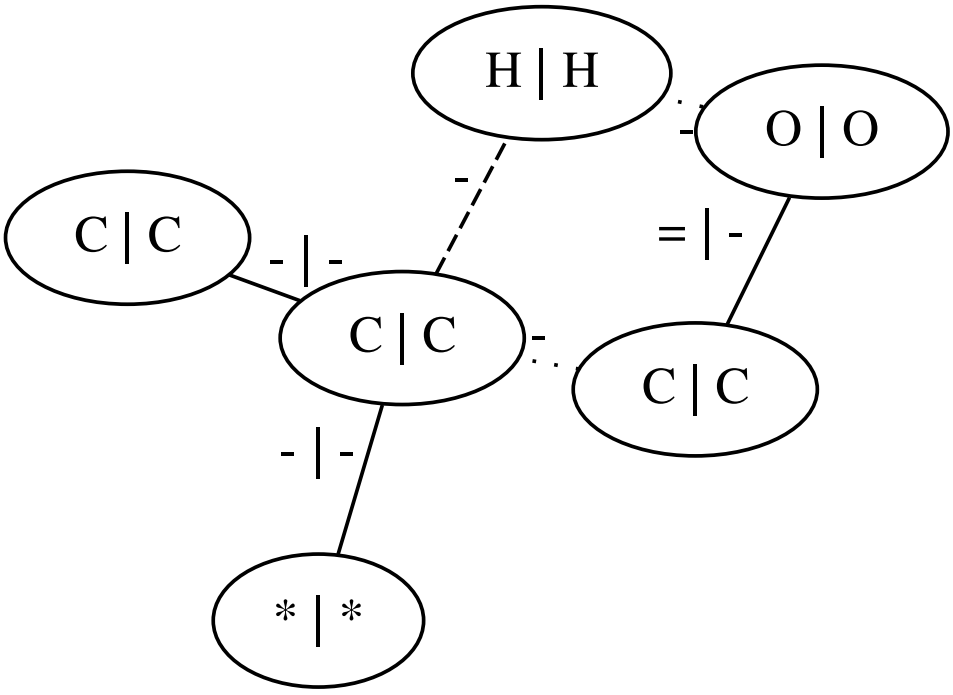
0.0.19 Knoevenagel H



Files: out/091_r_17_10300000_{L, K, R}



Files: out/092_r_17_11300100_{L, K, R}



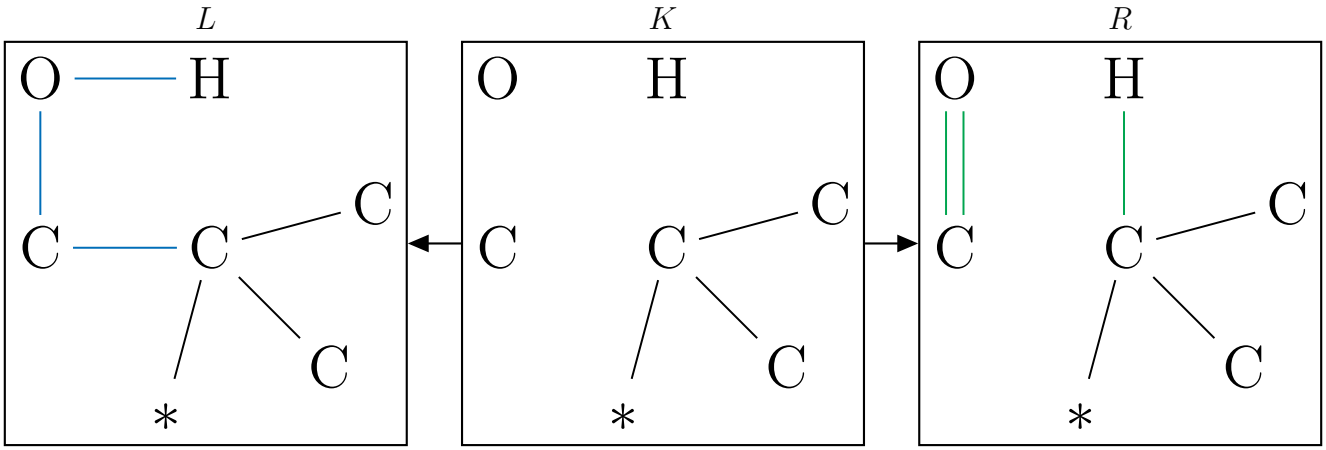
File: out/093_r_17_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

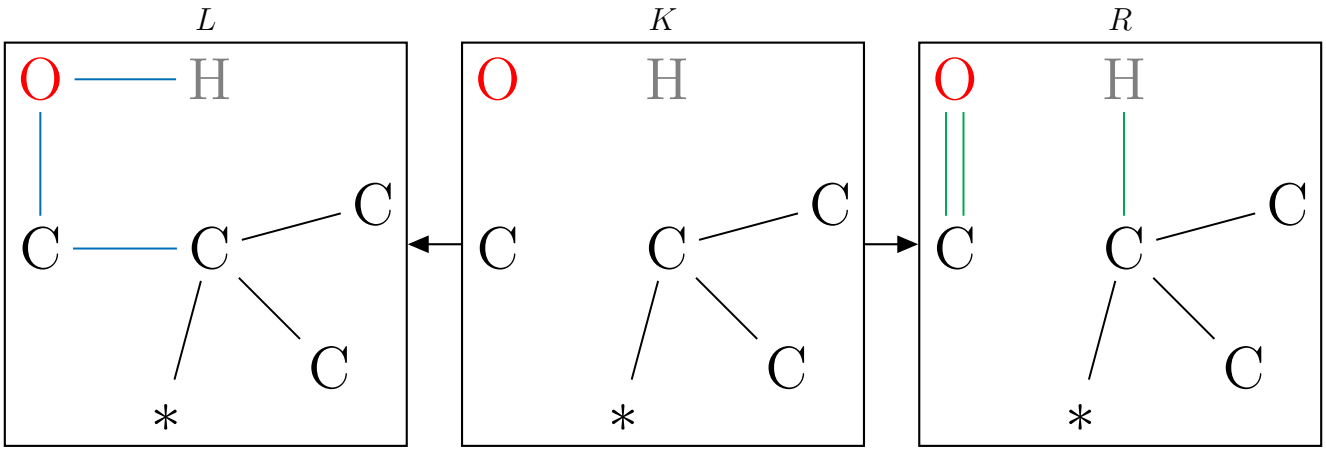
$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`-'}, \text{`='}\} \\
&\}| \geq 1
\end{aligned}
$$

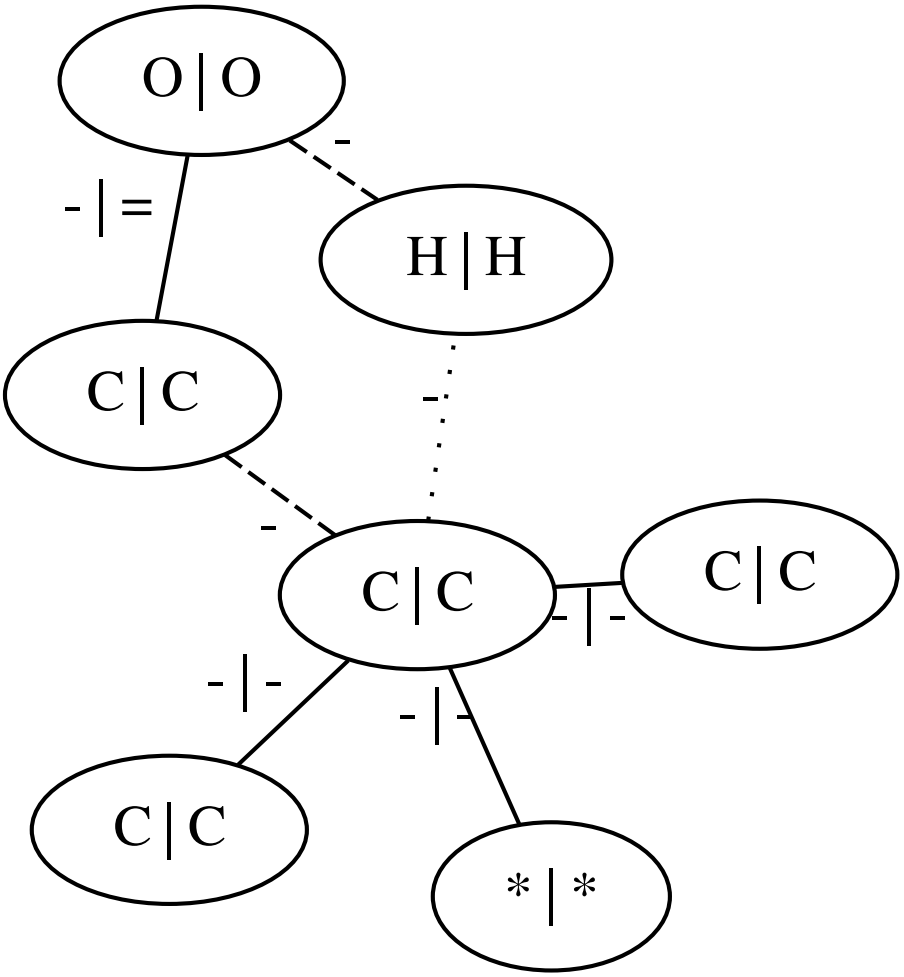
0.0.20 Knoevenagel C (inverse)



Files: out/096_r_18_10300000_{L, K, R}



Files: out/097_r_18_11300100_{L, K, R}



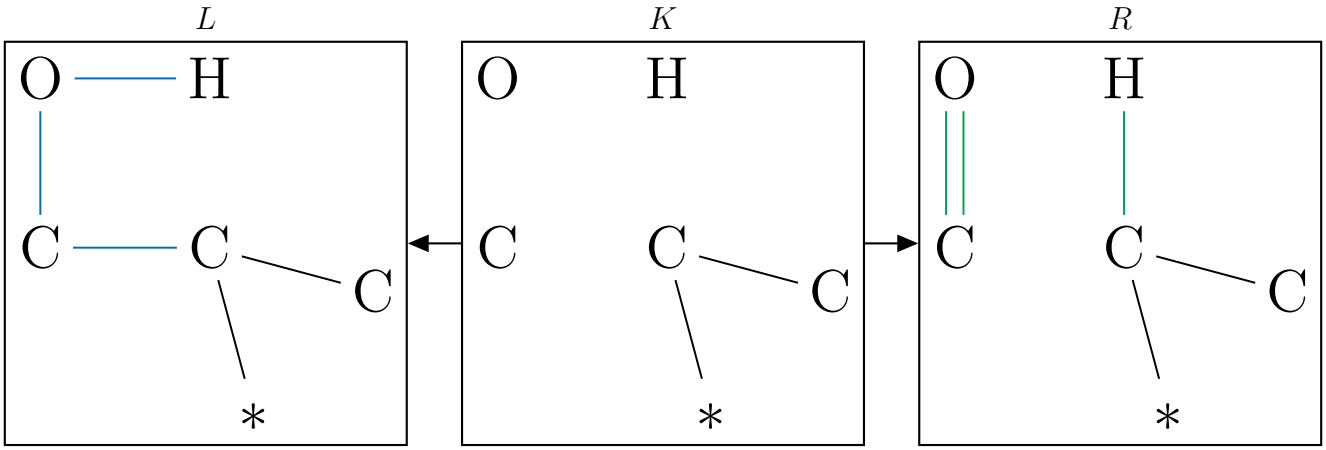
File: out/098_r_18_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

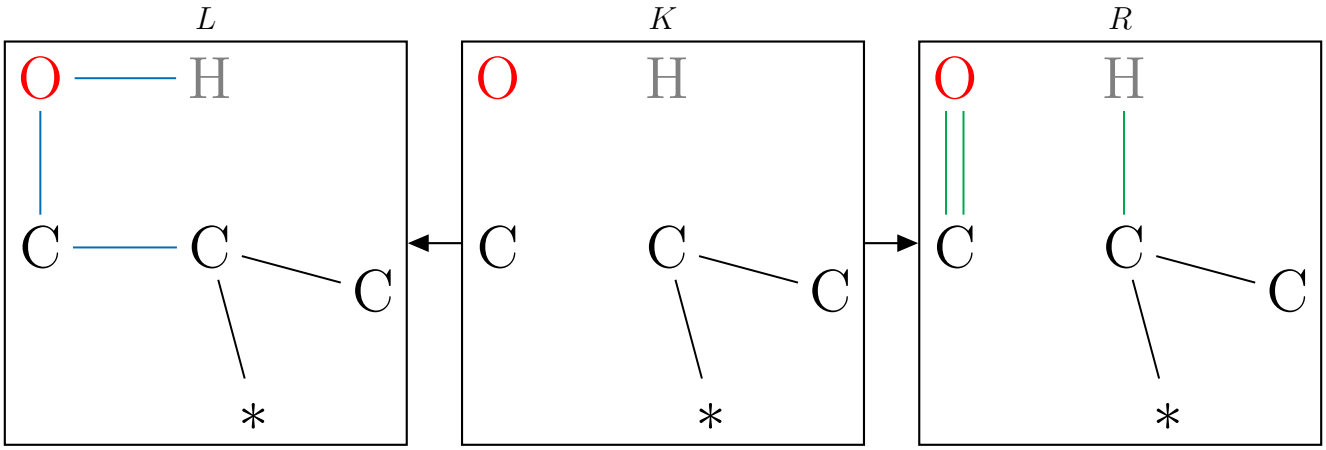
$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`='}\}\}| = 1$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`-'}, \text{`='}\}\}| \geq 1$$

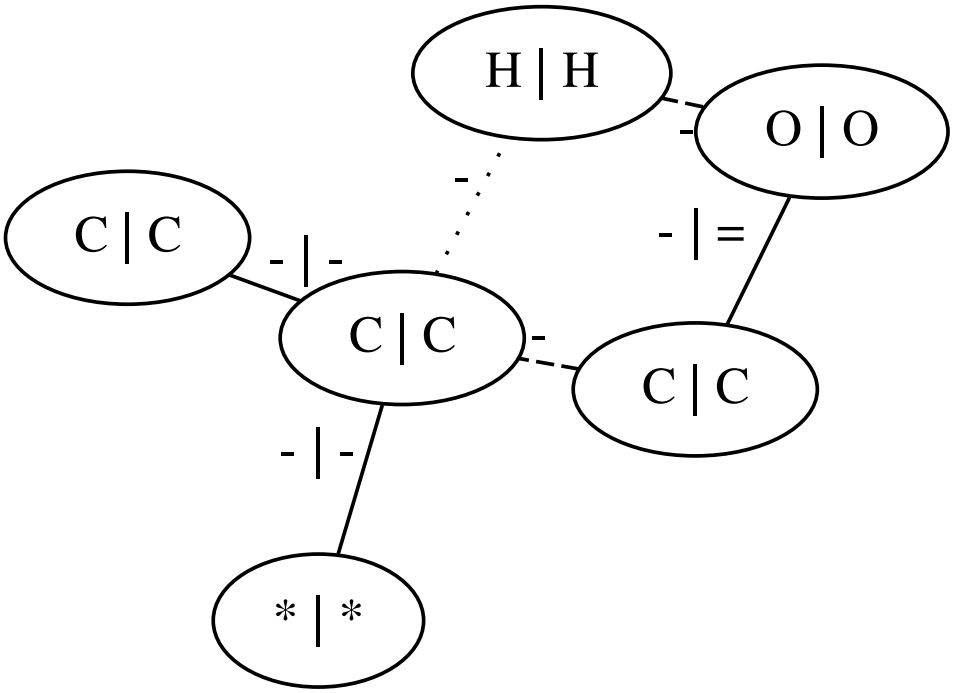
0.0.21 Knoevenagel H (inv)



Files: out/101_r_19_10300000_{L, K, R}



Files: out/102_r_19_11300100_{L, K, R}



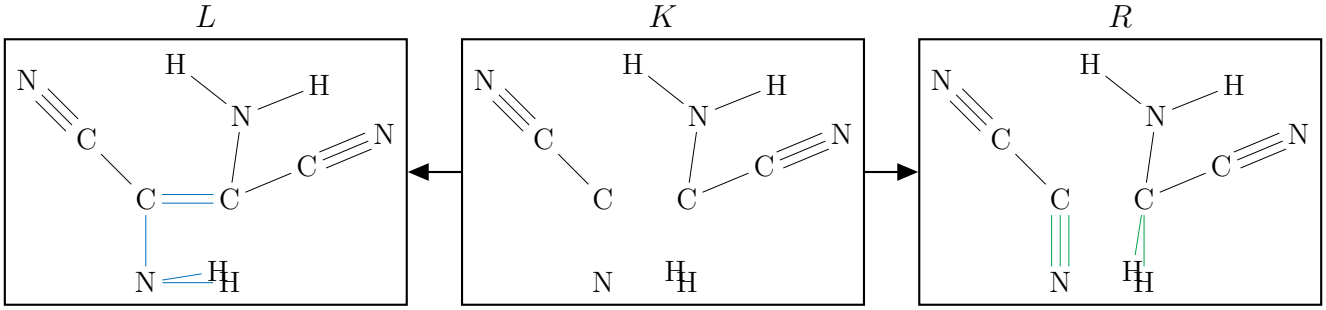
File: out/103_r_19_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

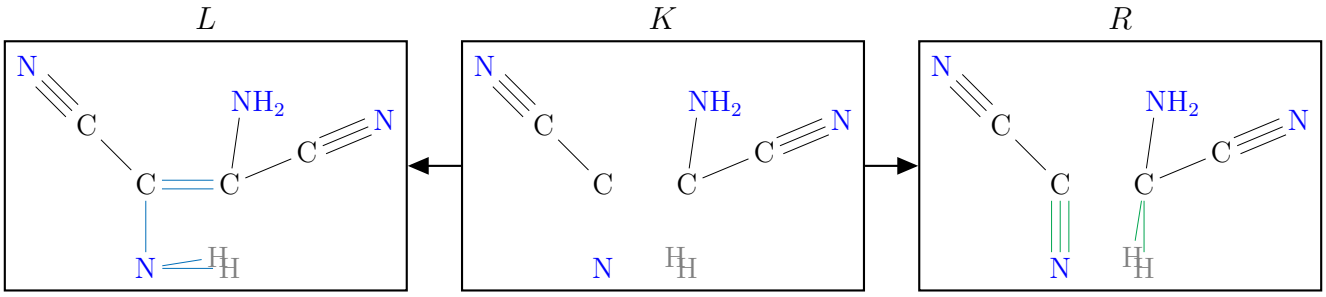
$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`-'}, \text{`='}\} \\
&\}| \geq 1
\end{aligned}
$$

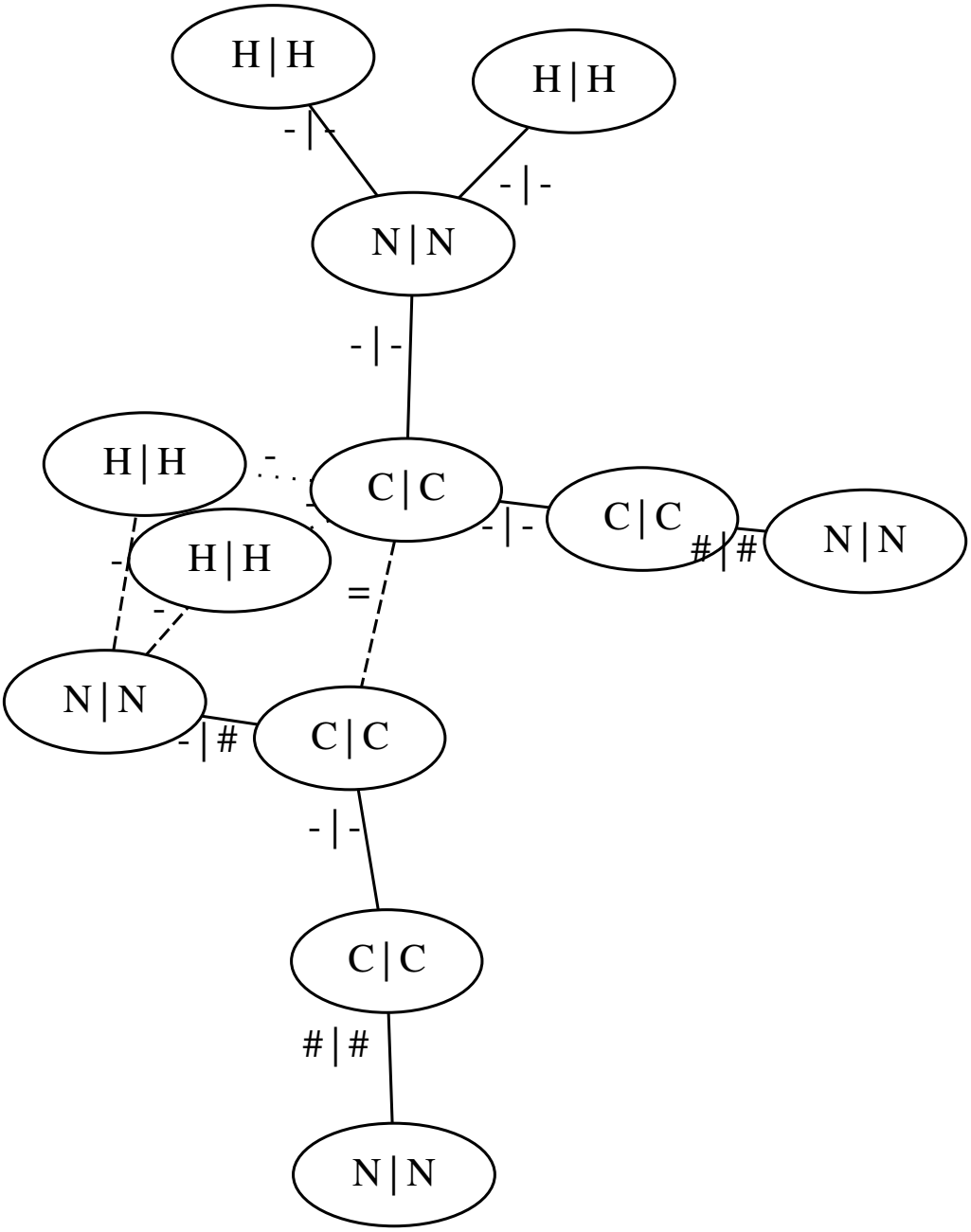
0.0.22 DAMN Scission



Files: out/106_r_20_10300000_{L, K, R}

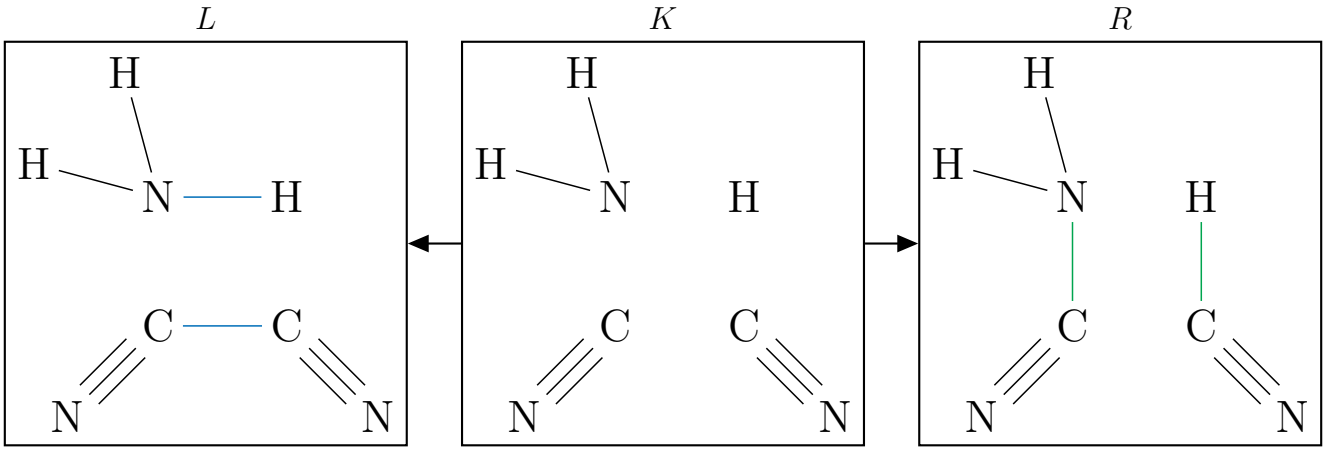


Files: out/107_r_20_11300100_{L, K, R}

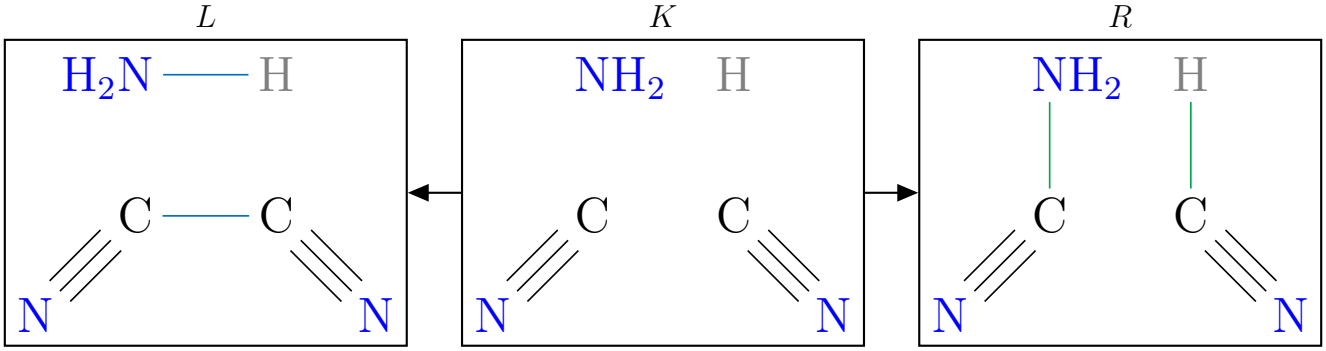


File: out/108_r_20_combined

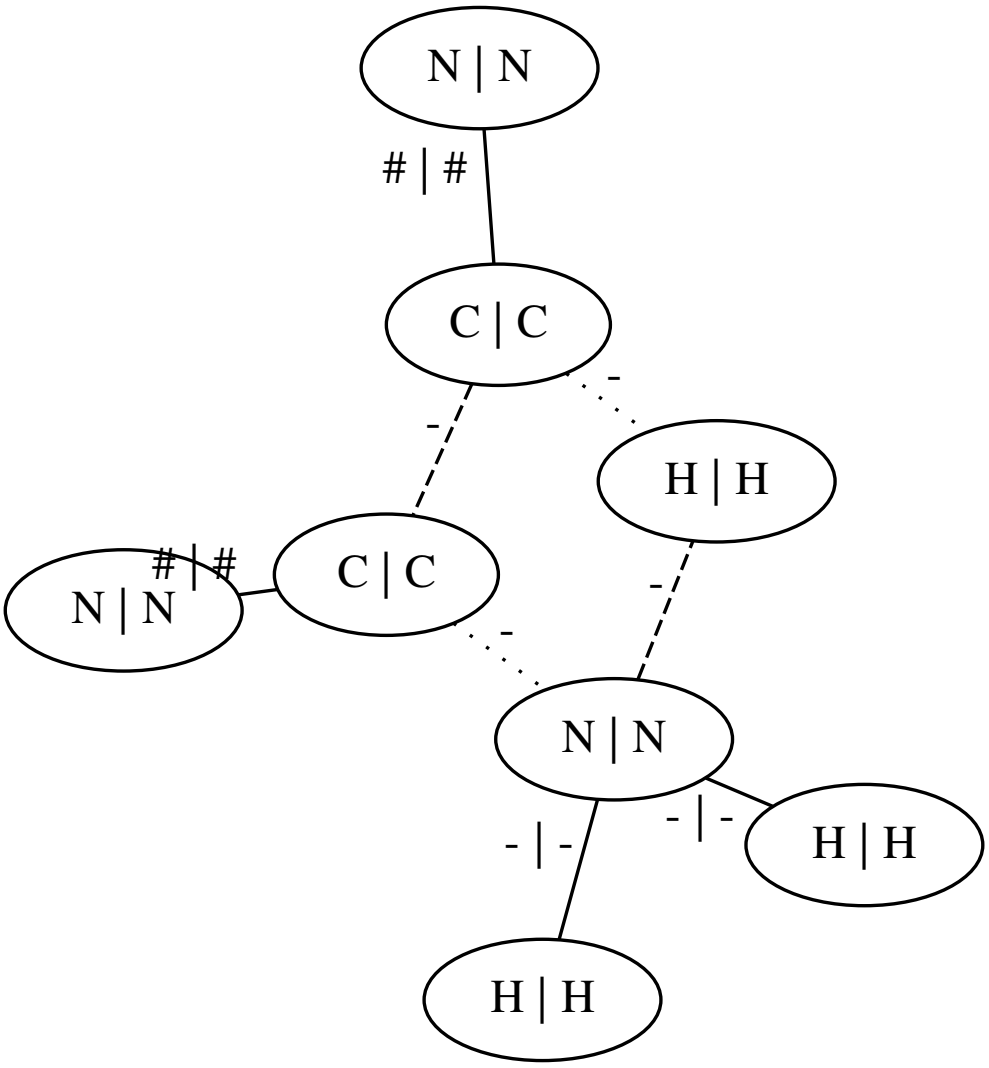
0.0.23 Cyanogen Ammonolysis



Files: out/111_r_21_10300000_{L, K, R}

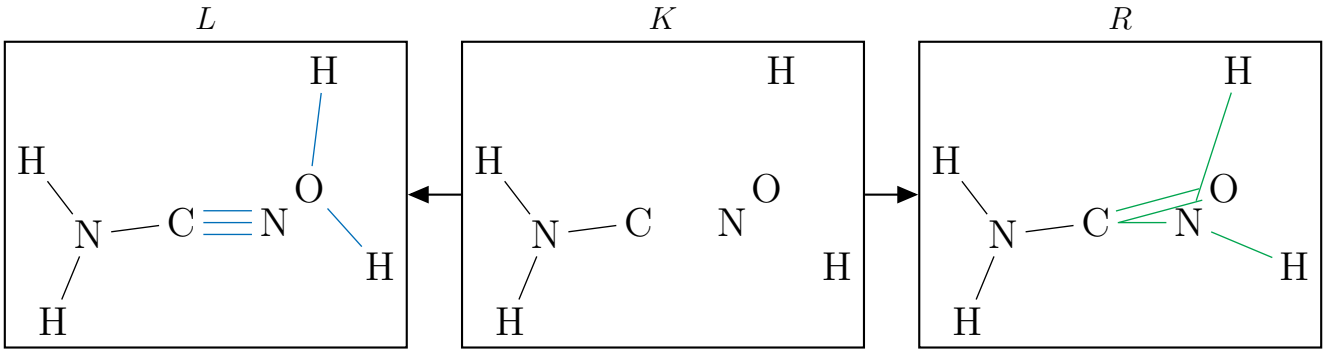


Files: out/112_r_21_11300100_{L, K, R}

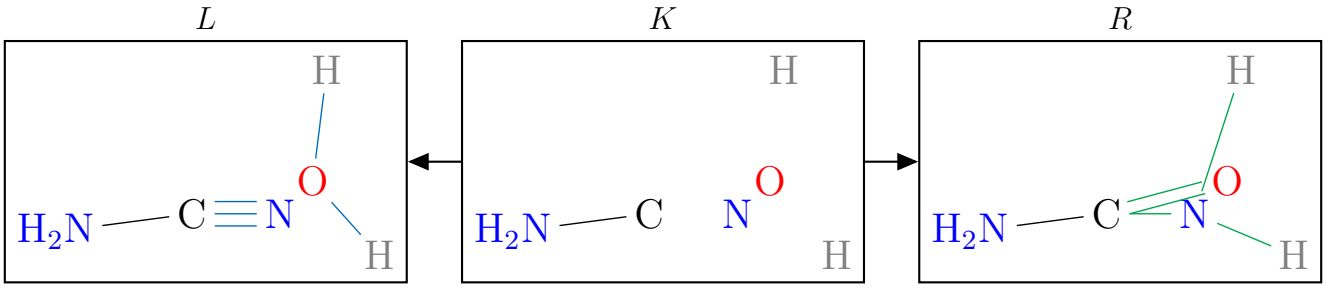


File: out/113_r_21_combined

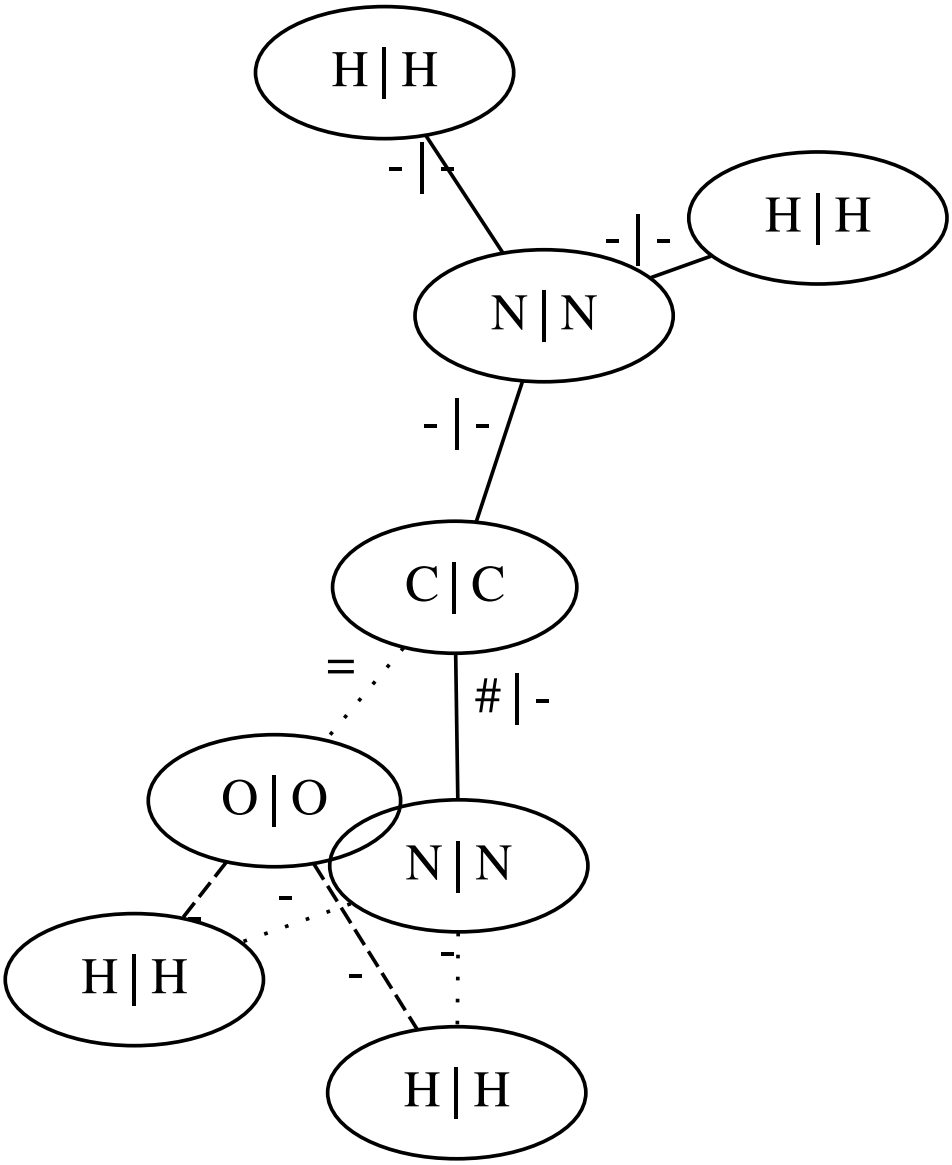
0.0.24 Cyanamide Hydration



Files: out/116_r_22_10300000_{L, K, R}

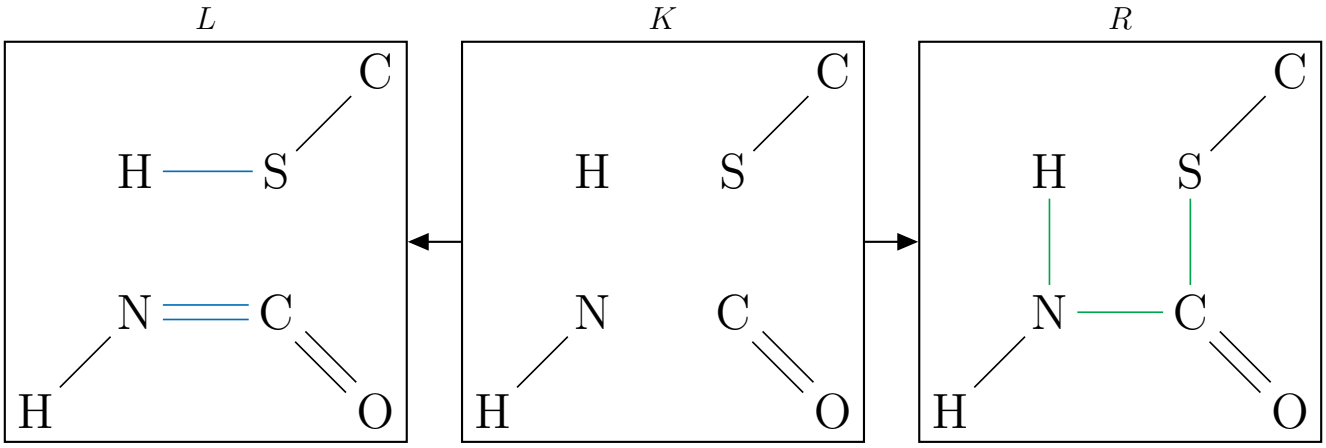


Files: out/117_r_22_11300100_{L, K, R}

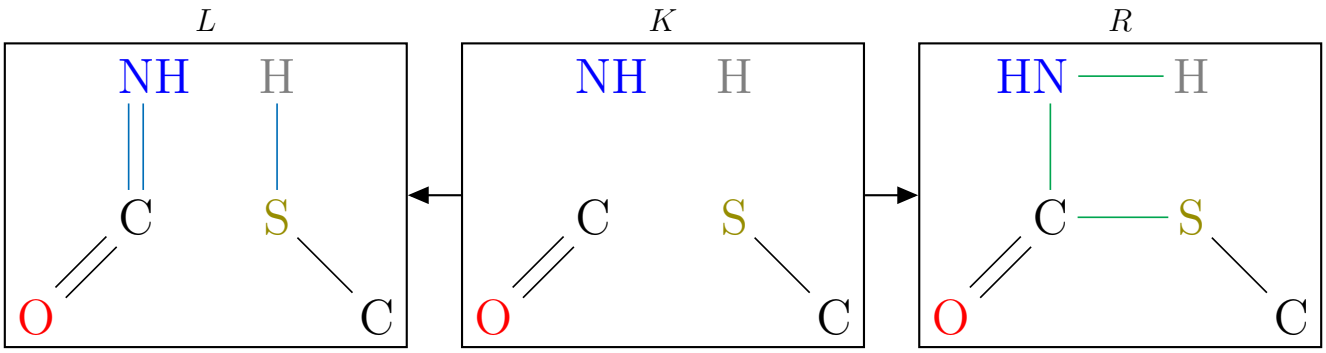


File: out/118_r_22_combined

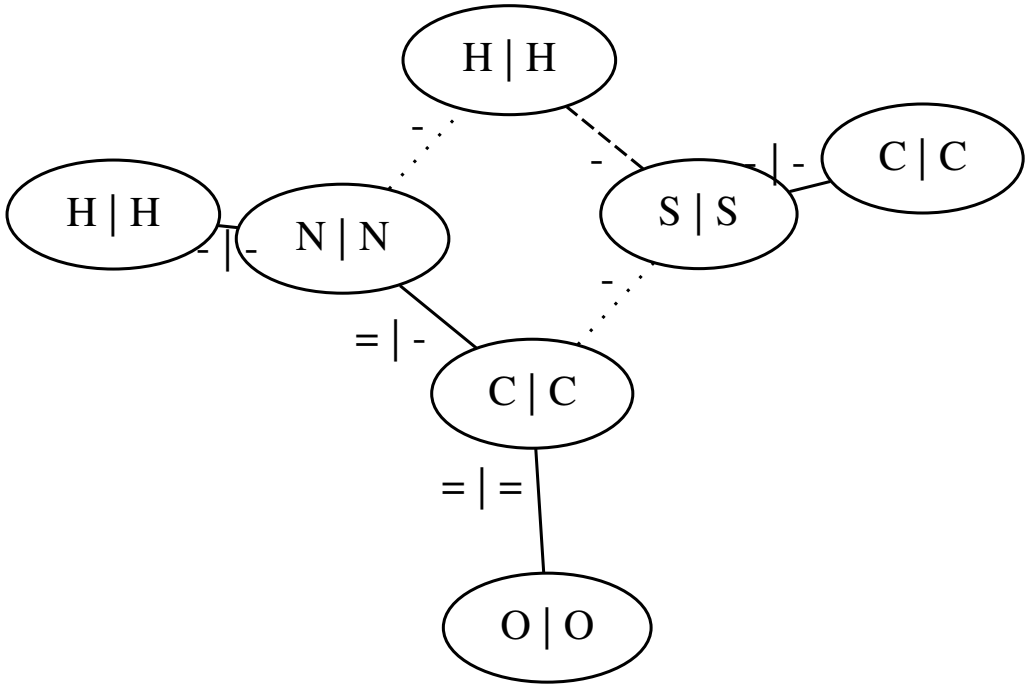
0.0.25 Carbamylation, SC



Files: out/121_r_23_10300000_{L, K, R}

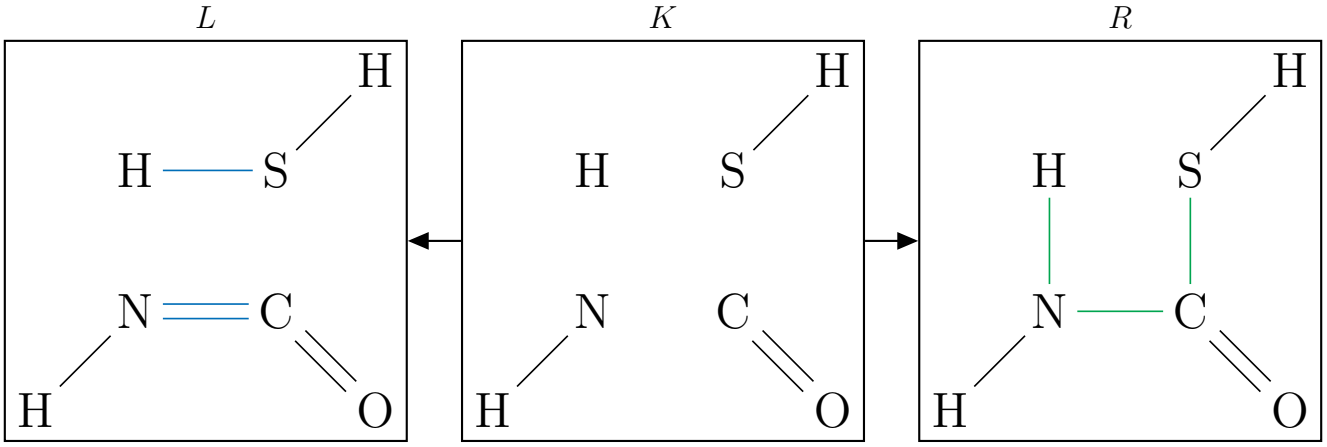


Files: out/122_r_23_11300100_{L, K, R}

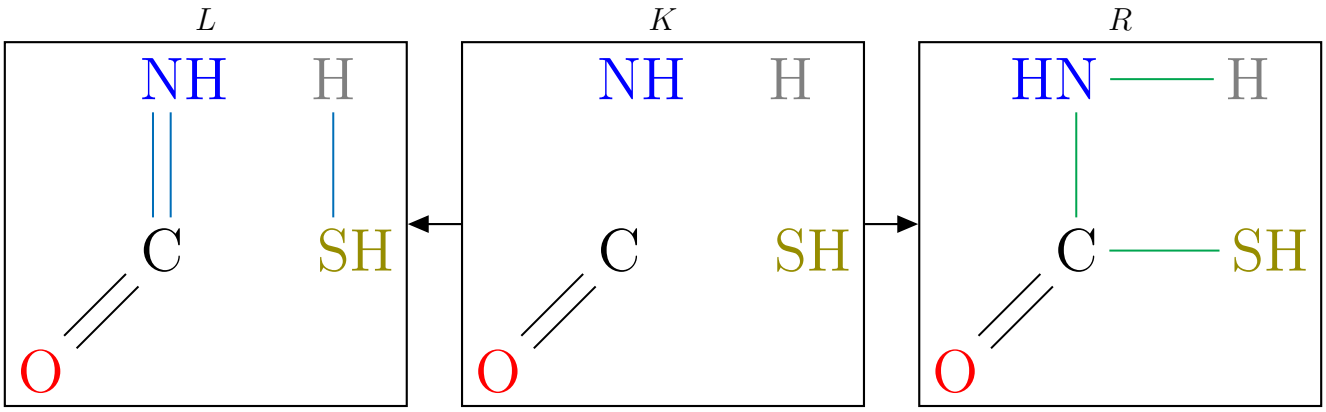


File: out/123_r_23_combined

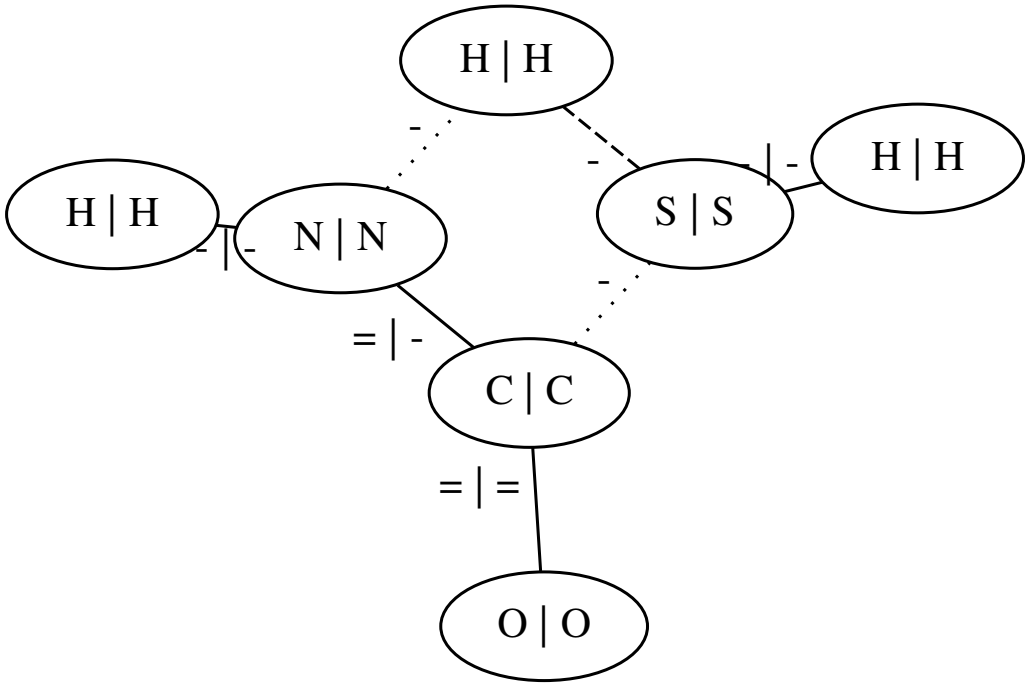
0.0.26 Carbamylation, SH



Files: out/126_r_24_10300000_{L, K, R}

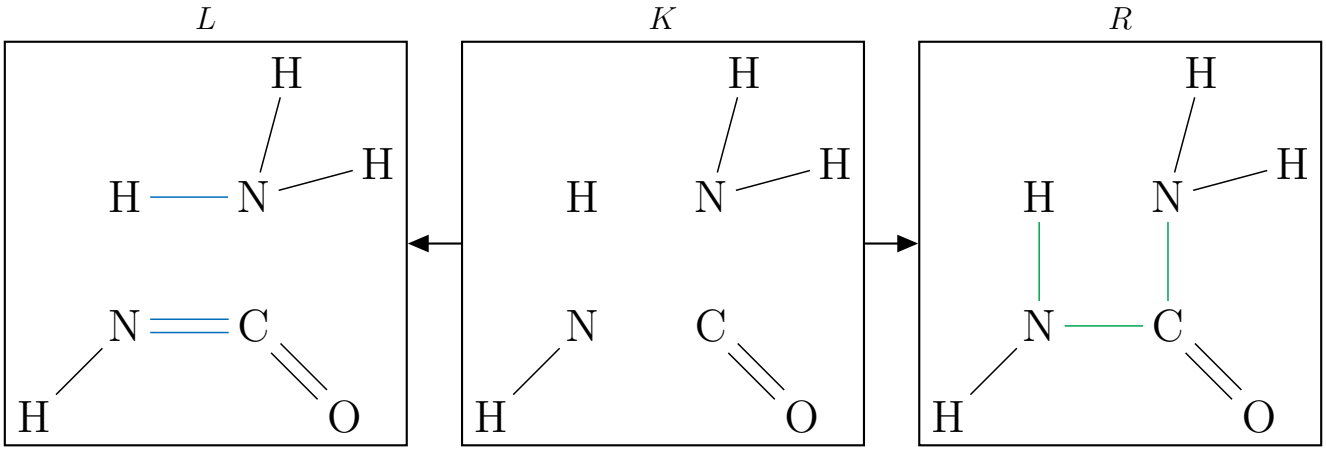


Files: out/127_r_24_11300100_{L, K, R}

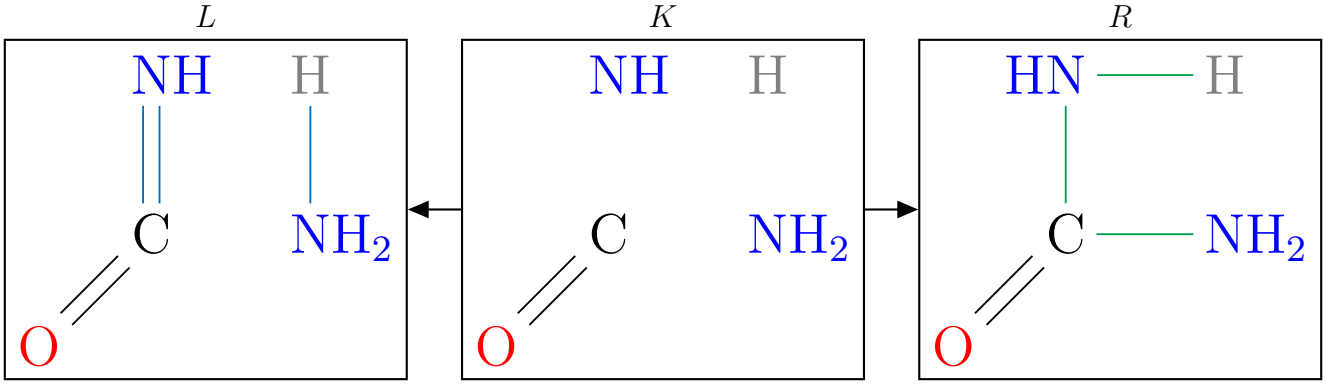


File: out/128_r_24_combined

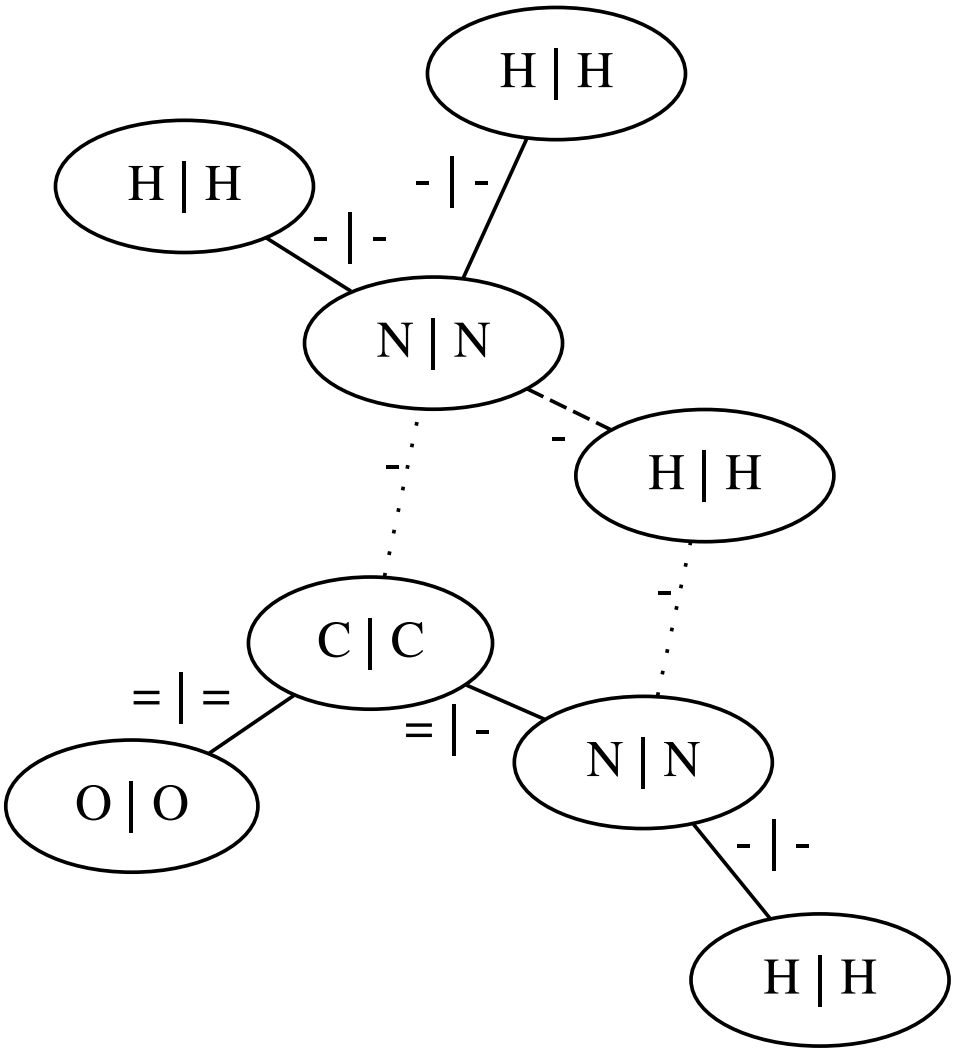
0.0.27 Carbamylation, N, HH



Files: out/131_r_25_10300000_{L, K, R}

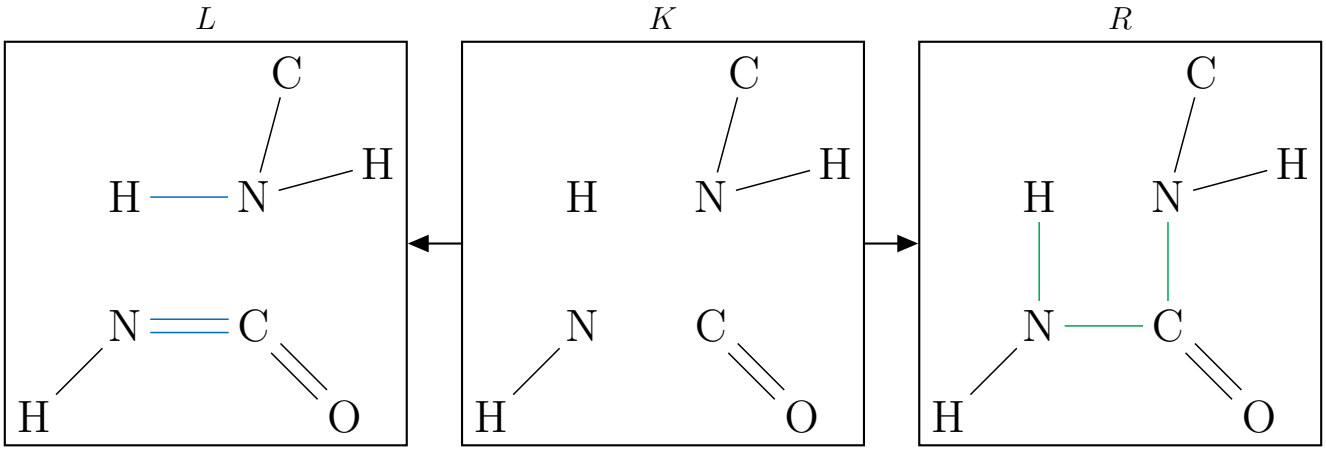


Files: out/132_r_25_11300100_{L, K, R}

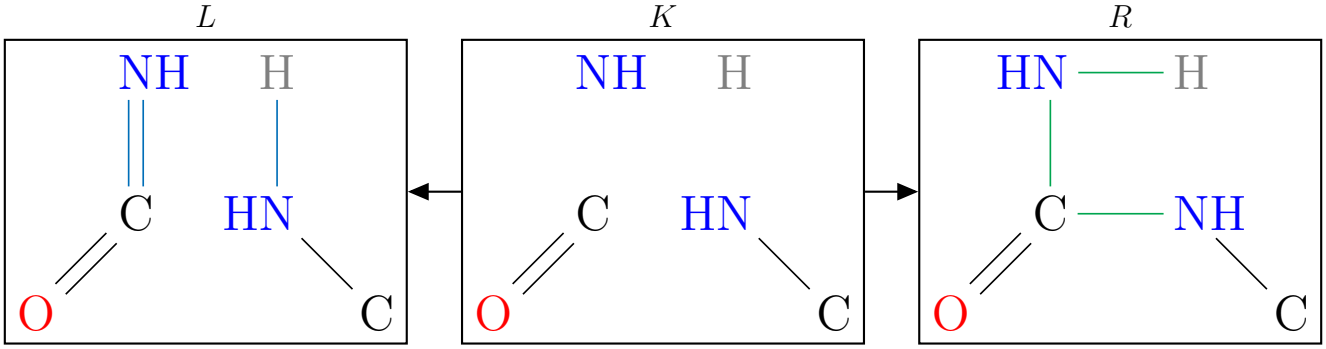


File: out/133_r_25_combined

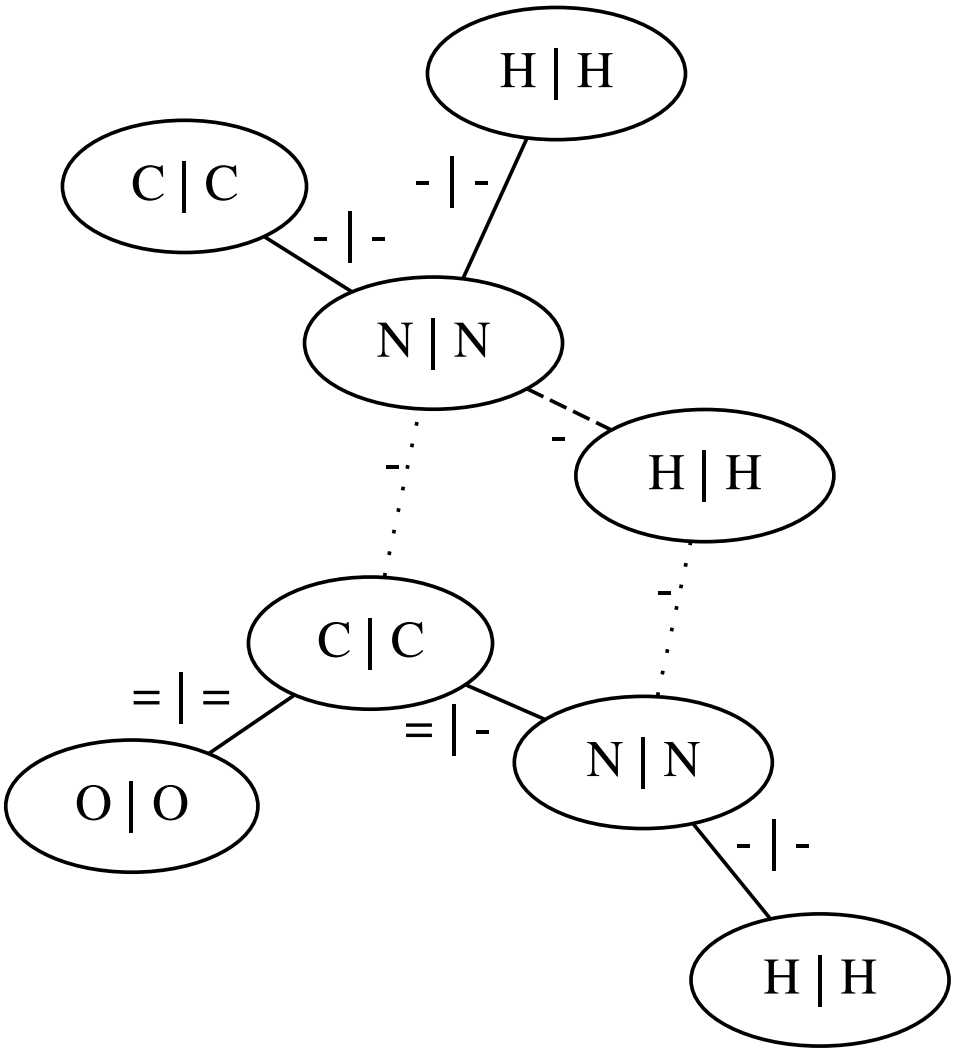
0.0.28 Carbamylation, N, HC



Files: out/136_r_26_10300000_{L, K, R}



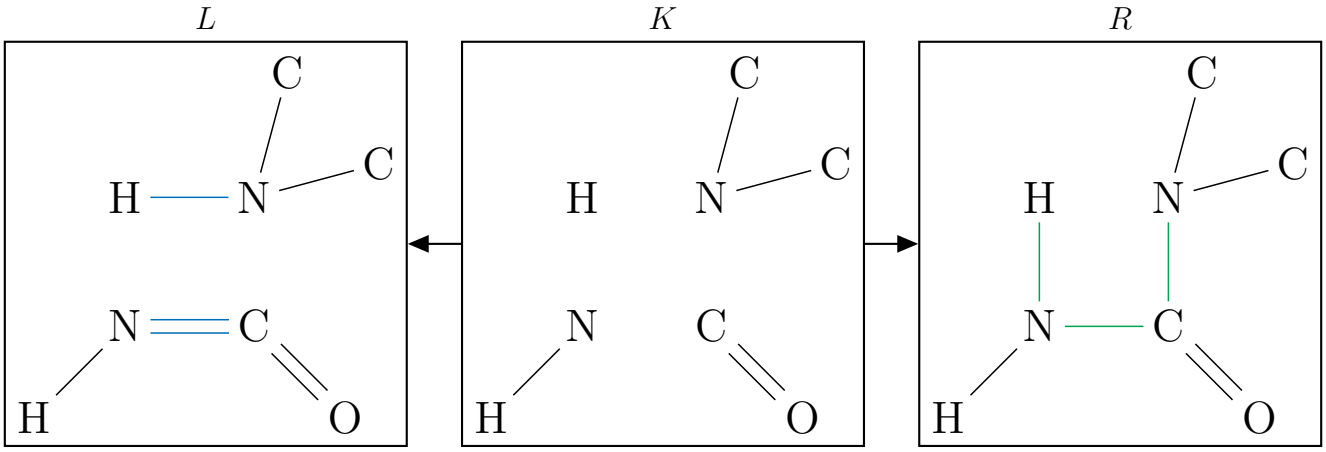
Files: out/137_r_26_11300100_{L, K, R}



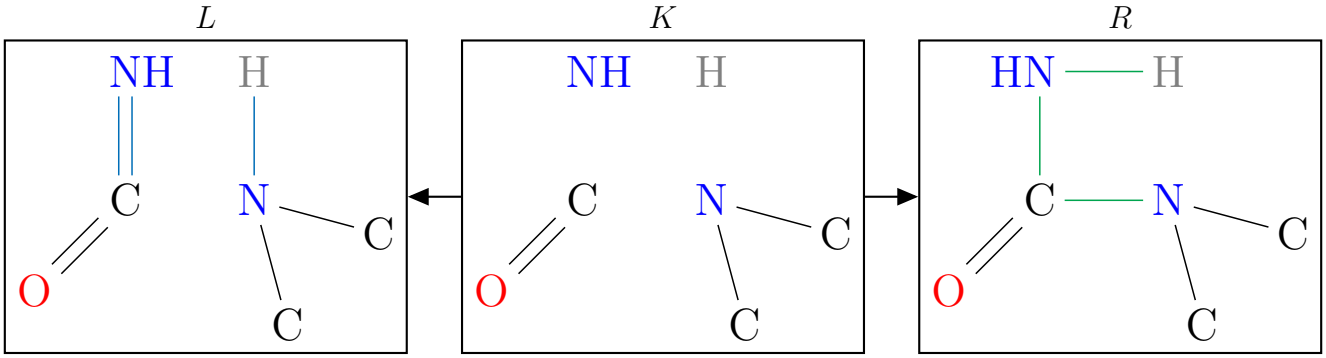
File: out/138_r_26_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

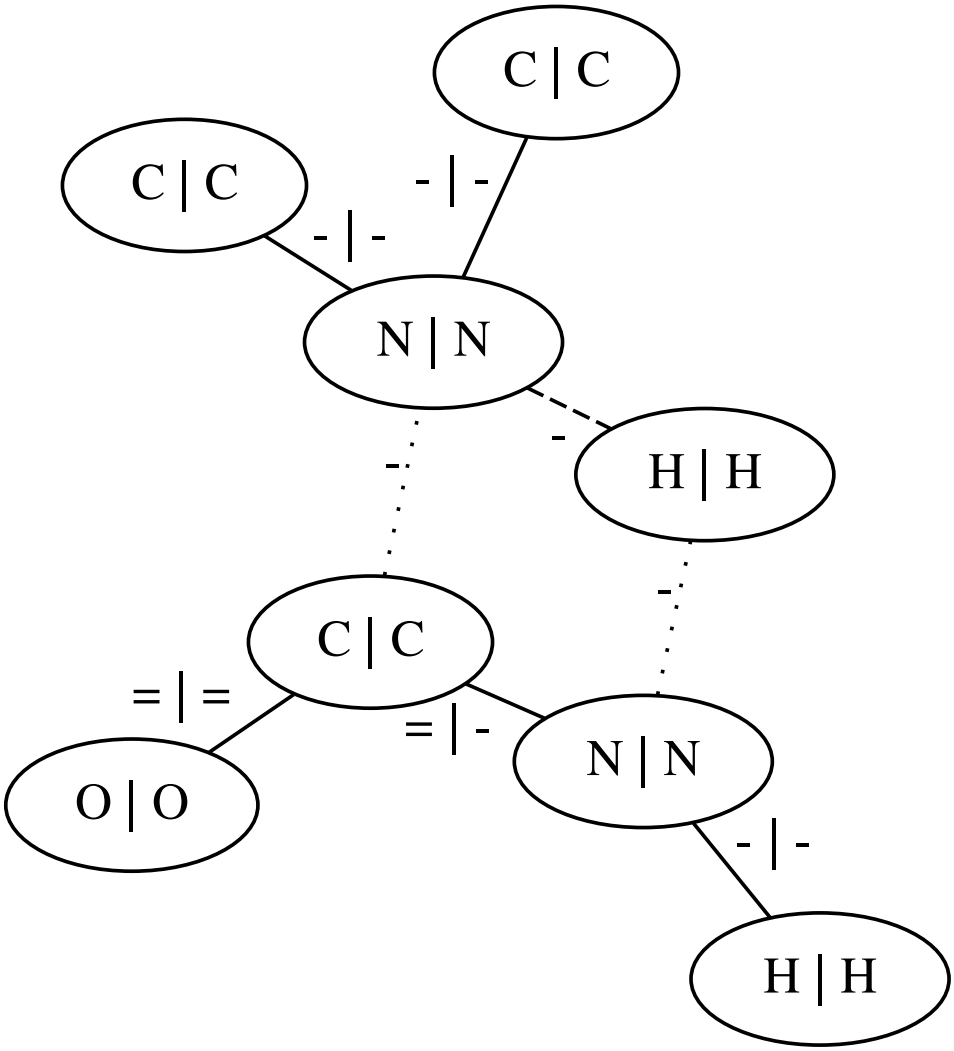
0.0.29 Carbamylation, N, CC



Files: out/141_r_27_10300000_{L, K, R}



Files: out/142_r_27_11300100_{L, K, R}

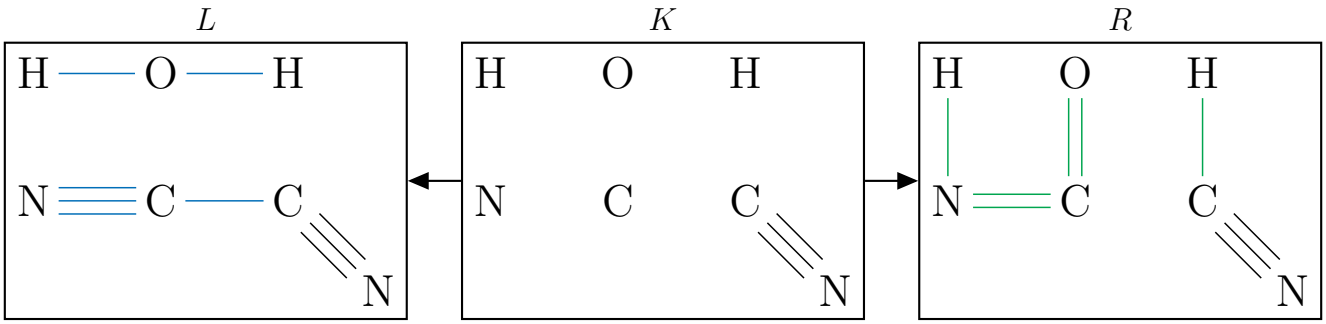


File: out/143_r_27_combined

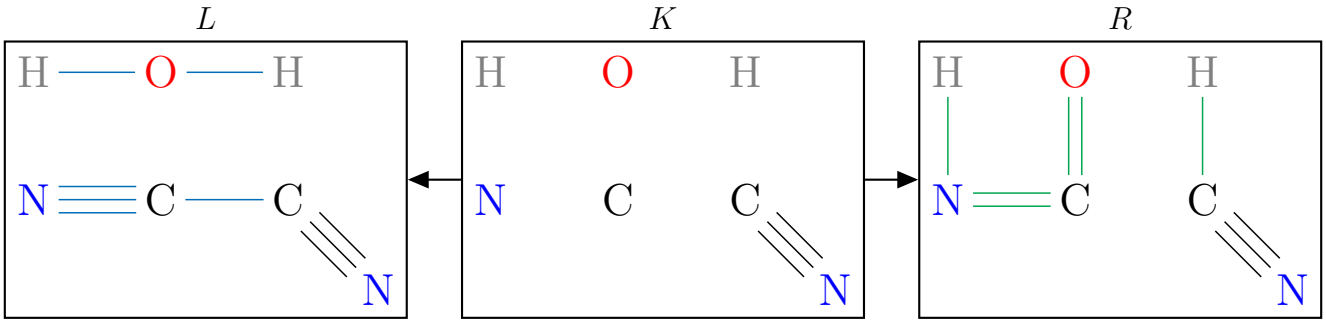
$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

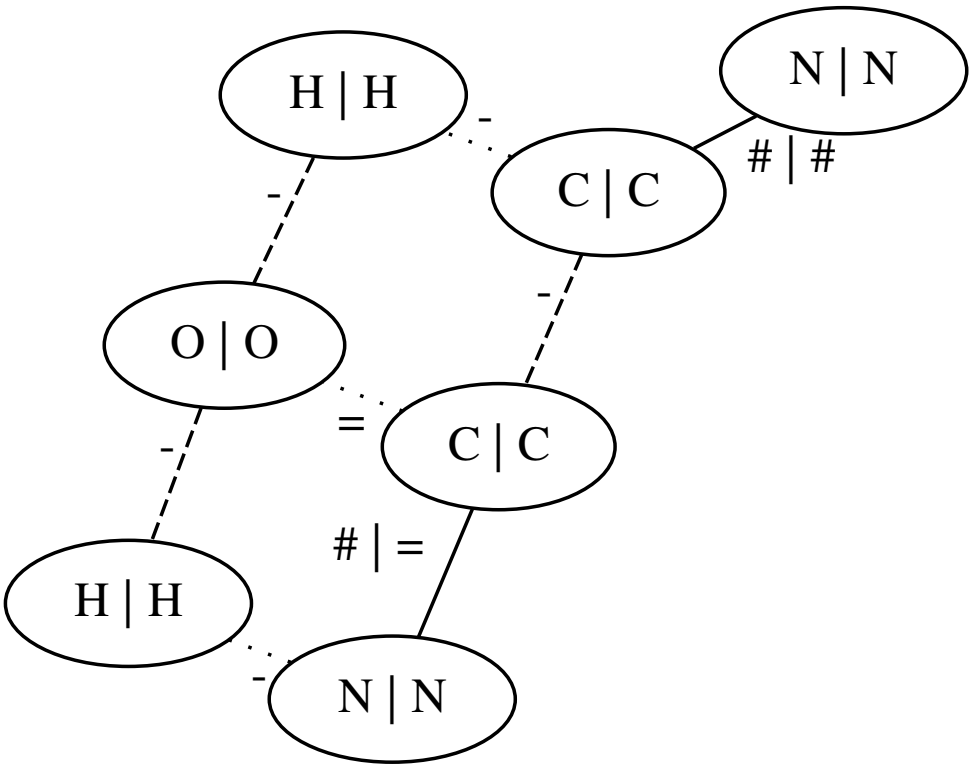
0.0.30 Cyanate from cyanogen



Files: out/146_r_28_10300000_{L, K, R}

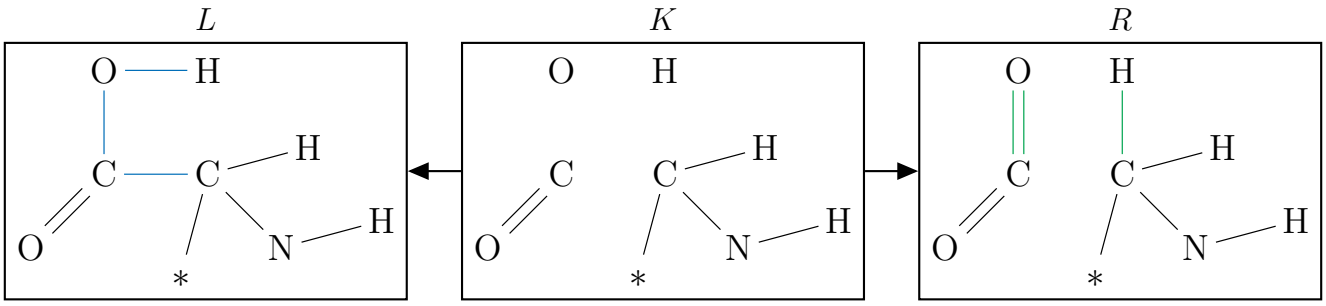


Files: out/147_r_28_11300100_{L, K, R}

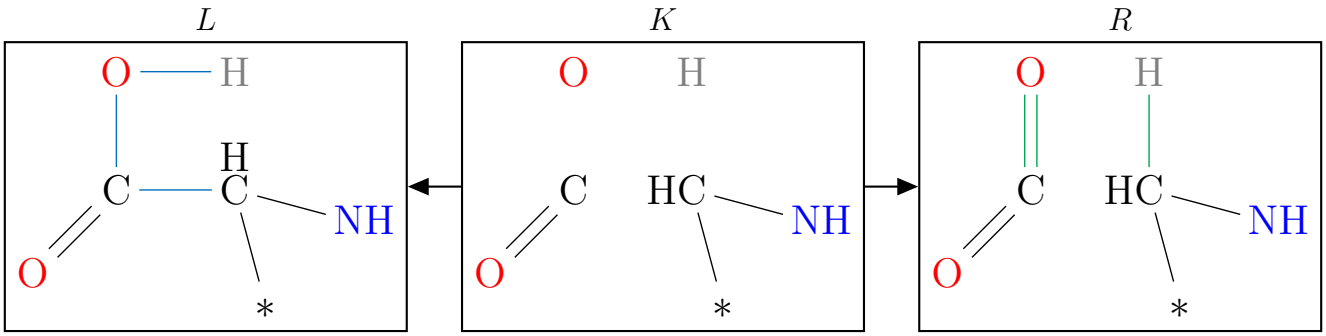


File: out/148_r_28_combined

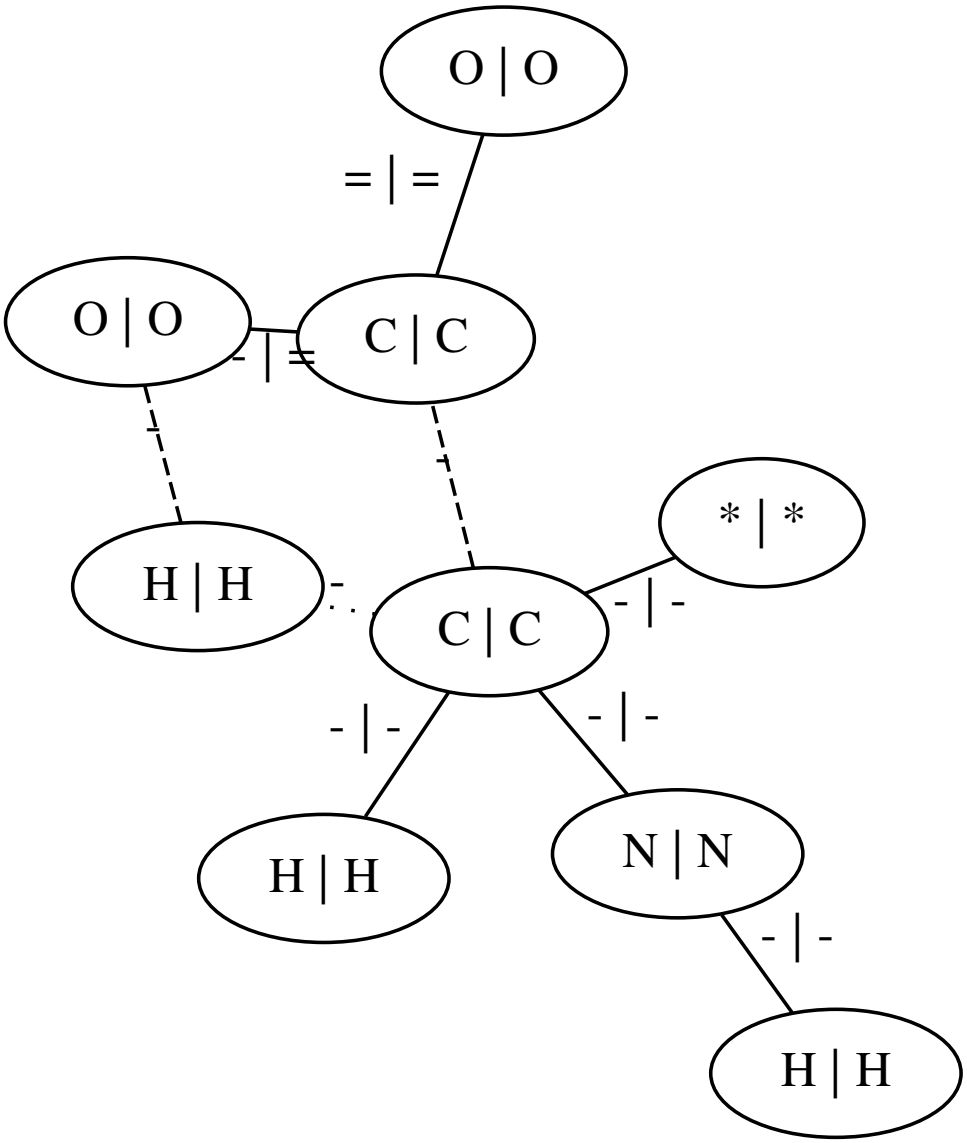
0.0.31 Ketone-Catalyzed Decarboxylation



Files: out/151_r_29_10300000_{L, K, R}

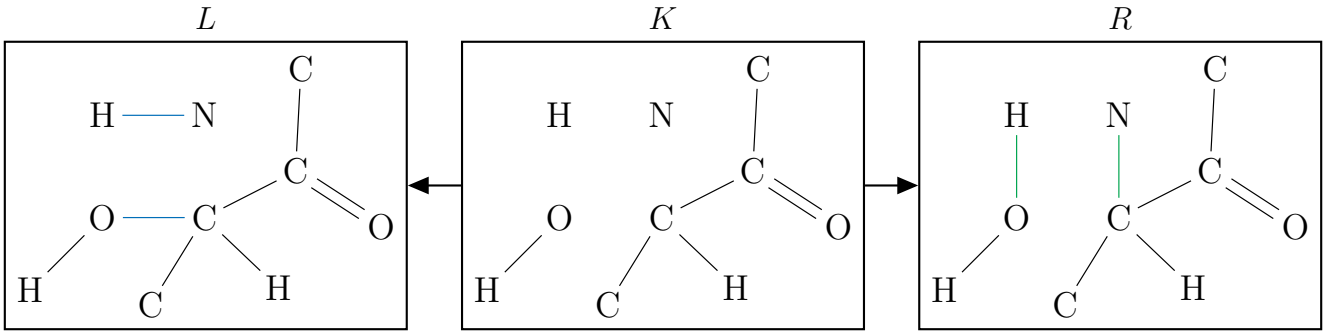


Files: out/152_r_29_11300100_{L, K, R}

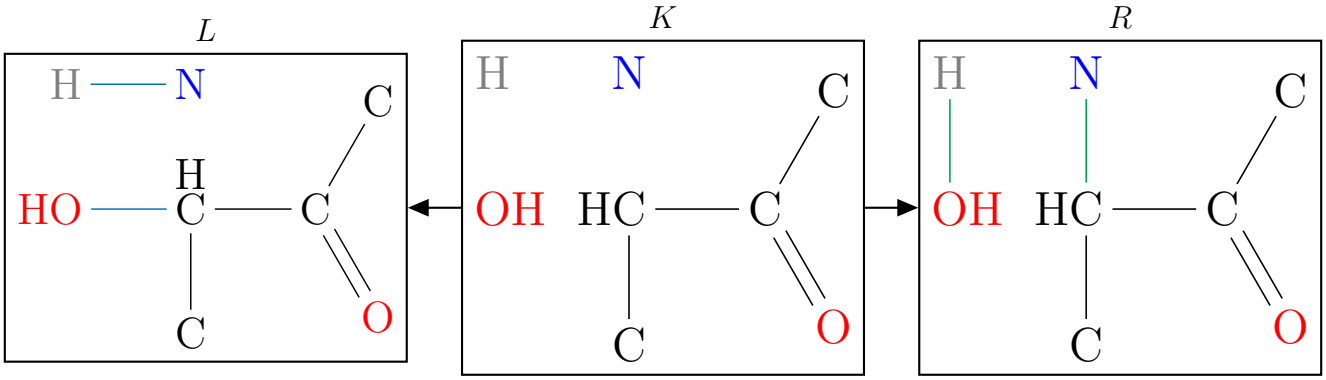


File: out/153_r_29_combined

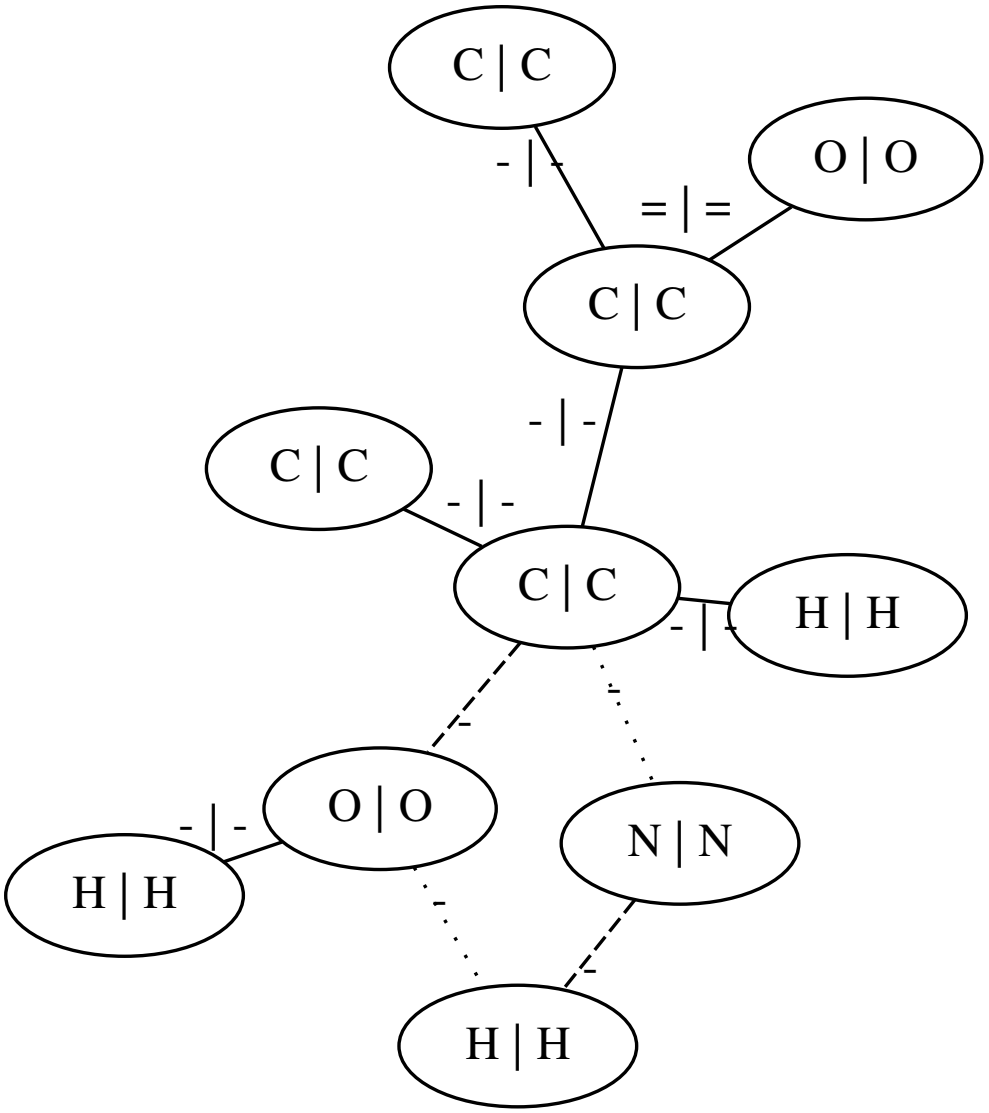
0.0.32 Amadori Rearrangement



Files: out/156_r_30_10300000_{L, K, R}

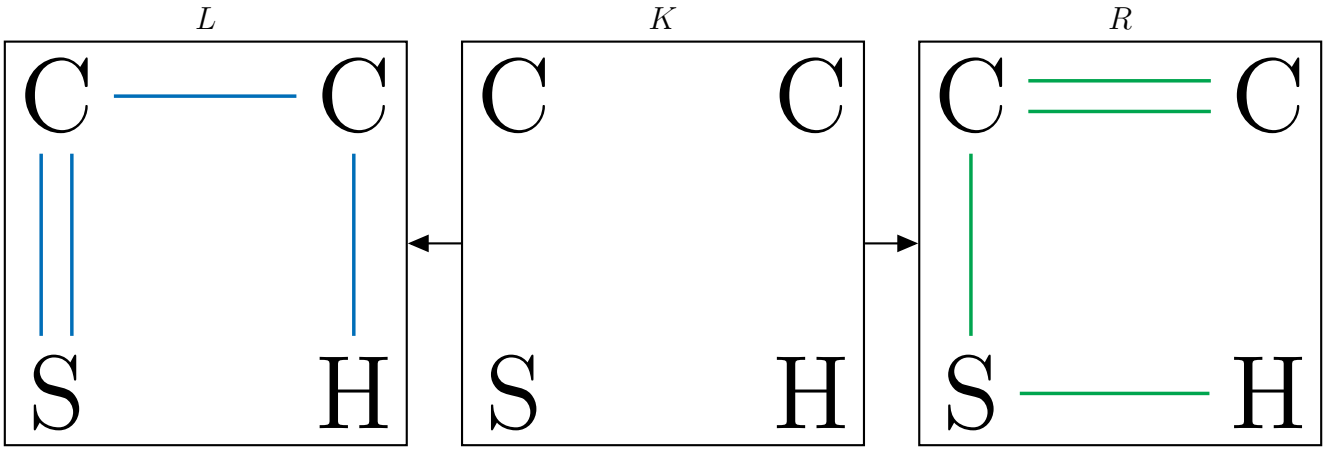


Files: out/157_r_30_11300100_{L, K, R}

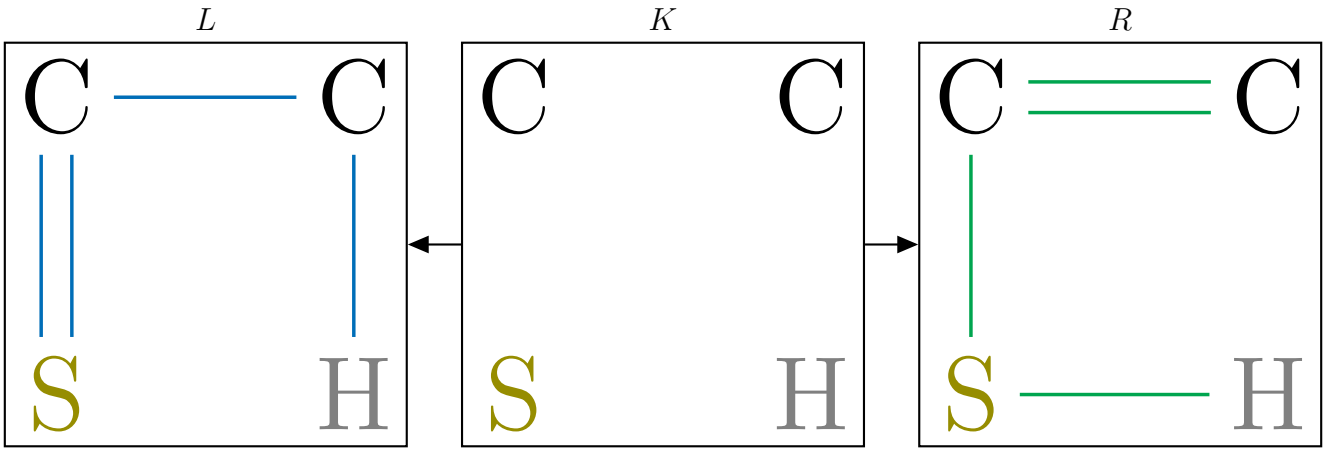


File: out/158_r_30_combined

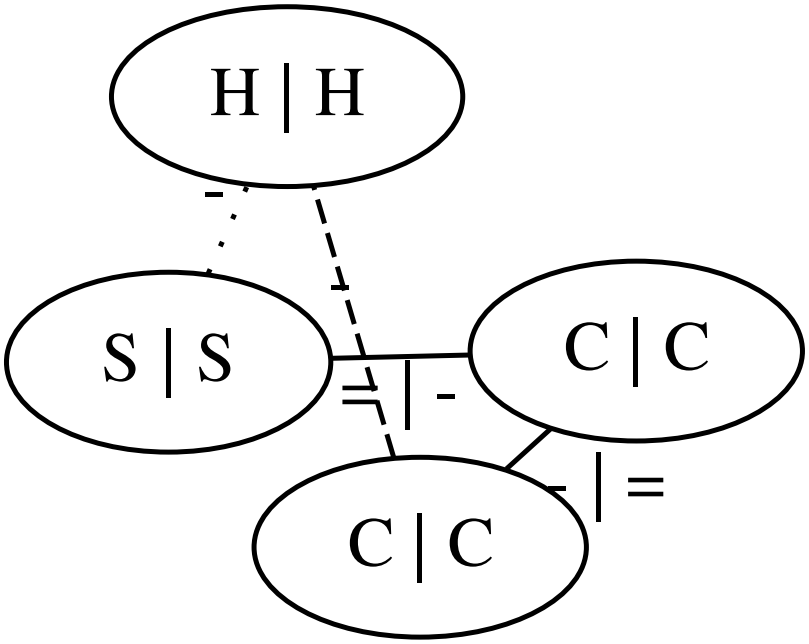
0.0.33 Thial -> Thiene



Files: out/161_r_31_10300000_{L, K, R}

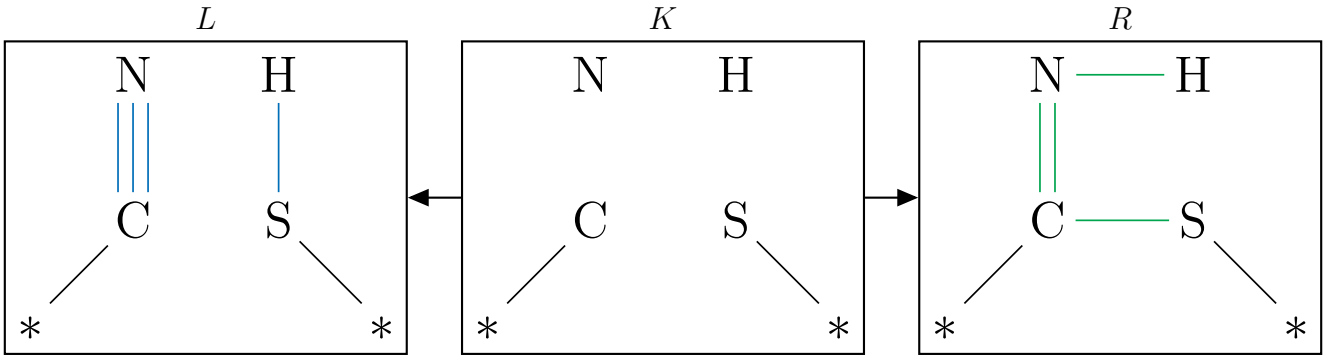


Files: out/162_r_31_11300100_{L, K, R}

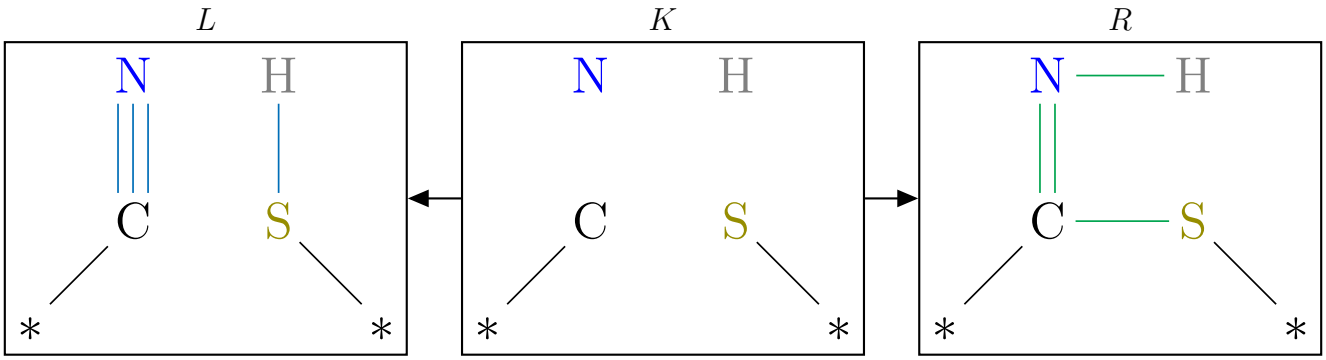


File: out/163_r_31_combined

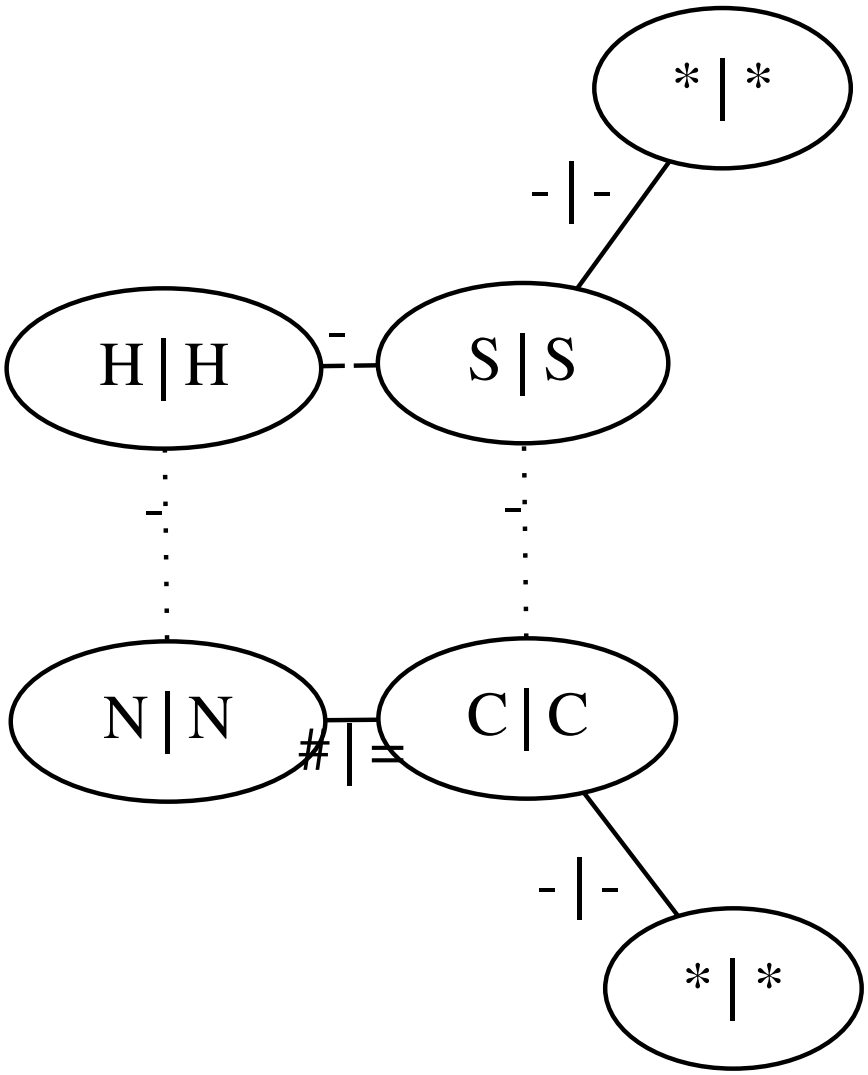
0.0.34 Sulfide to Nitrile Addition



Files: out/166_r_32_10300000_{L, K, R}

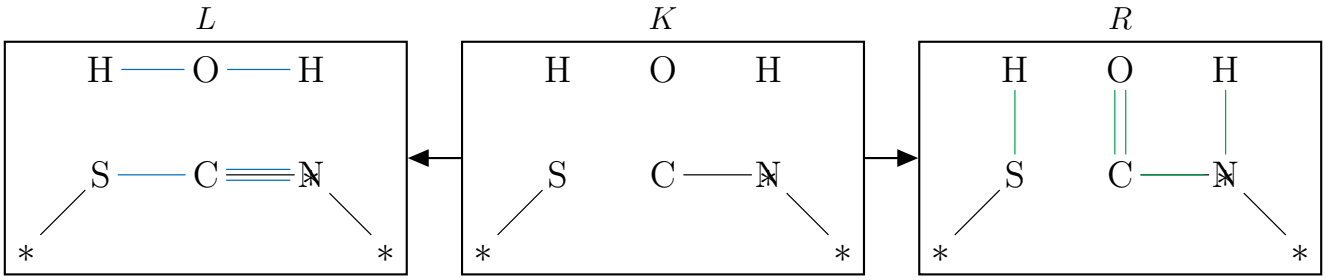


Files: out/167_r_32_11300100_{L, K, R}

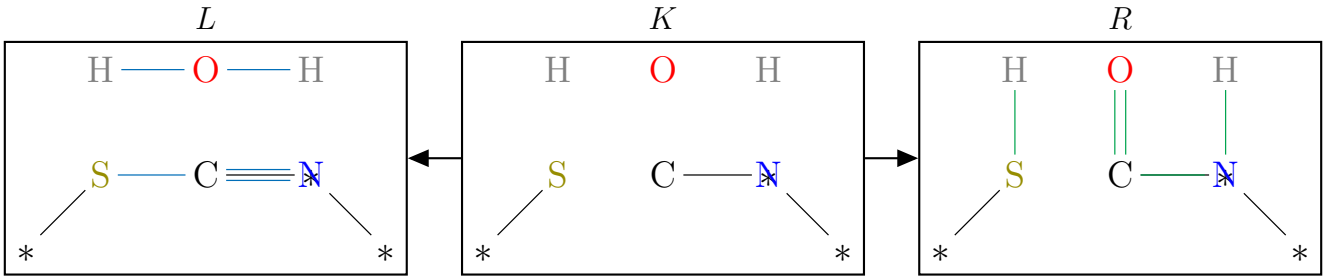


File: out/168_r_32_combined

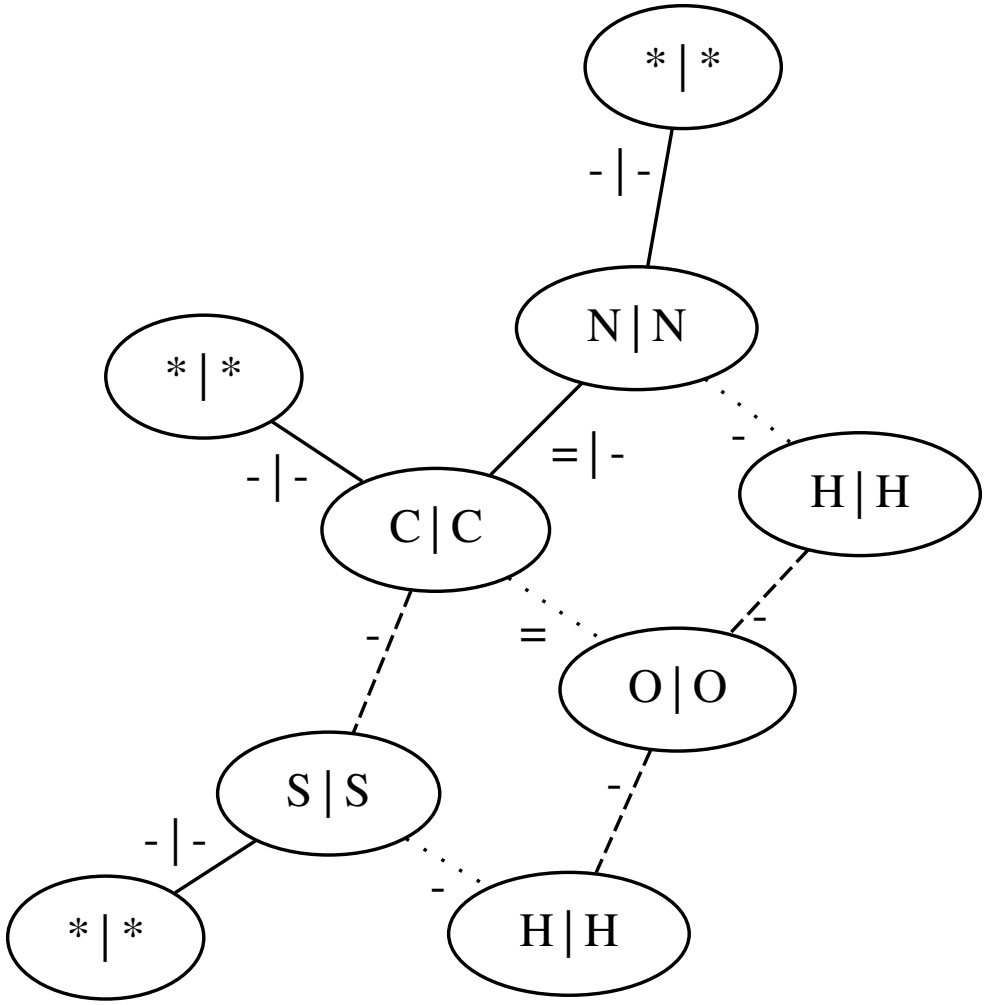
0.0.35 Thioamidine to Amide Hydrolysis



Files: out/171_r_33_10300000_{L, K, R}

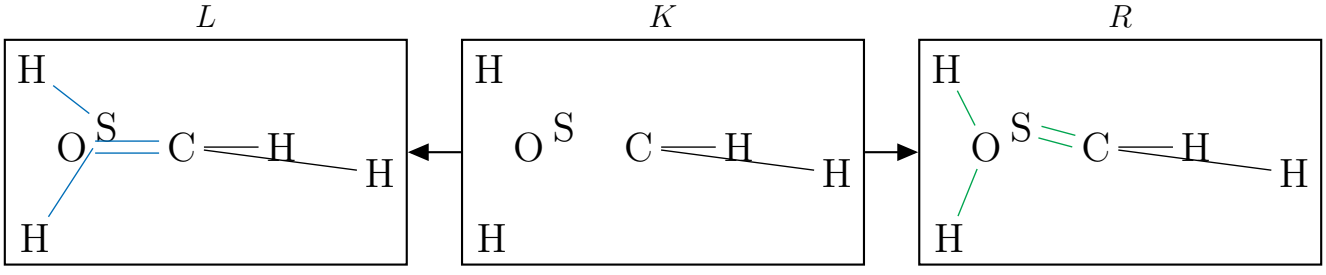


Files: out/172_r_33_11300100_{L, K, R}

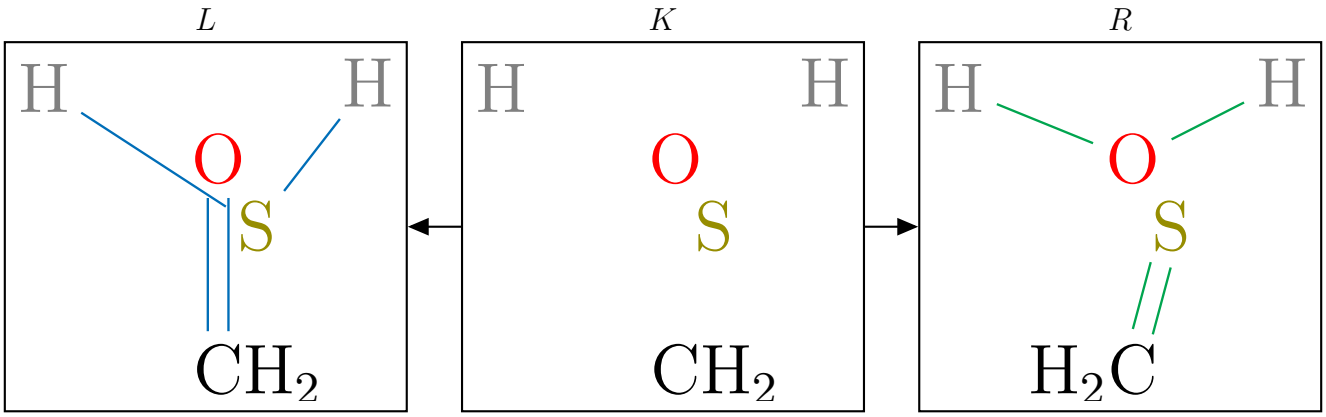


File: out/173_r_33_combined

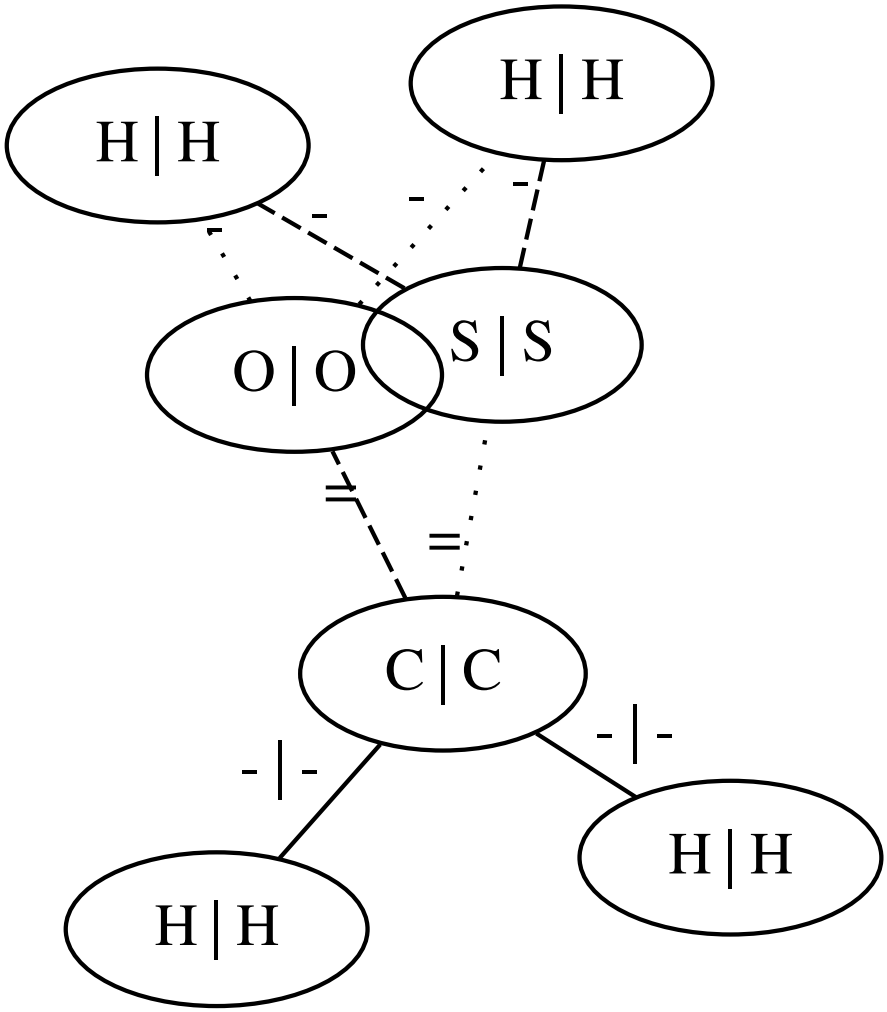
0.0.36 Ketone/Aldehyde to Thioketone/Thial, HH



Files: out/176_r_34_10300000_{L, K, R}

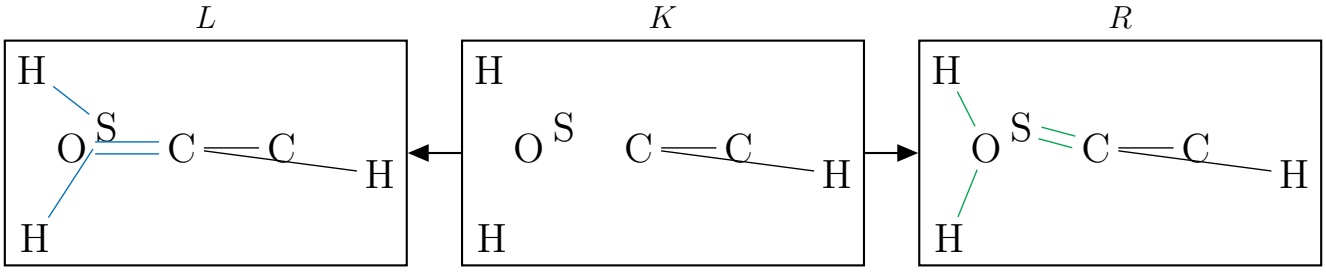


Files: out/177_r_34_11300100_{L, K, R}

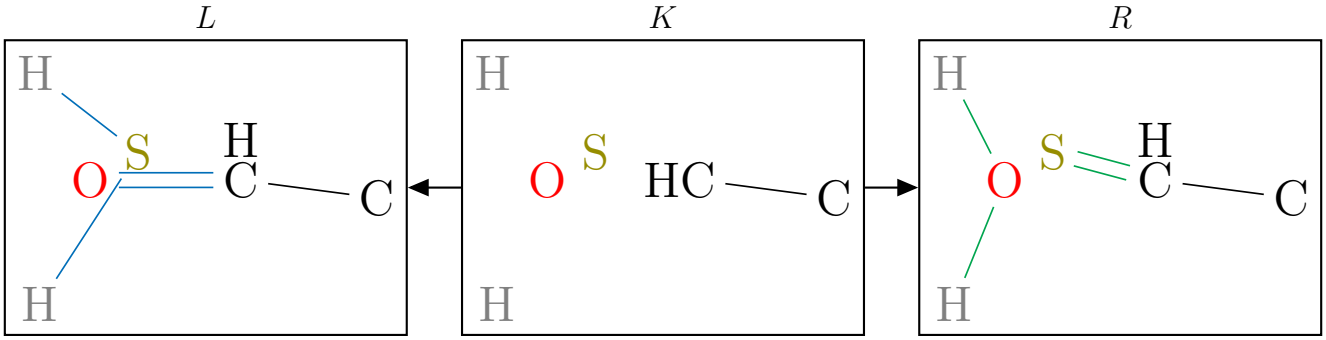


File: out/178_r_34_combined

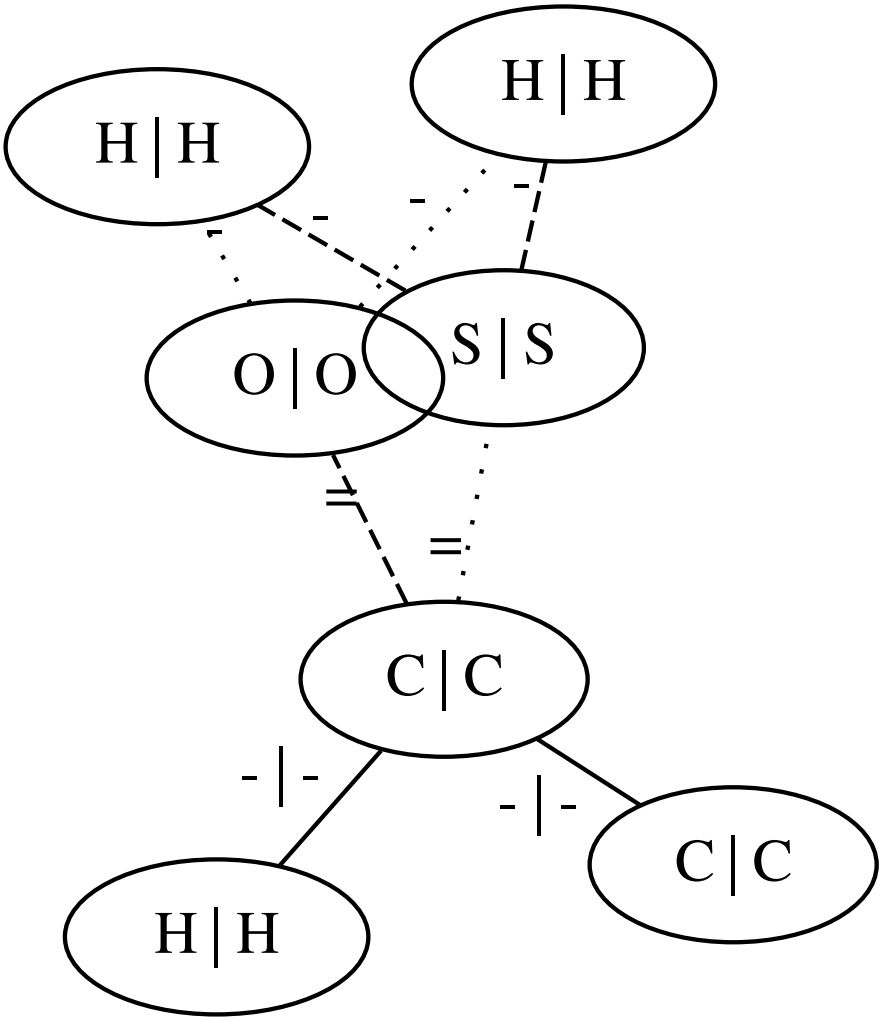
0.0.37 Ketone/Aldehyde to Thioketone/Thial, HC



Files: out/181_r_35_10300000_{L, K, R}



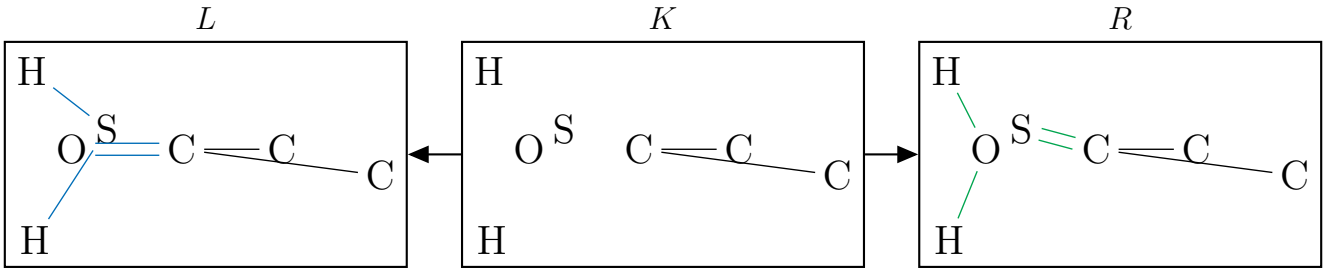
Files: out/182_r_35_11300100_{L, K, R}



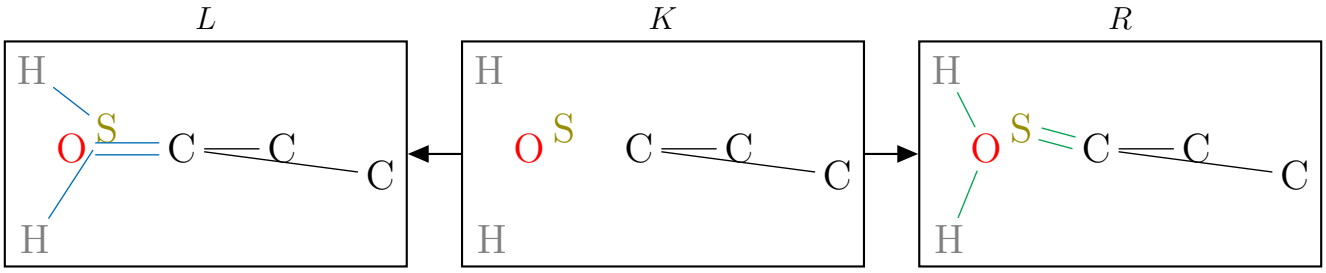
File: out/183_r_35_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

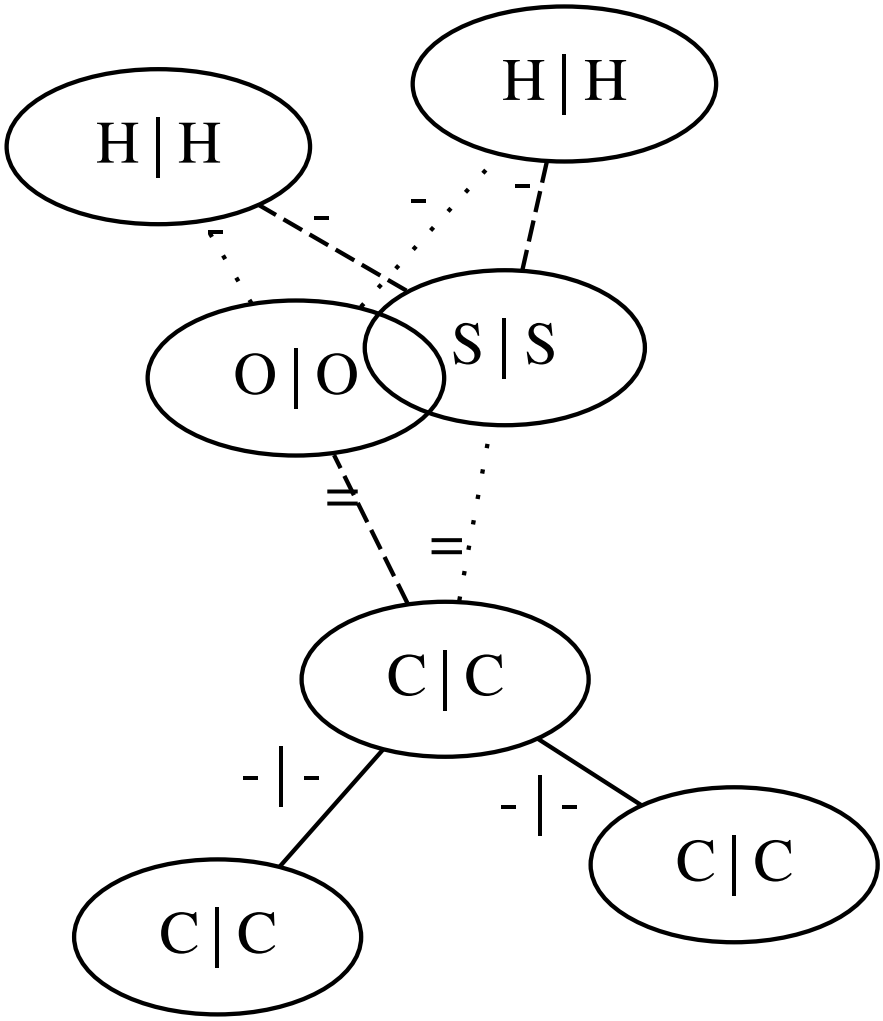
0.0.38 Ketone/Aldehyde to Thioketone/Thial, CC



Files: out/186_r_36_10300000_{L, K, R}



Files: out/187_r_36_11300100_{L, K, R}



File: out/188_r_36_combined

$$
\begin{aligned}
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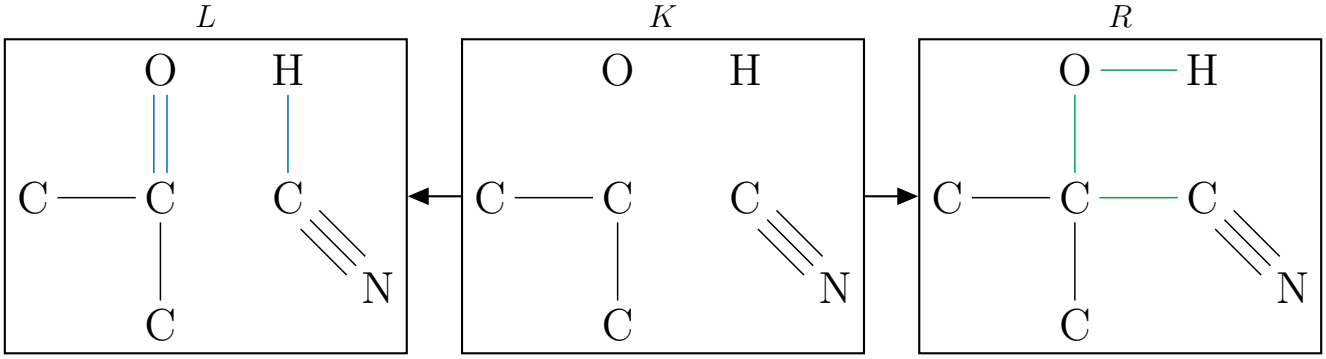
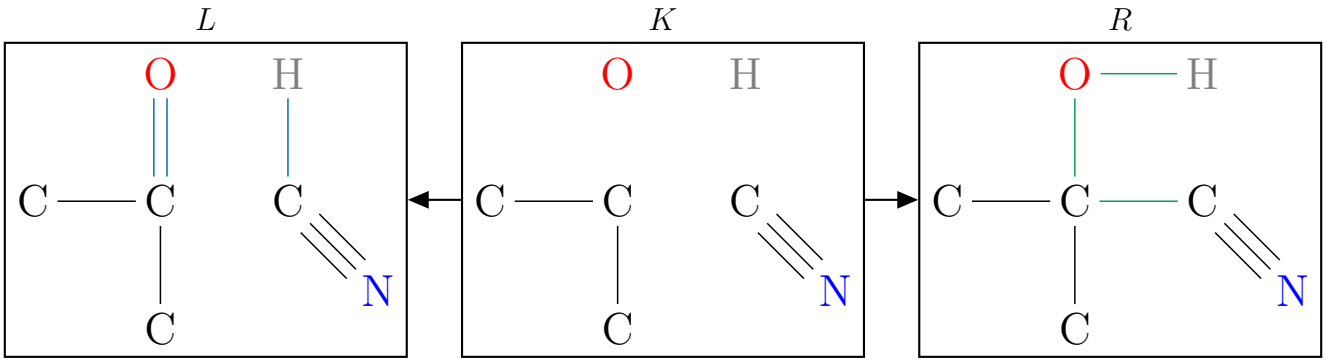
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

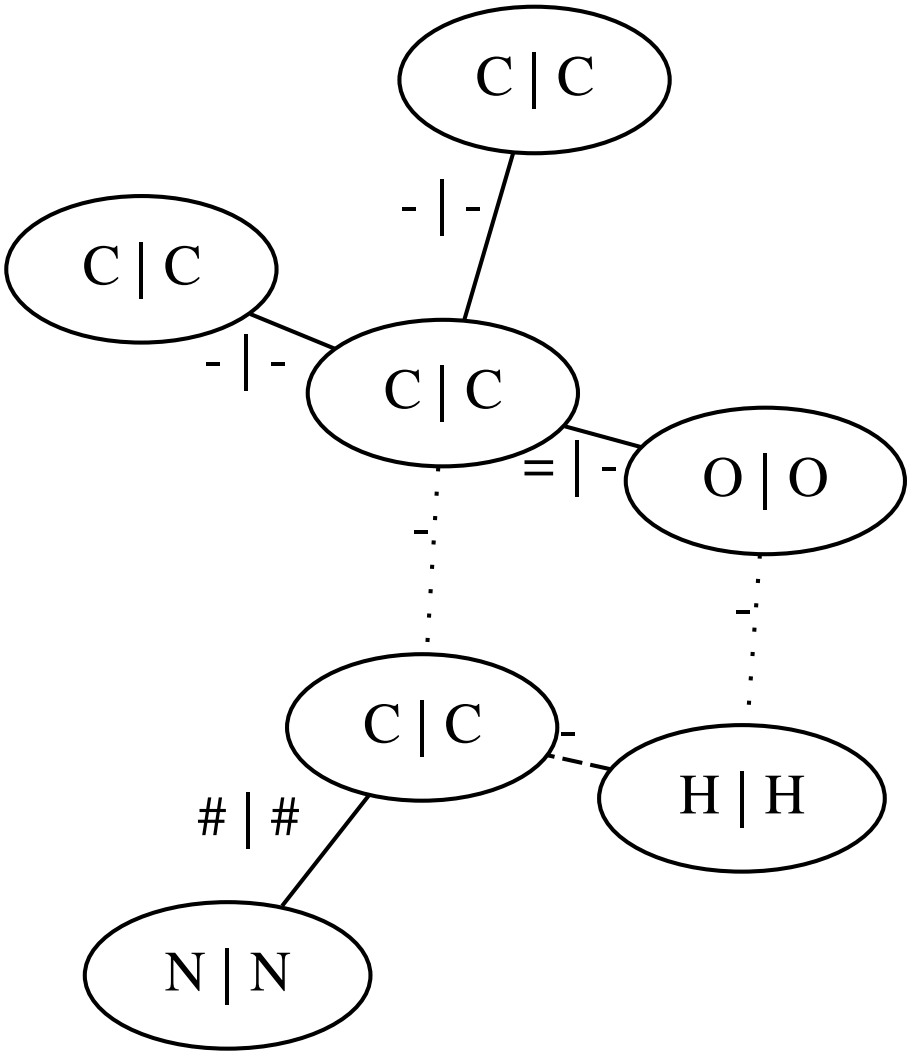
0.0.39 HCN to Ketone



Files: out/191_r_37_10300000_{L, K, R}

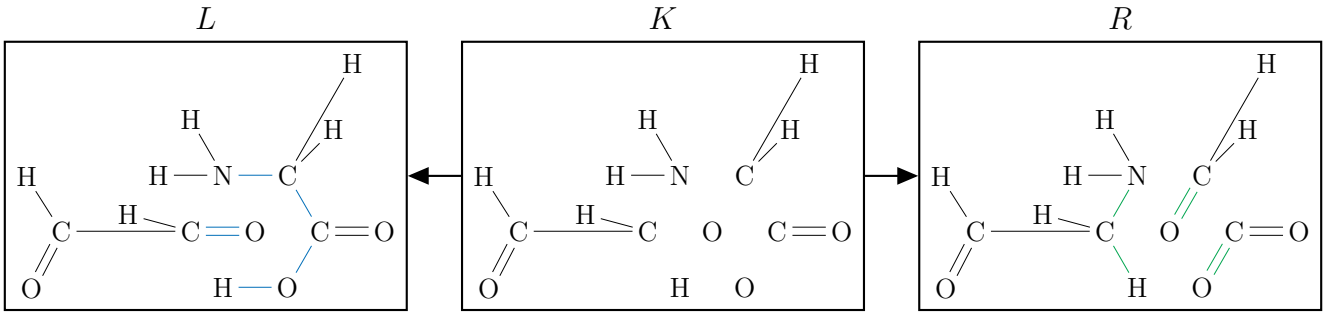


Files: out/192_r_37_11300100_{L, K, R}

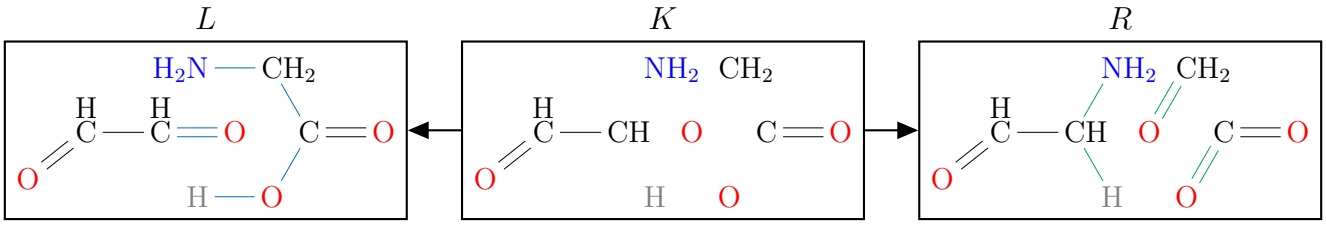


File: out/193_r_37_combined

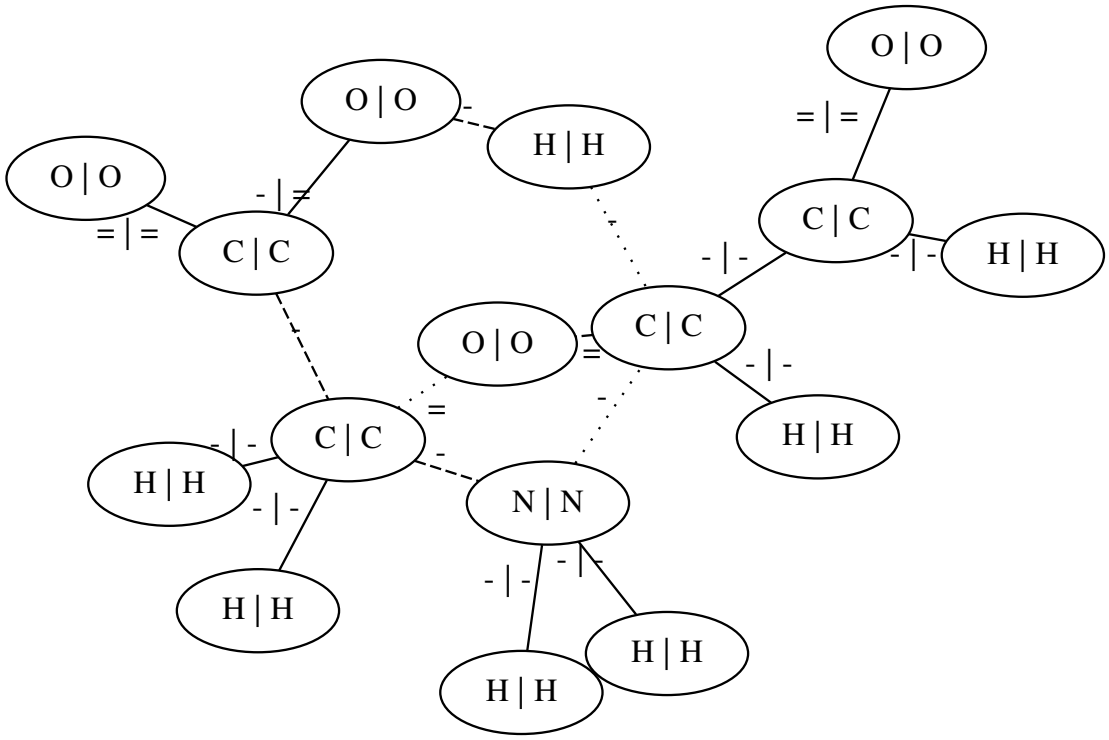
0.0.40 Strecker Degradation Dicarbonyl, H, H, H, H



Files: out/196_r_38_10300000_{L, K, R}

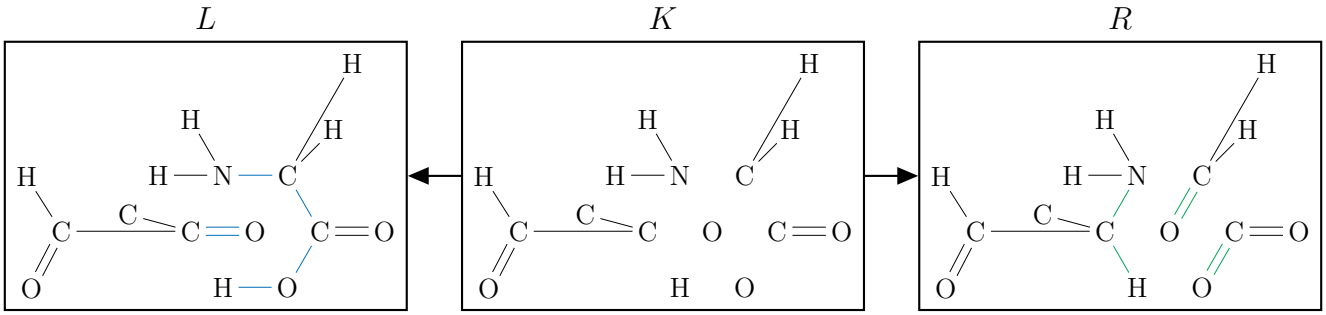


Files: out/197_r_38_11300100_{L, K, R}

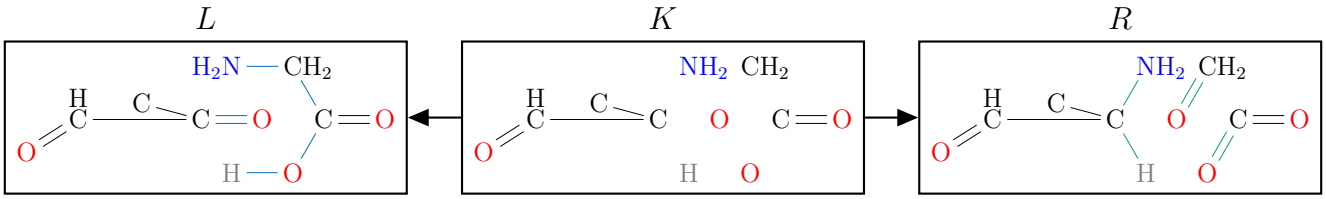


File: out/198_r_38_combined

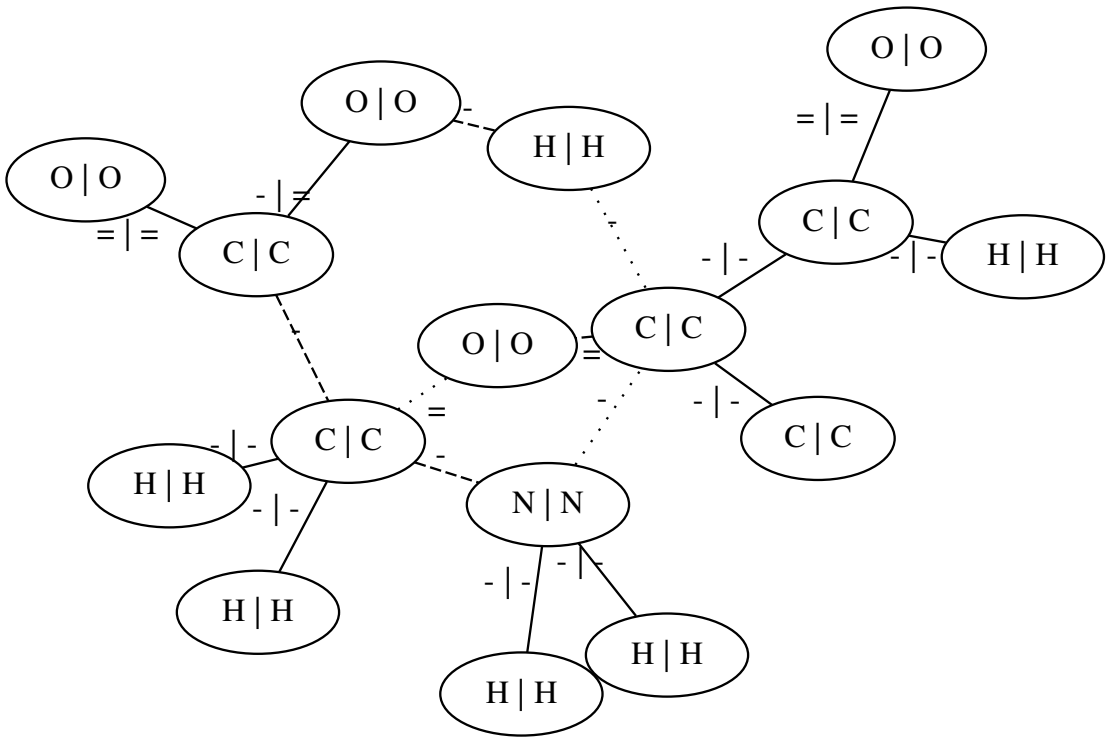
0.0.41 Strecker Degradation Dicarbonyl, H, H, H, C



Files: out/201_r_39_10300000_{L, K, R}



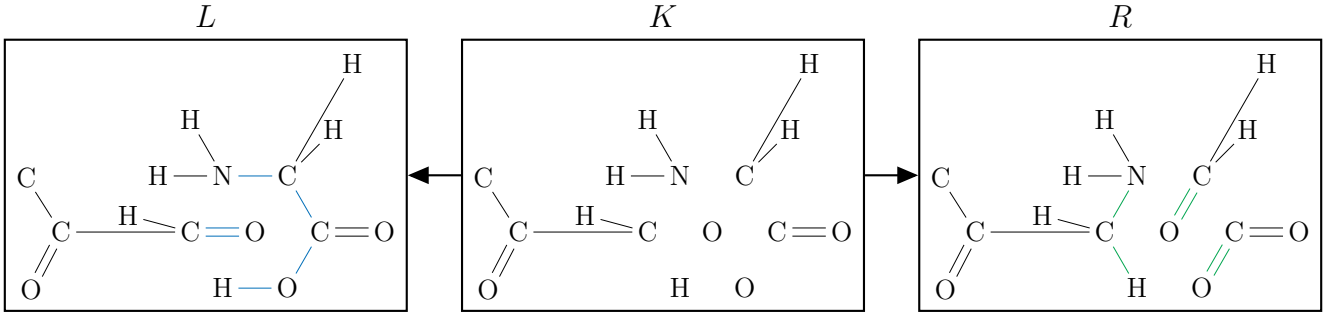
Files: out/202_r_39_11300100_{L, K, R}



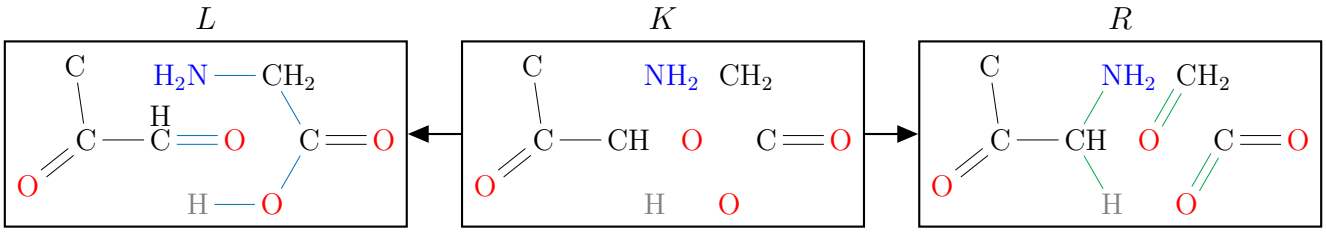
File: out/203_r_39_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

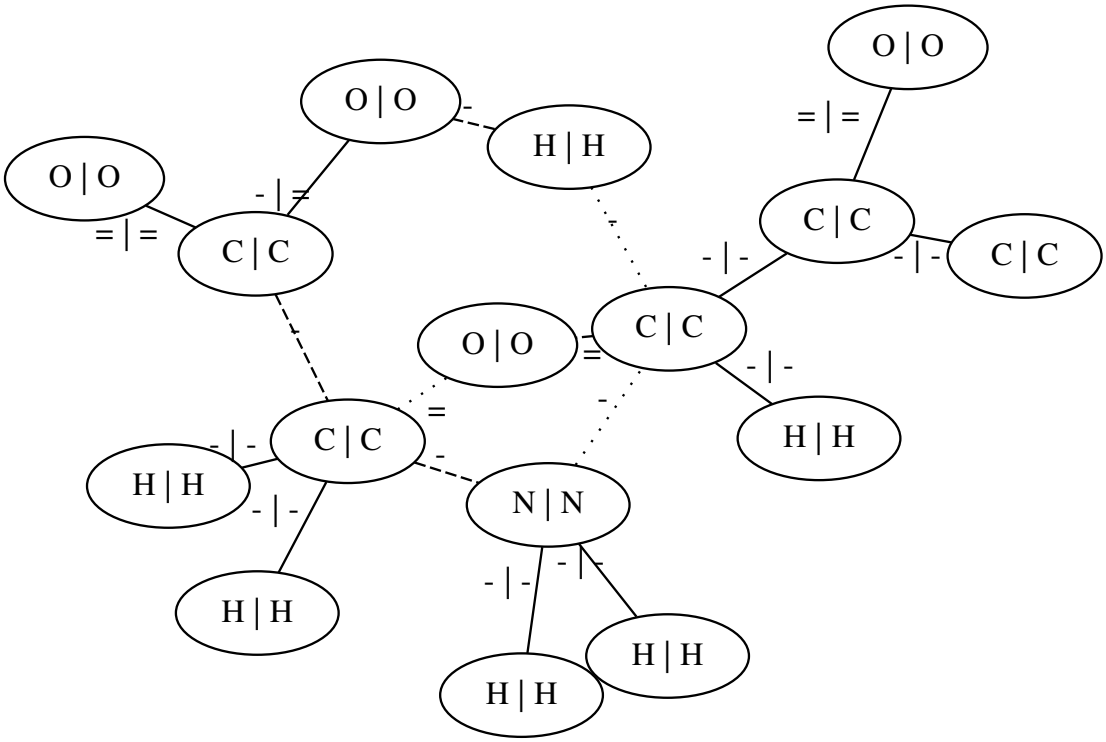
0.0.42 Strecker Degradation Dicarbonyl, H, H, C, H



Files: out/206_r_40_10300000_{L, K, R}



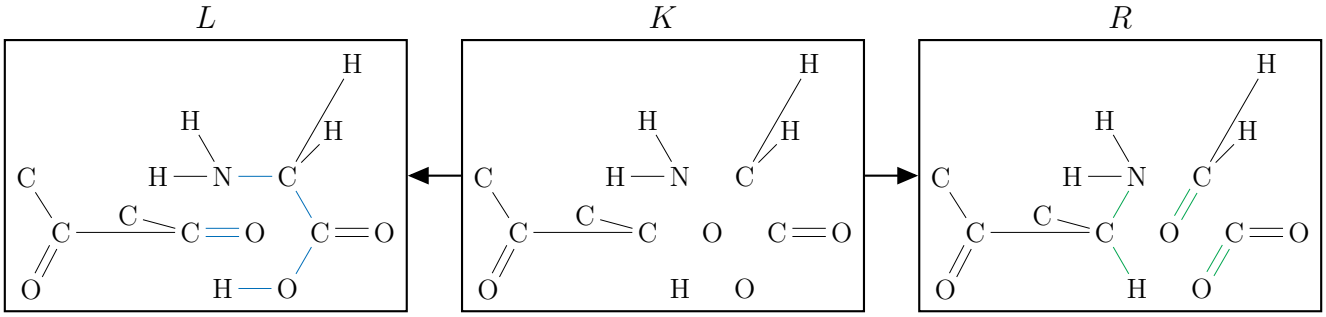
Files: out/207_r_40_11300100_{L, K, R}



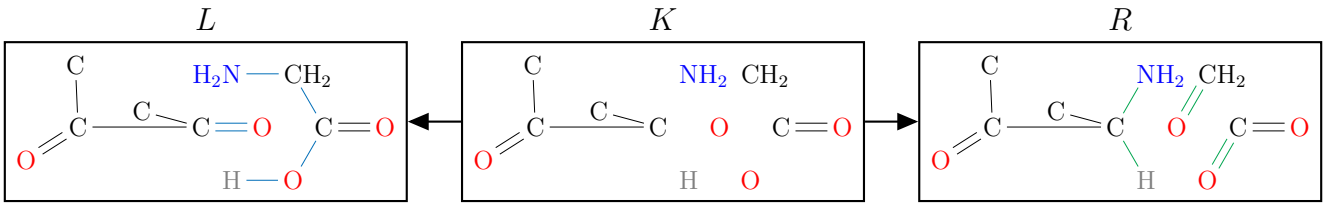
File: out/208_r_40_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

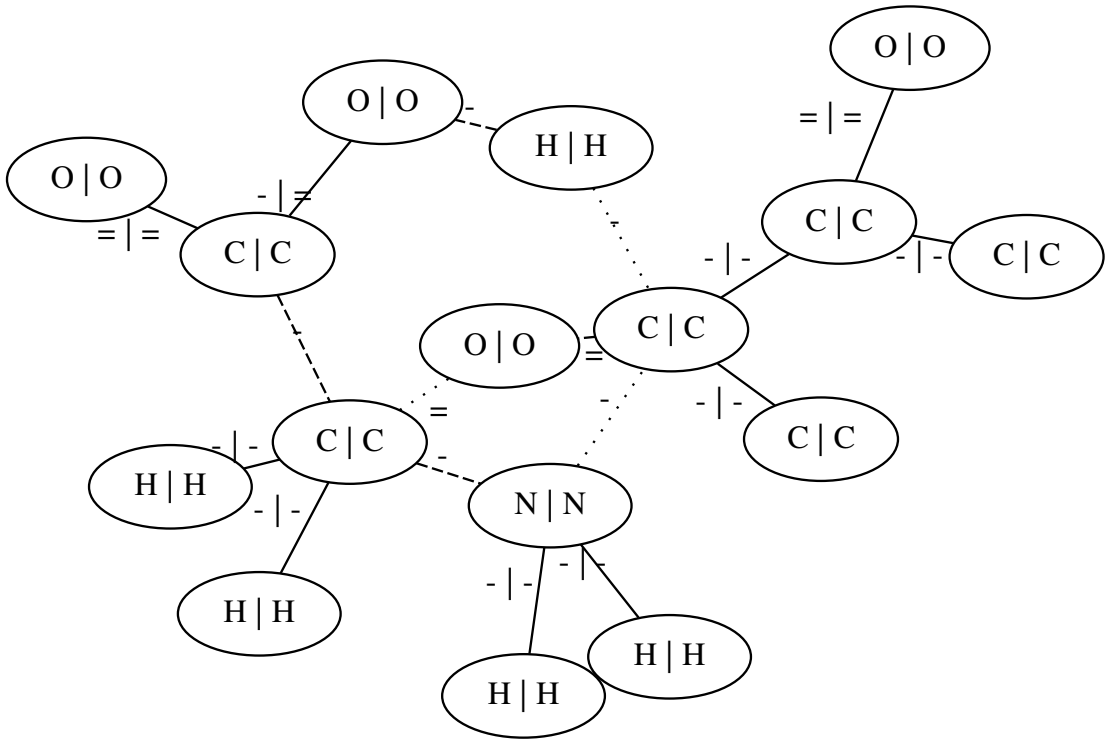
0.0.43 Strecker Degradation Dicarbonyl, H, H, C, C



Files: out/211_r_41_10300000_{L, K, R}



Files: out/212_r_41_11300100_{L, K, R}

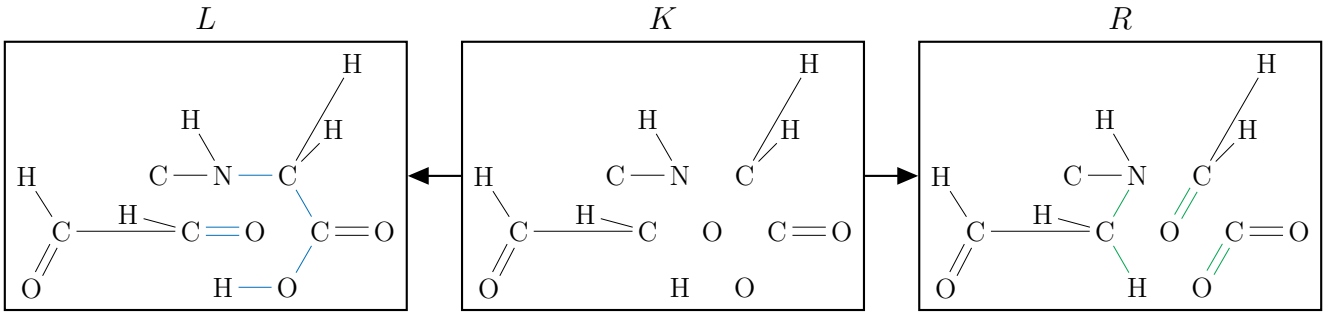


File: out/213_r_41_combined

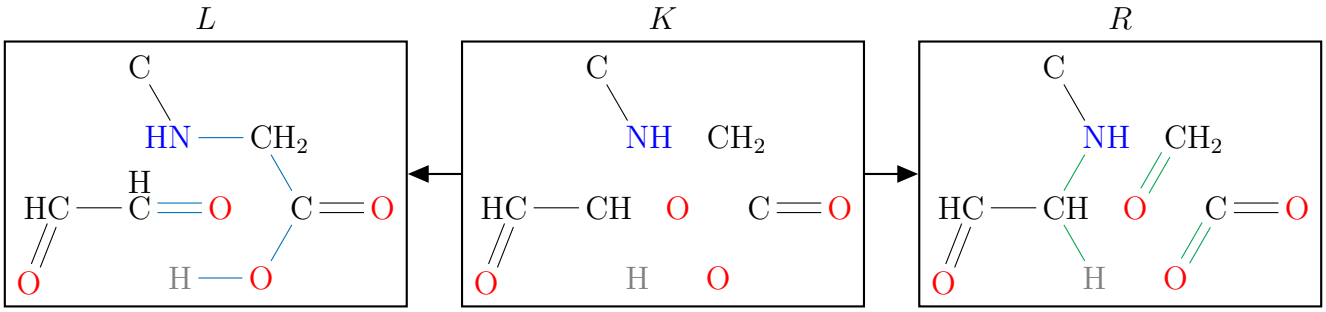
$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

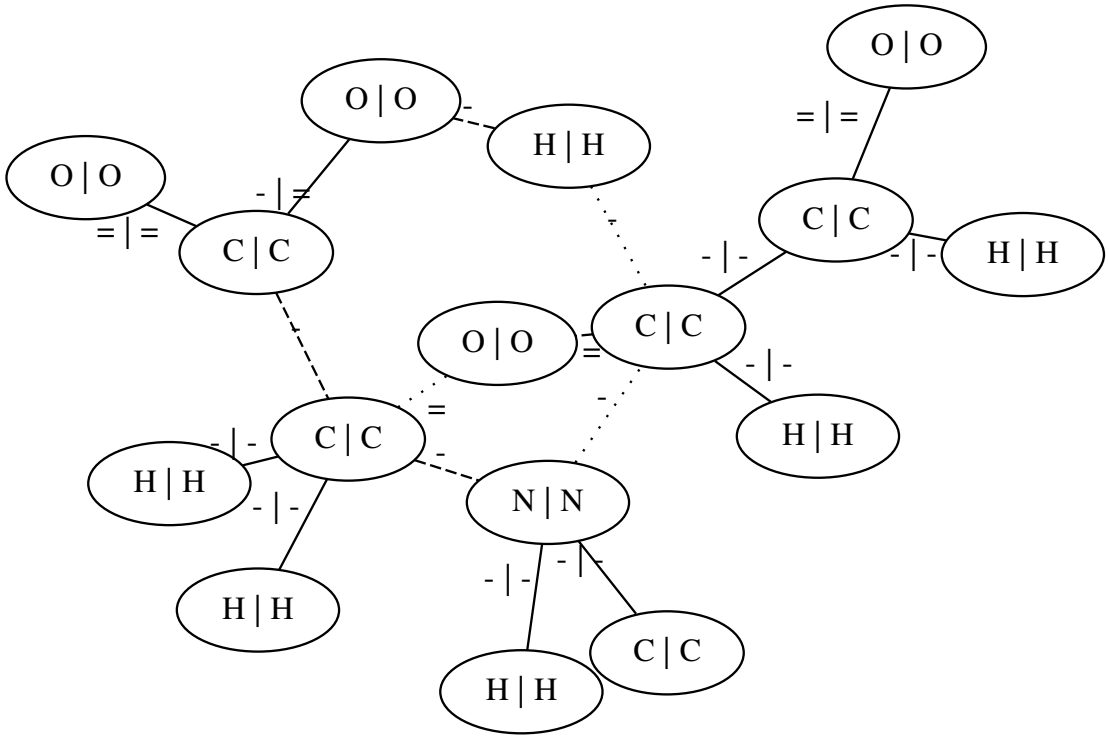
0.0.44 Strecker Degradation Dicarbonyl, H, C, H, H



Files: out/216_r_42_10300000_{L, K, R}



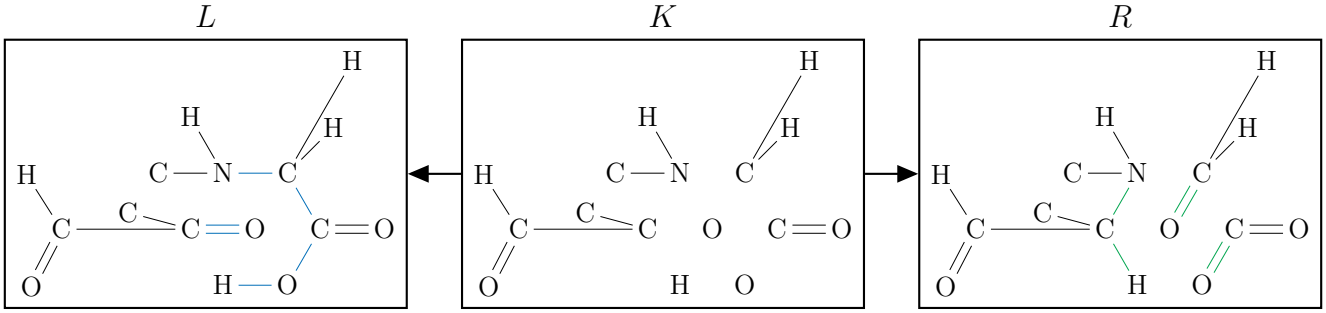
Files: out/217_r_42_11300100_{L, K, R}



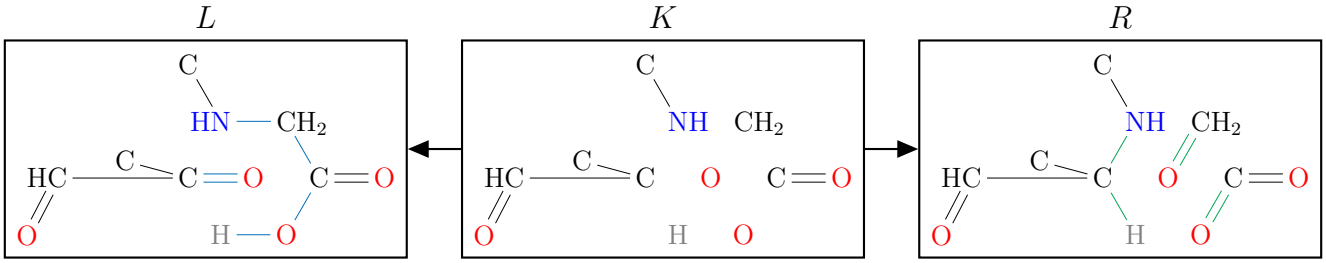
File: out/218_r_42_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

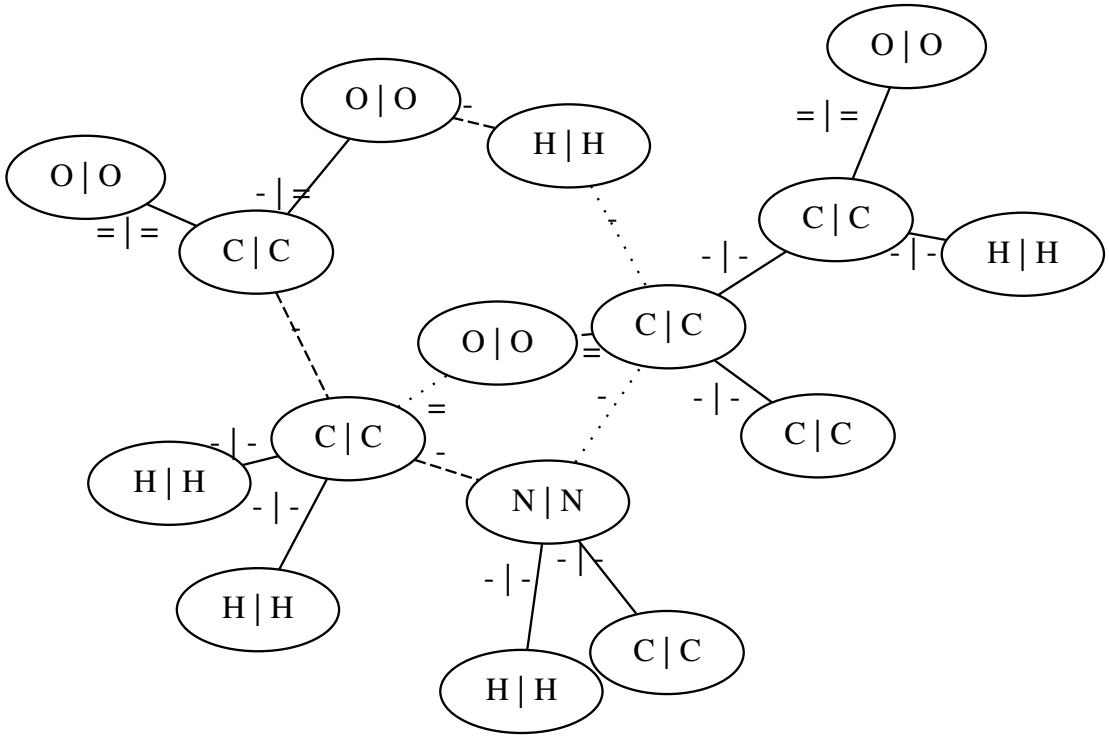
0.0.45 Strecker Degradation Dicarbonyl, H, C, H, C



Files: out/221_r_43_10300000_{L, K, R}



Files: out/222_r_43_11300100_{L, K, R}



File: out/223_r_43_combined

$$
\begin{aligned}
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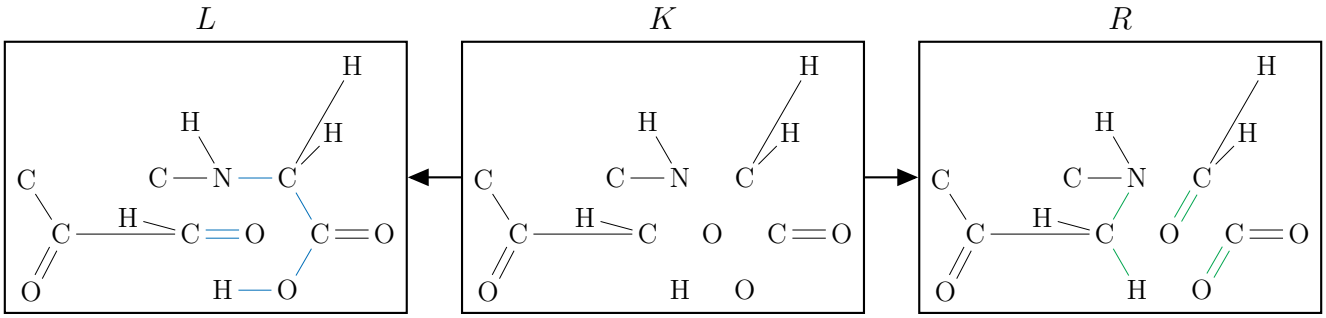
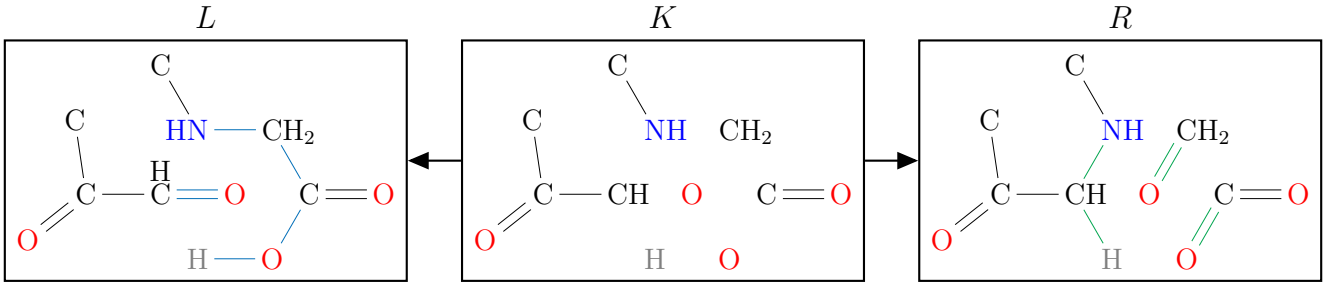
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

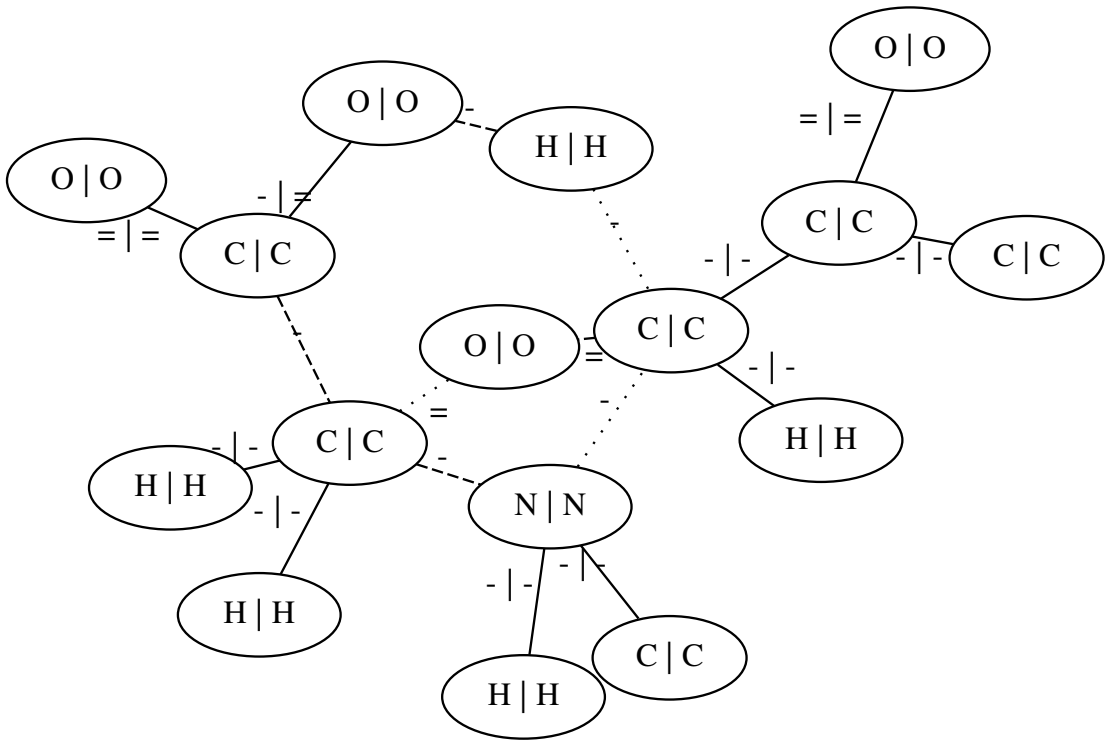
0.0.46 Strecker Degradation Dicarbonyl, H, C, C, H



Files: out/226_r_44_10300000_{L, K, R}



Files: out/227_r_44_11300100_{L, K, R}



File: out/228_r_44_combined

$$
\begin{aligned}
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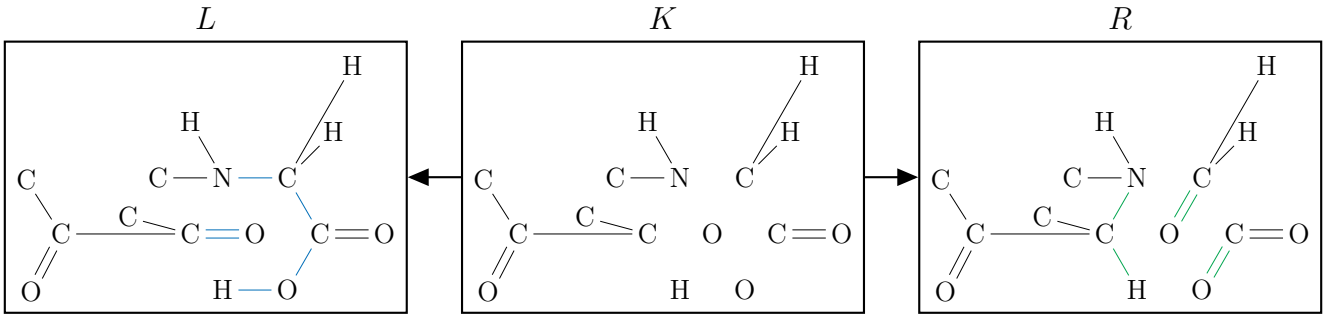
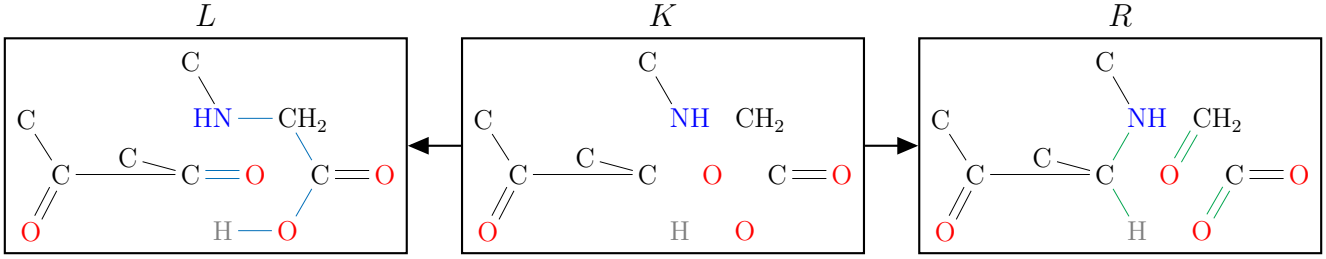
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

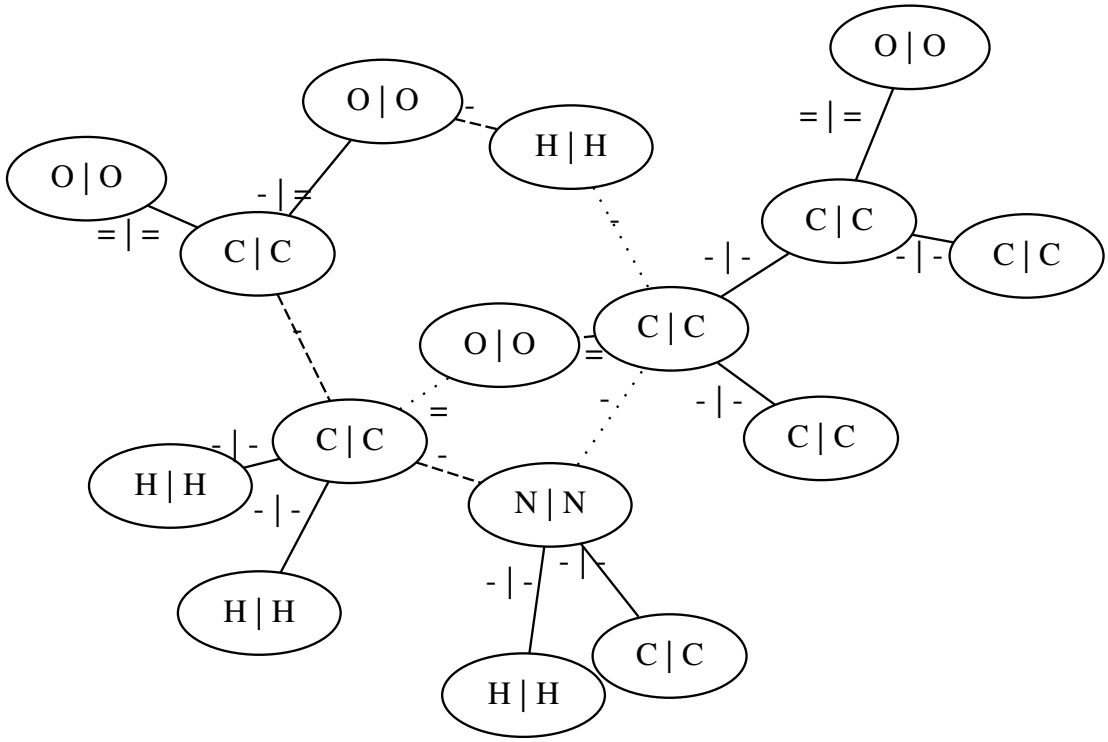
0.0.47 Strecker Degradation Dicarbonyl, H, C, C, C



Files: out/231_r_45_10300000_{L, K, R}



Files: out/232_r_45_11300100_{L, K, R}



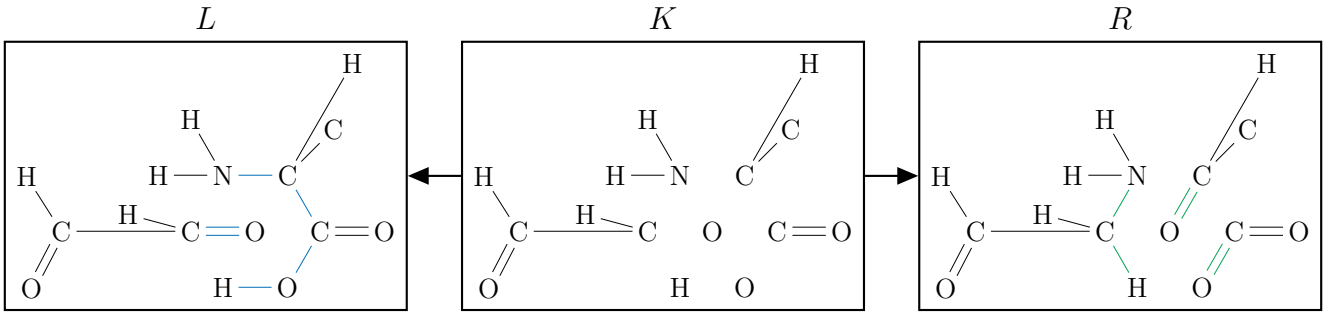
File: out/233_r_45_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

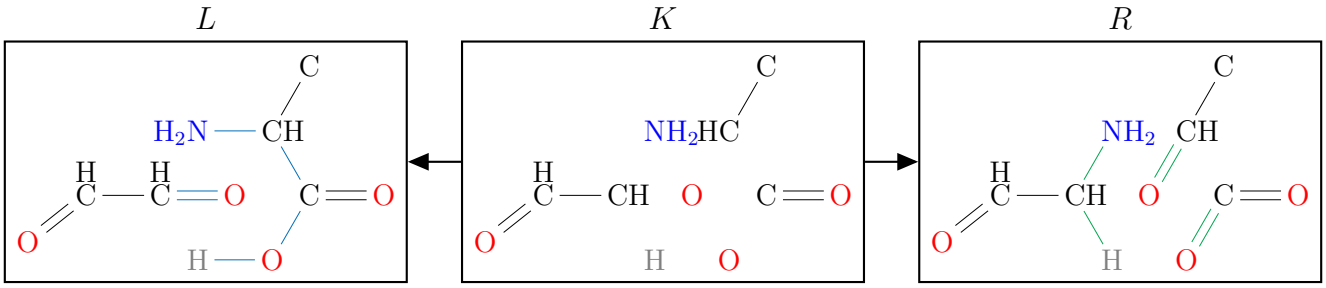
$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

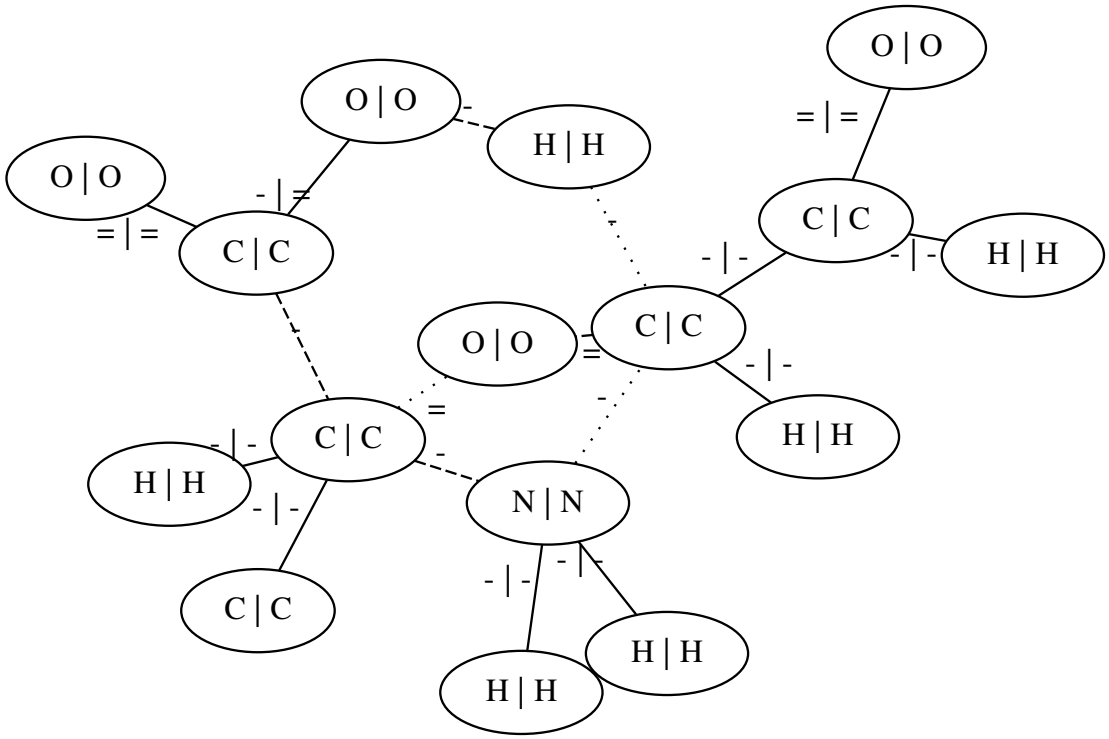
0.0.48 Strecker Degradation Dicarbonyl, C, H, H, H



Files: out/236_r_46_10300000_{L, K, R}



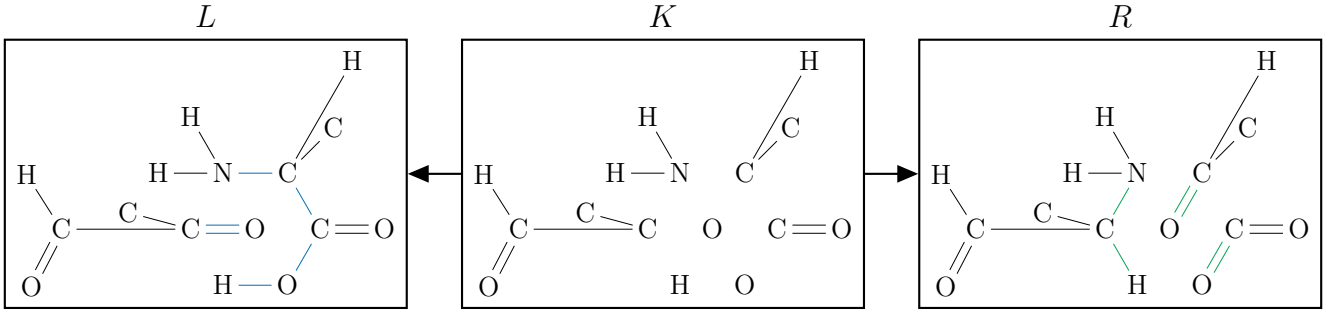
Files: out/237_r_46_11300100_{L, K, R}



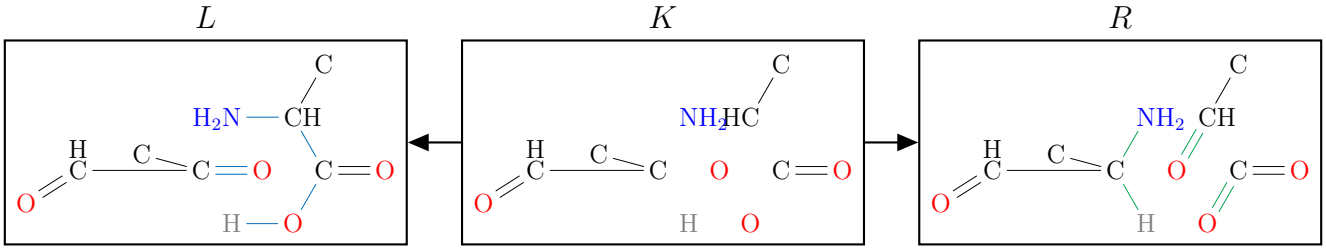
File: out/238_r_46_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

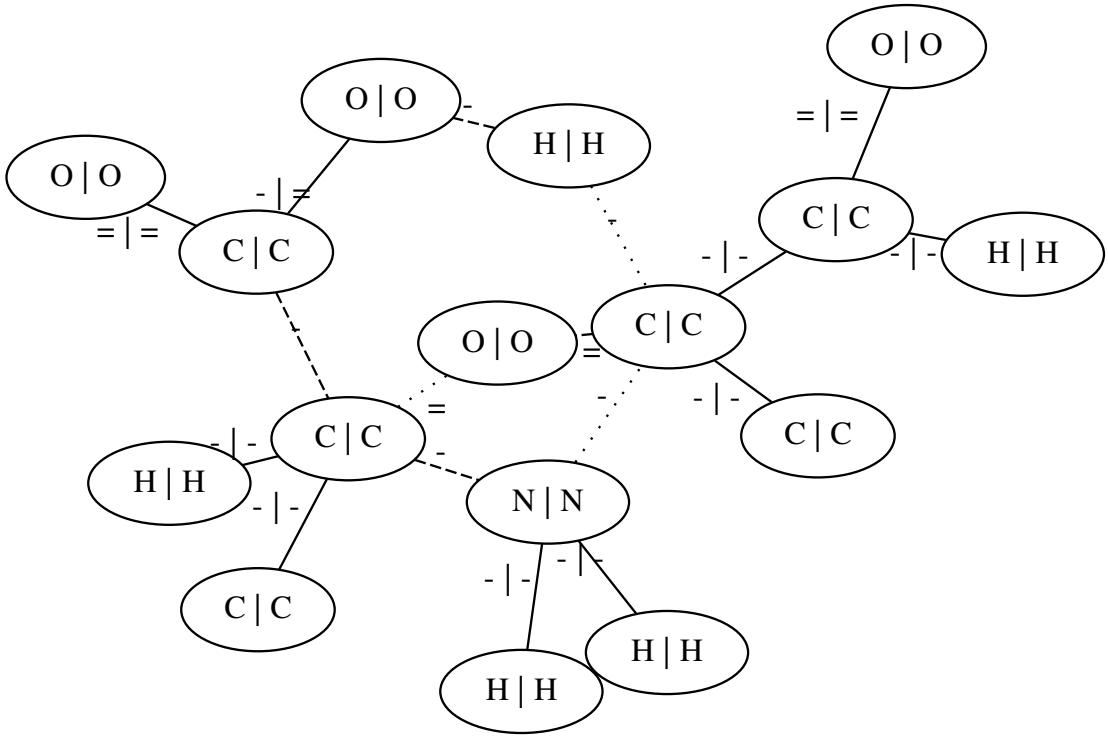
0.0.49 Strecker Degradation Dicarbonyl, C, H, H, C



Files: out/241_r_47_10300000_{L, K, R}



Files: out/242_r_47_11300100_{L, K, R}

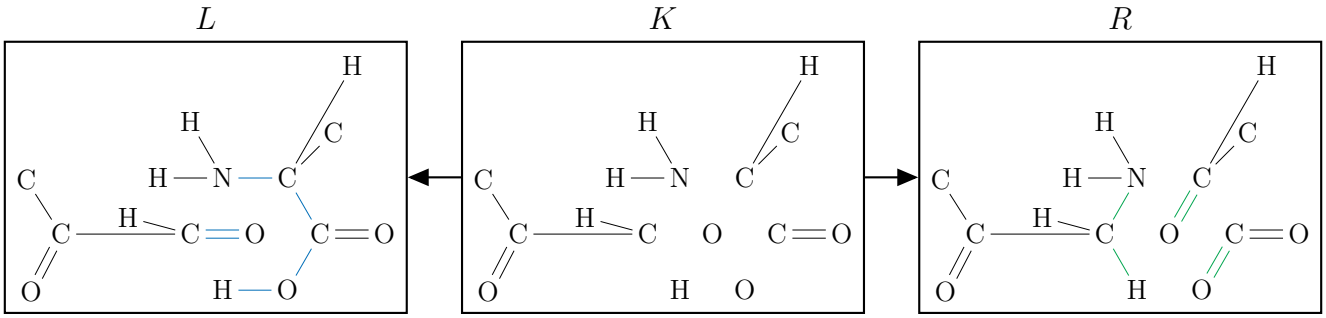


File: out/243_r_47_combined

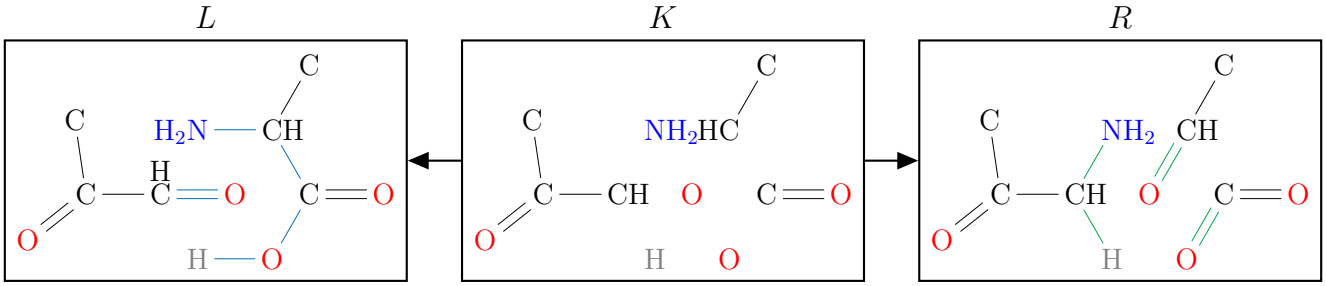
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

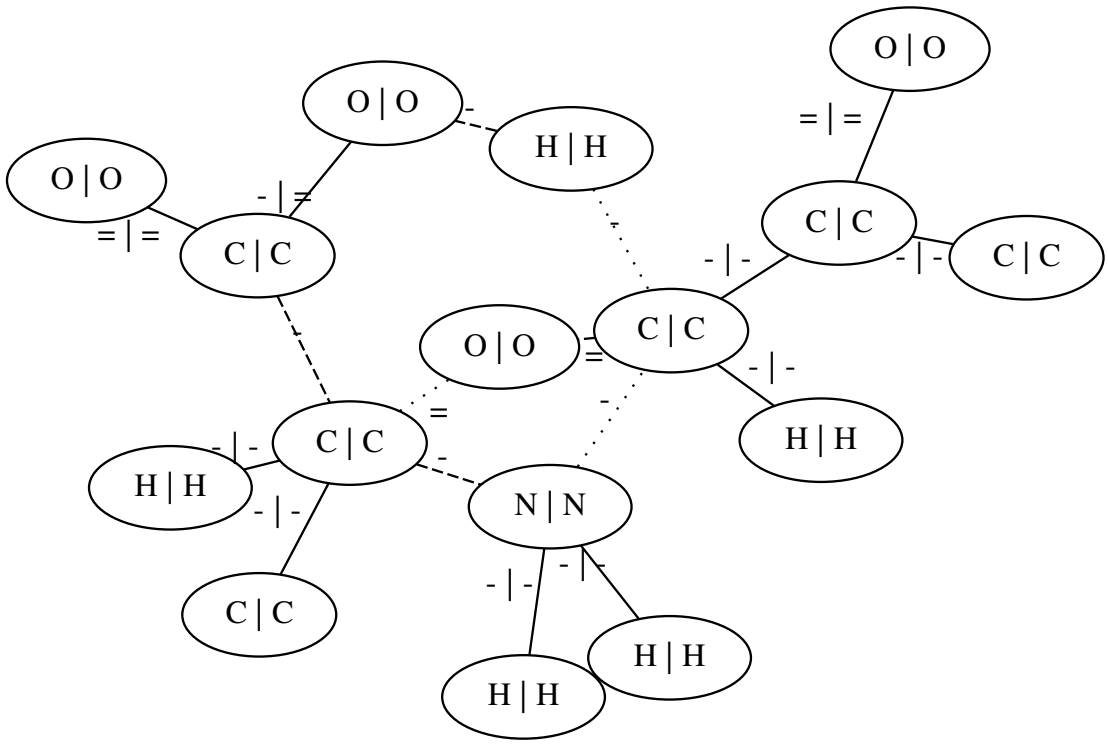
0.0.50 Strecker Degradation Dicarbonyl, C, H, C, H



Files: out/246_r_48_10300000_{L, K, R}



Files: out/247_r_48_11300100_{L, K, R}

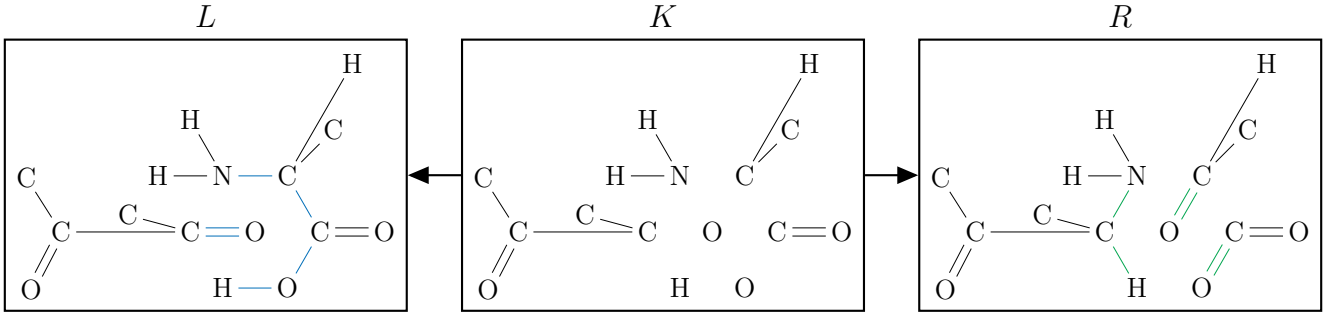


File: out/248_r_48_combined

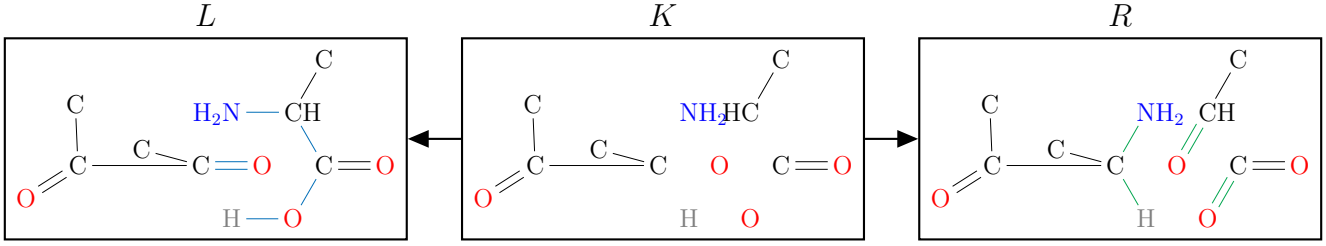
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

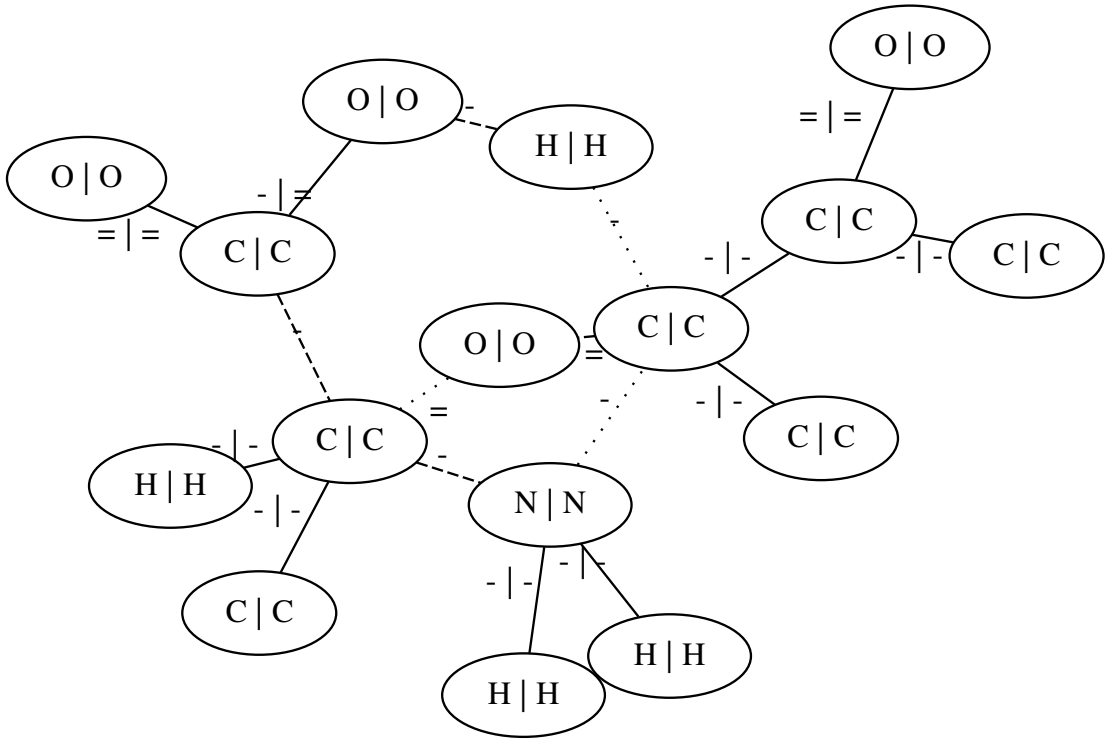
0.0.51 Strecker Degradation Dicarbonyl, C, H, C, C



Files: out/251_r_49_10300000_{L, K, R}



Files: out/252_r_49_11300100_{L, K, R}



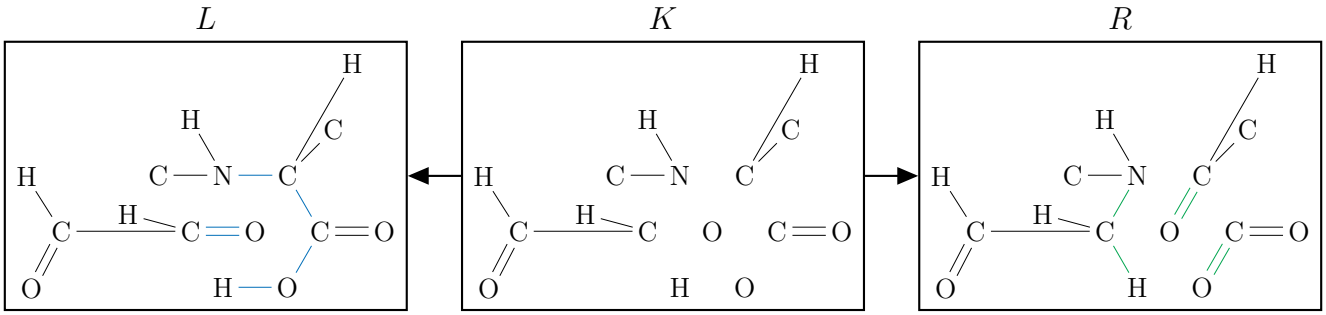
File: out/253_r_49_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

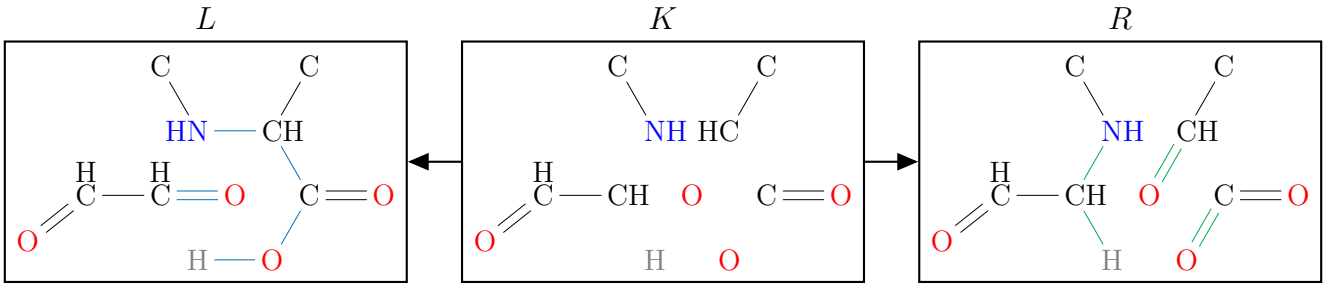
$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

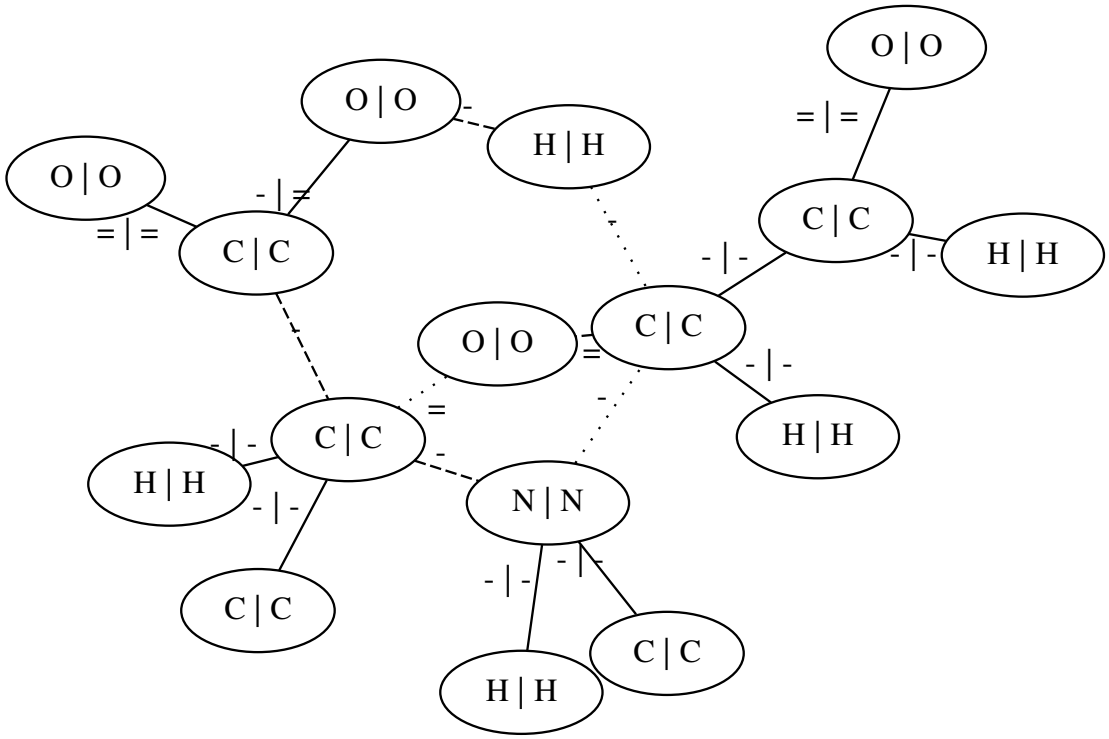
0.0.52 Strecker Degradation Dicarbonyl, C, C, H, H



Files: out/256_r_50_10300000_{L, K, R}



Files: out/257_r_50_11300100_{L, K, R}

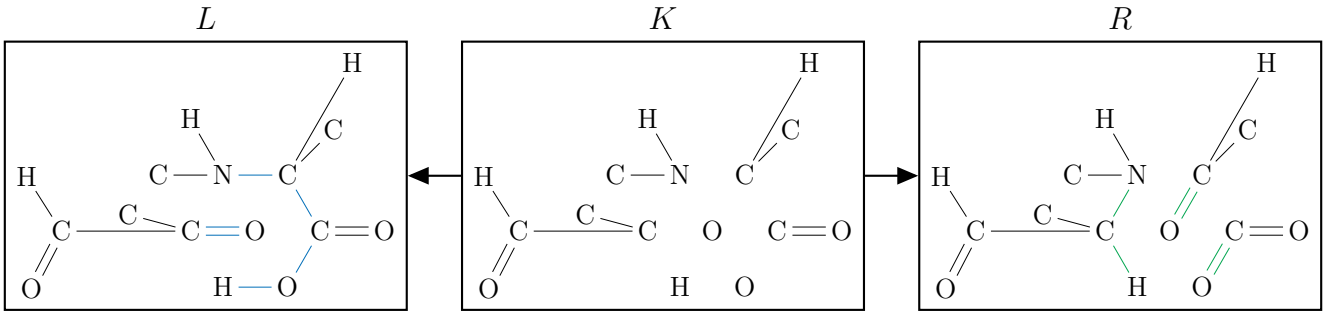


File: out/258_r_50_combined

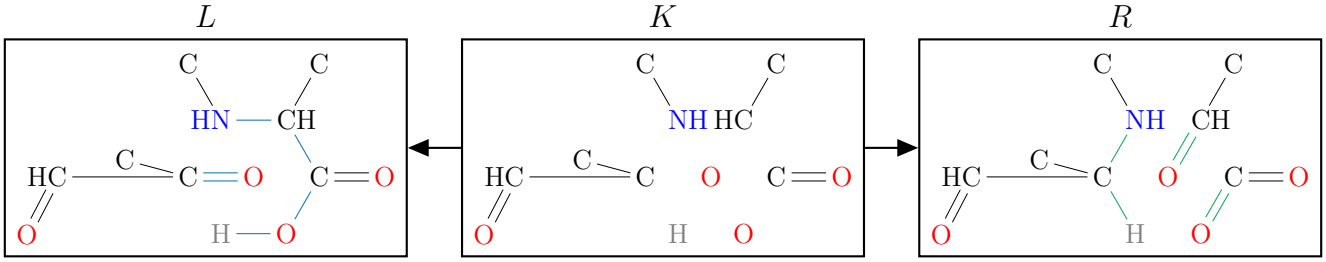
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

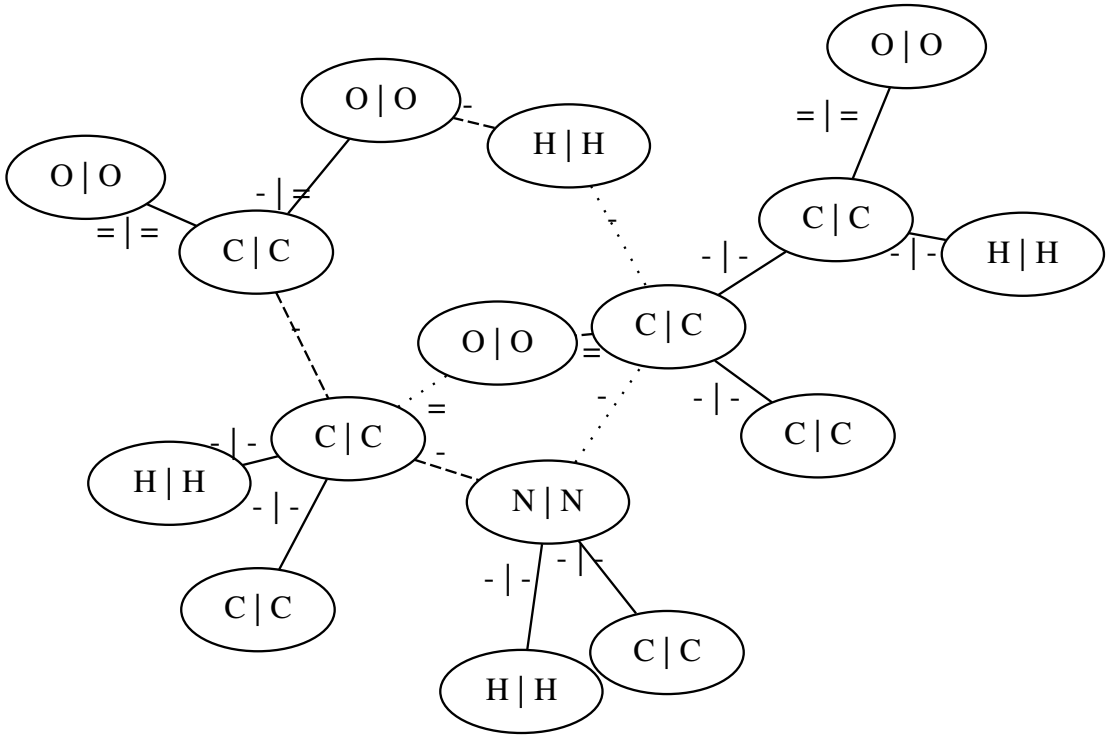
0.0.53 Strecker Degradation Dicarbonyl, C, C, H, C



Files: out/261_r_51_10300000_{L, K, R}



Files: out/262_r_51_11300100_{L, K, R}



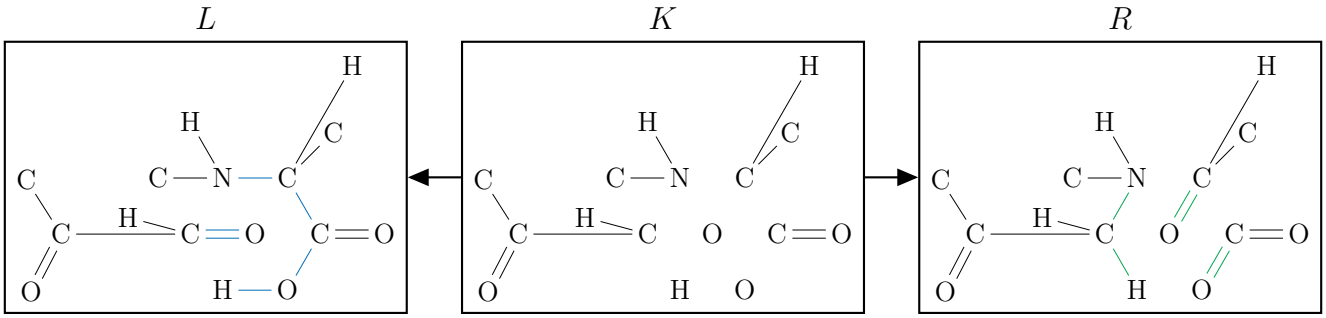
File: out/263_r_51_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

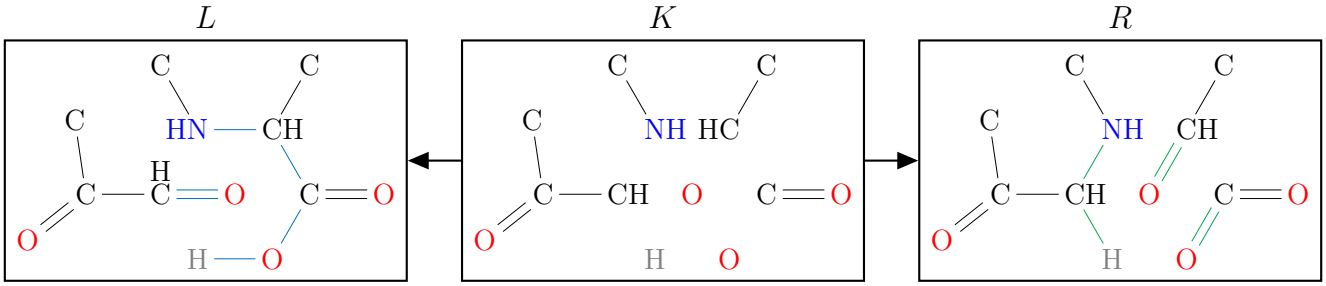
$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

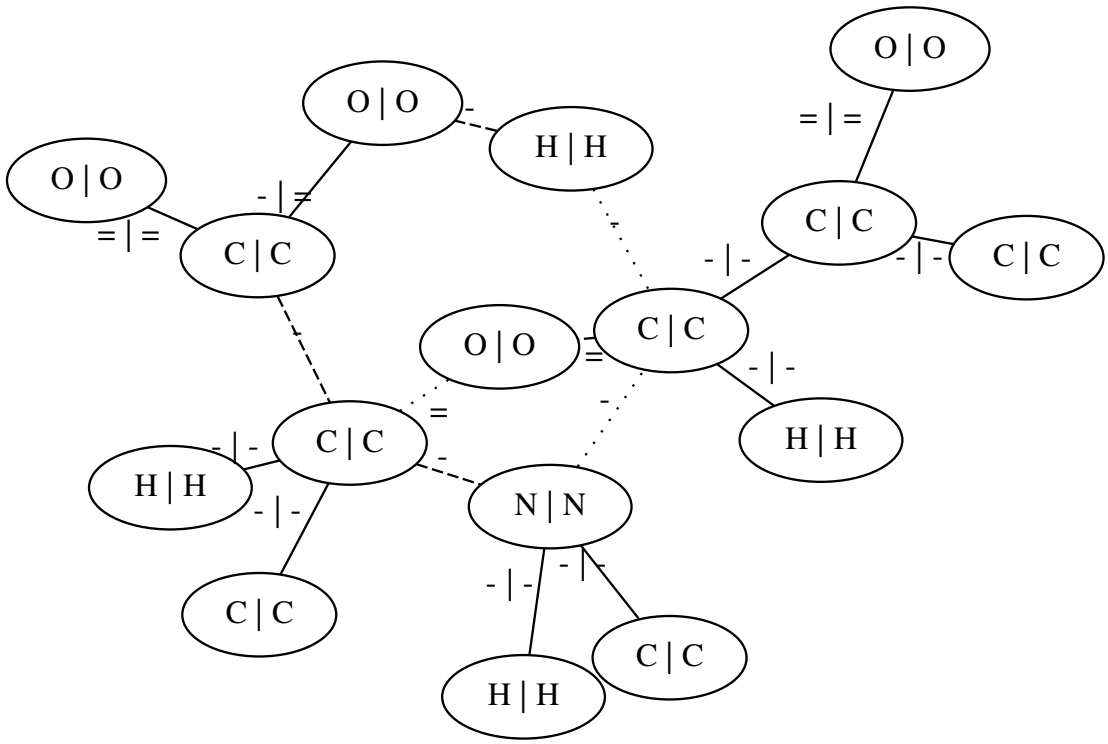
0.0.54 Strecker Degradation Dicarbonyl, C, C, C, H



Files: out/266_r_52_10300000_{L, K, R}



Files: out/267_r_52_11300100_{L, K, R}



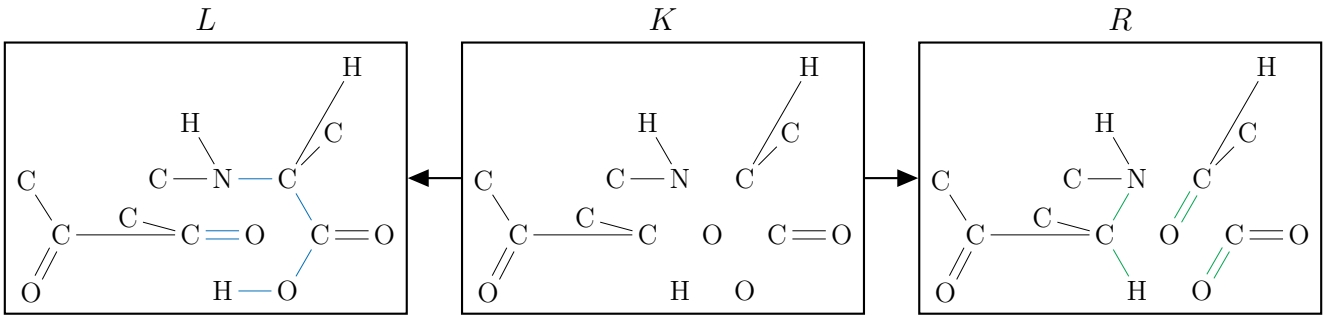
File: out/268_r_52_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

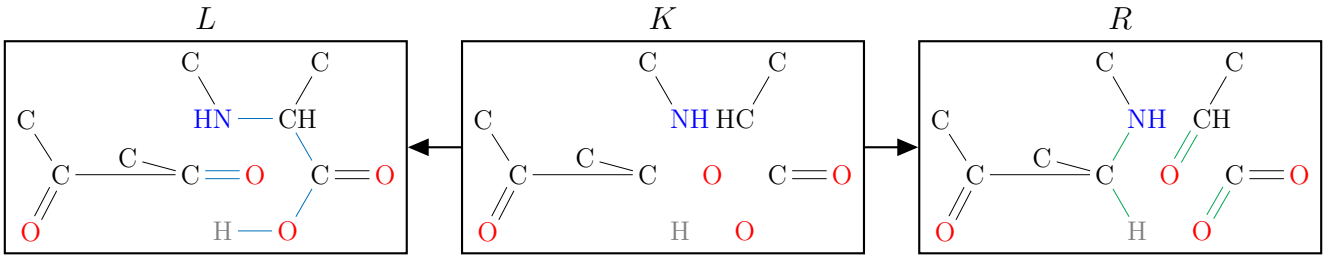
$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

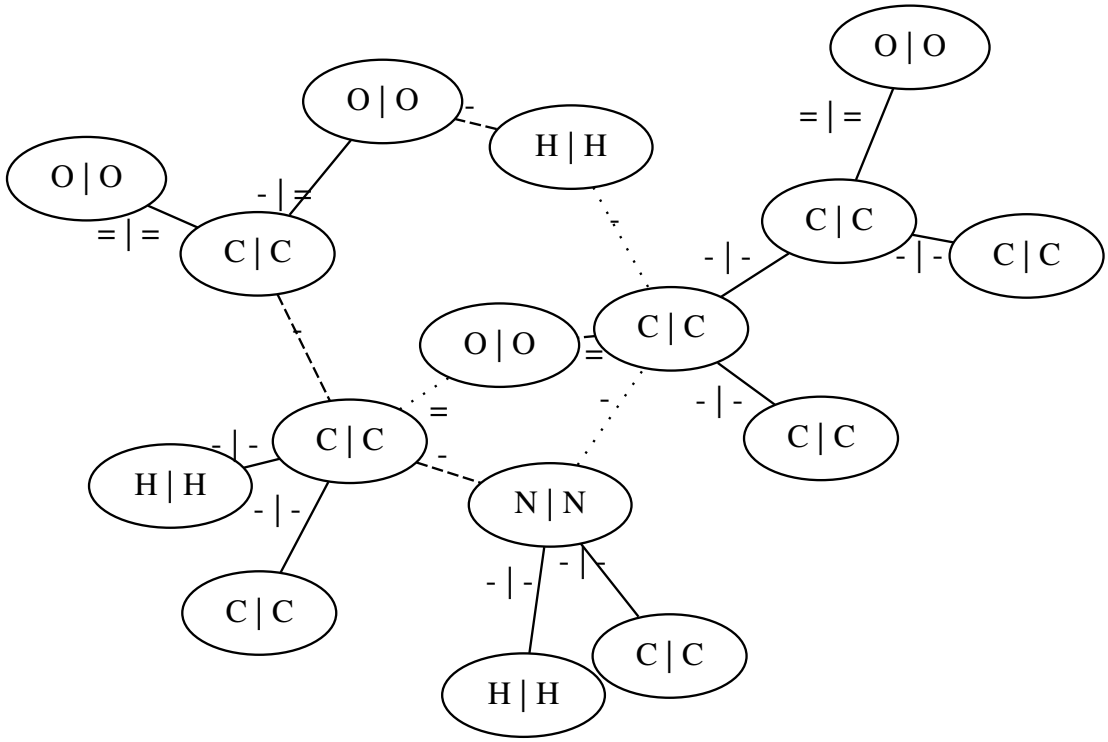
0.0.55 Strecker Degradation Dicarbonyl, C, C, C, C



Files: out/271_r_53_10300000_{L, K, R}



Files: out/272_r_53_11300100_{L, K, R}



File: out/273_r_53_combined

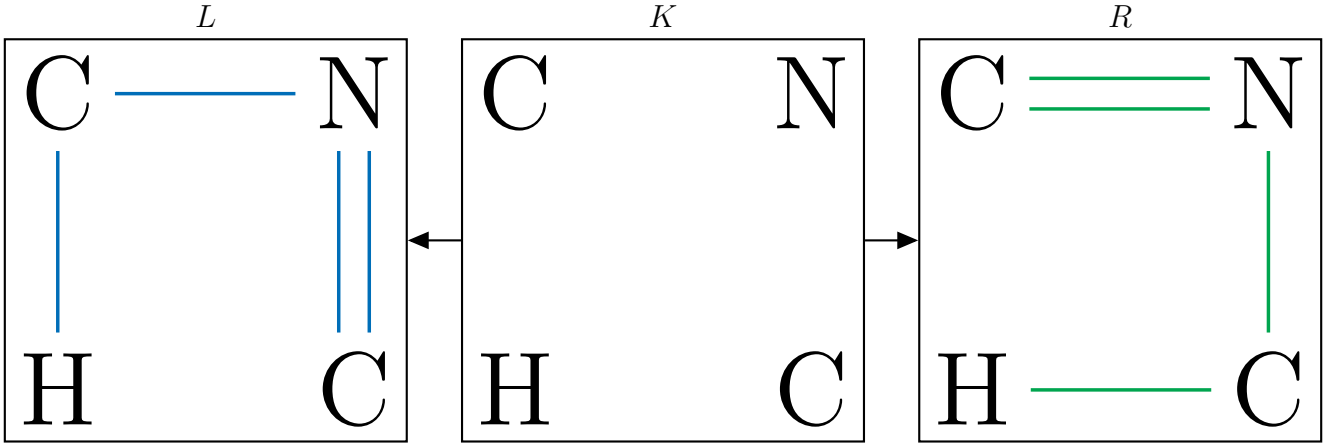
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

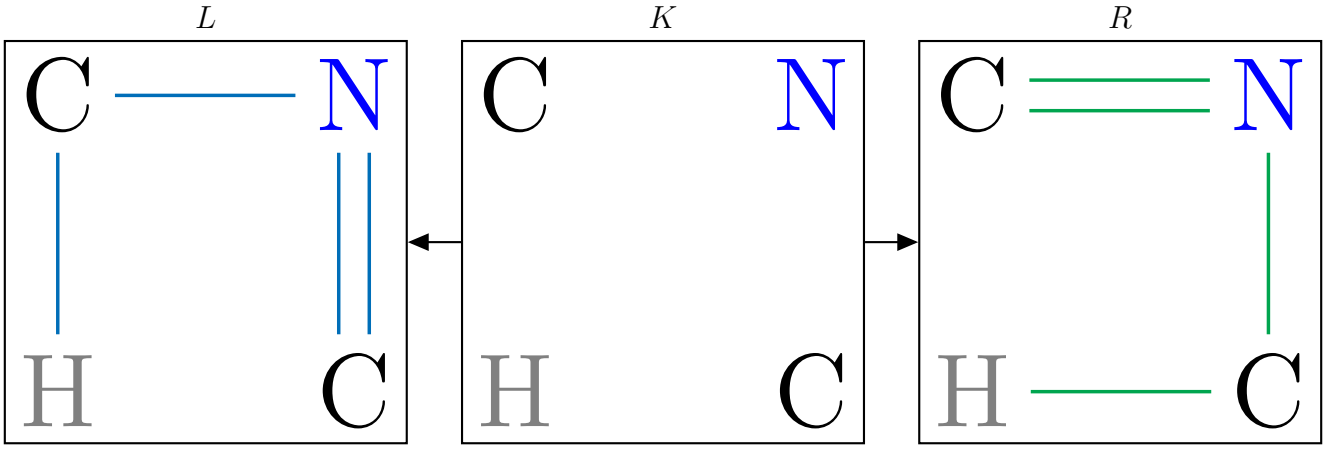
$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(15) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

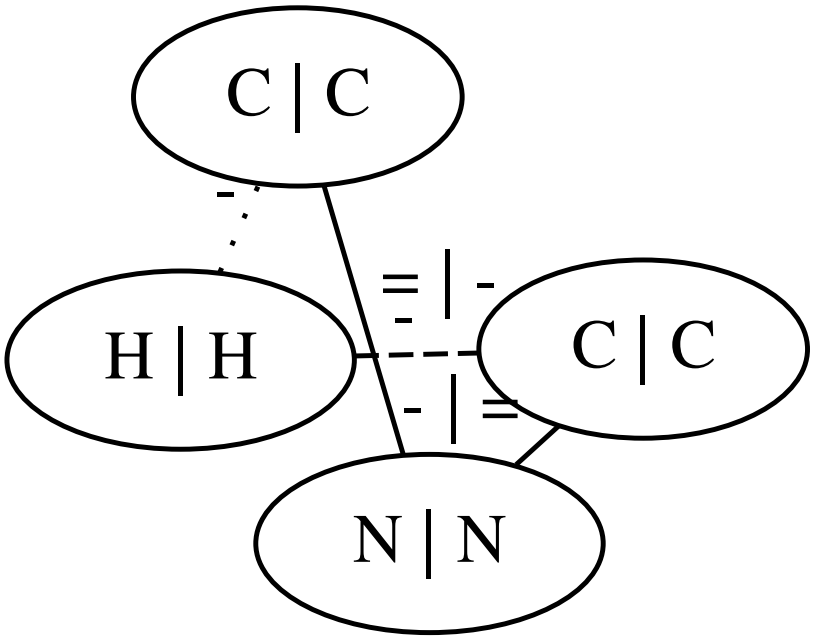
0.0.56 Schiff Tautomerization



Files: out/276_r_54_10300000_{L, K, R}

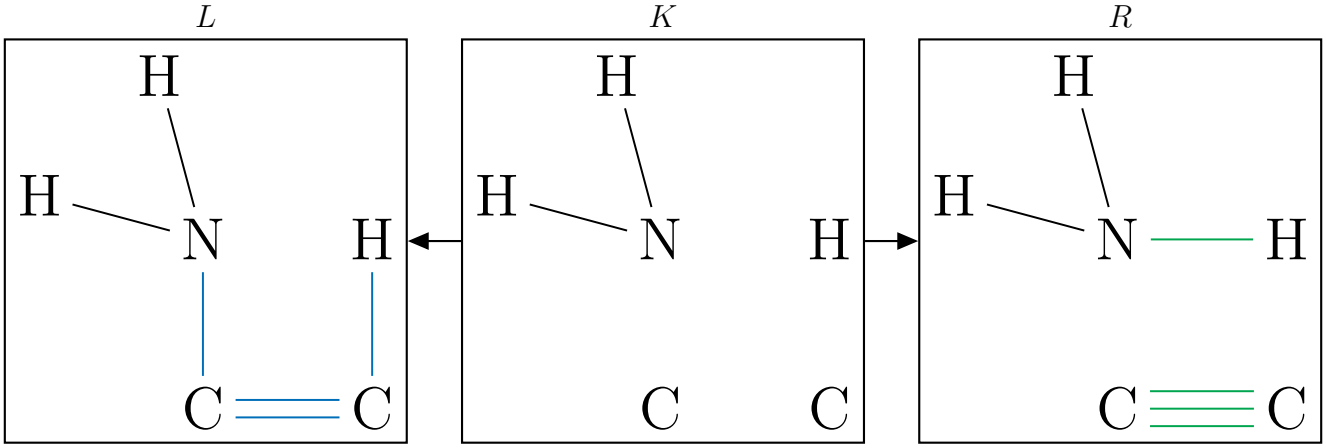


Files: out/277_r_54_11300100_{L, K, R}

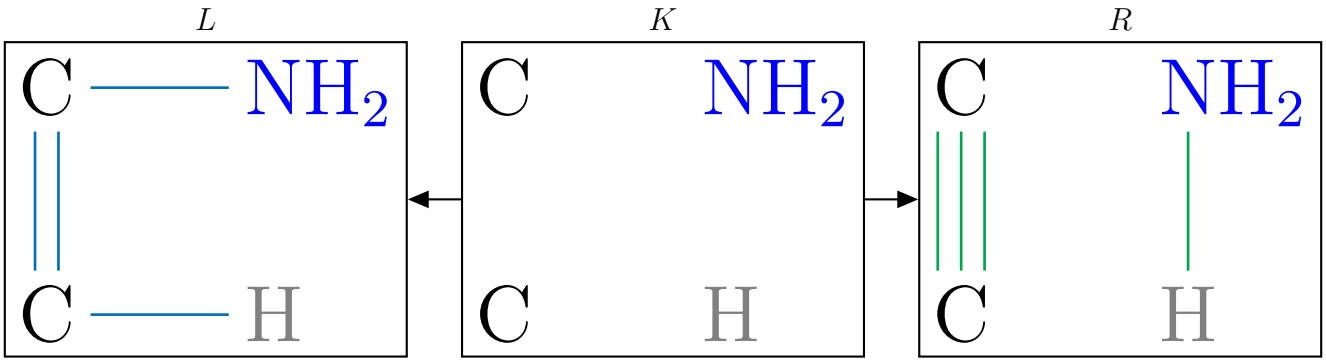


File: out/278_r_54_combined

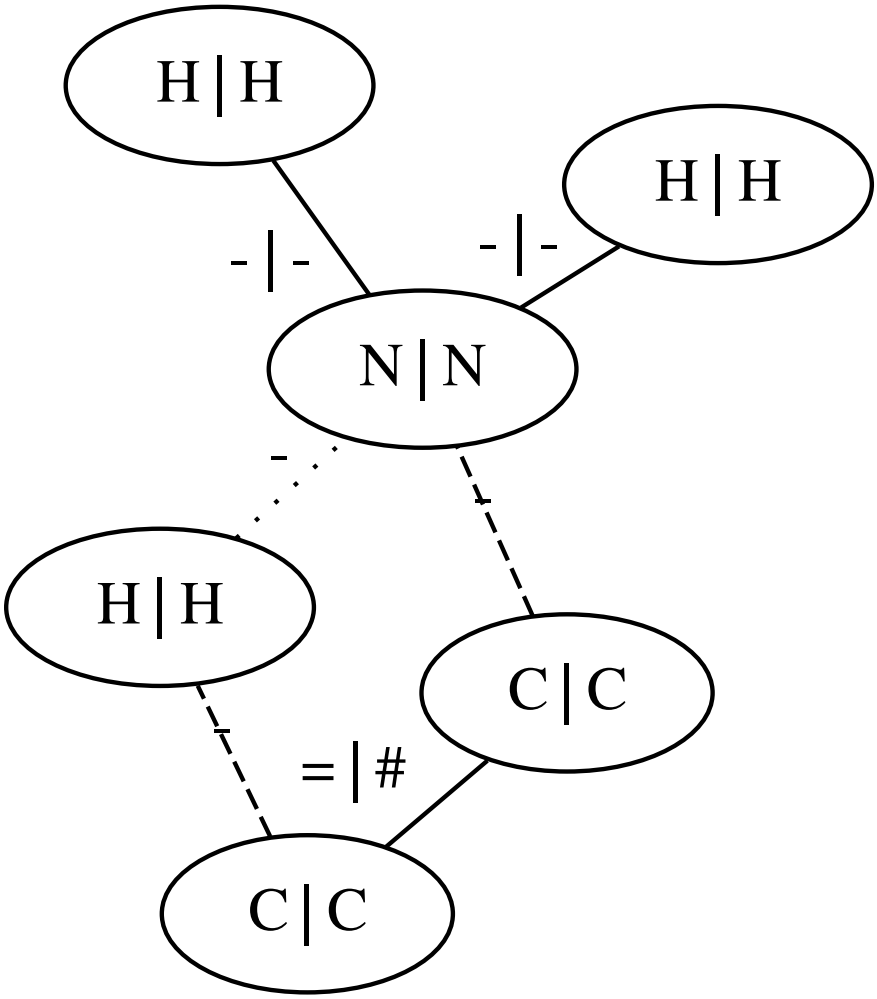
0.0.57 Alkyne Addition, N, HH, inverse



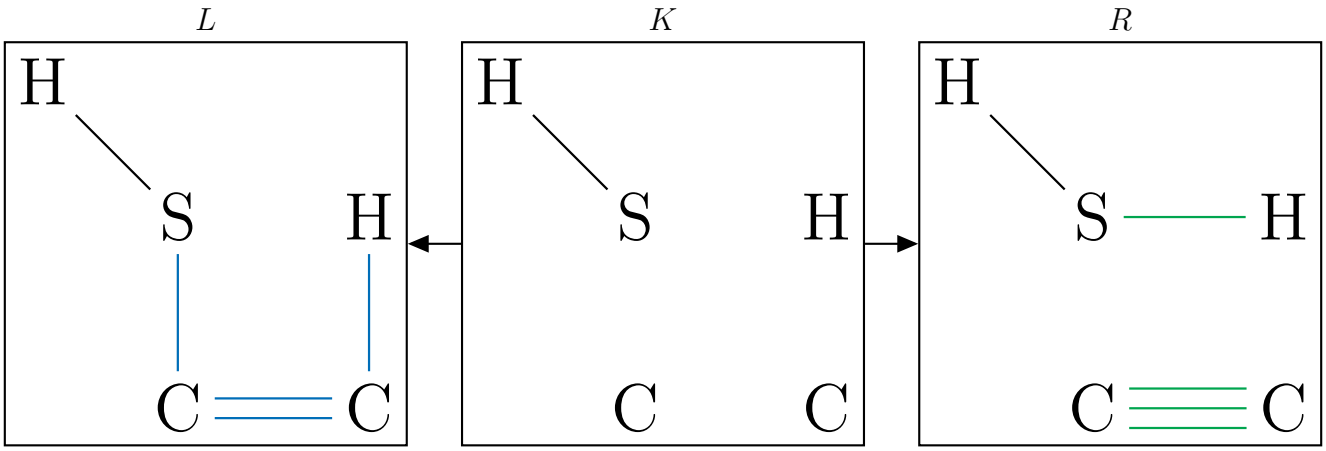
Files: out/281_r_55_10300000_{L, K, R}



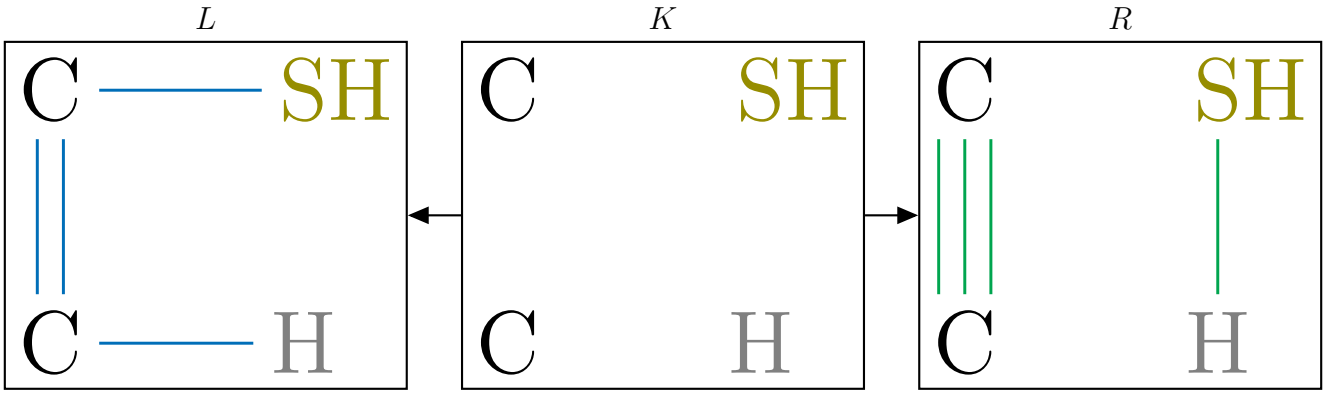
Files: out/282_r_55_11300100_{L, K, R}



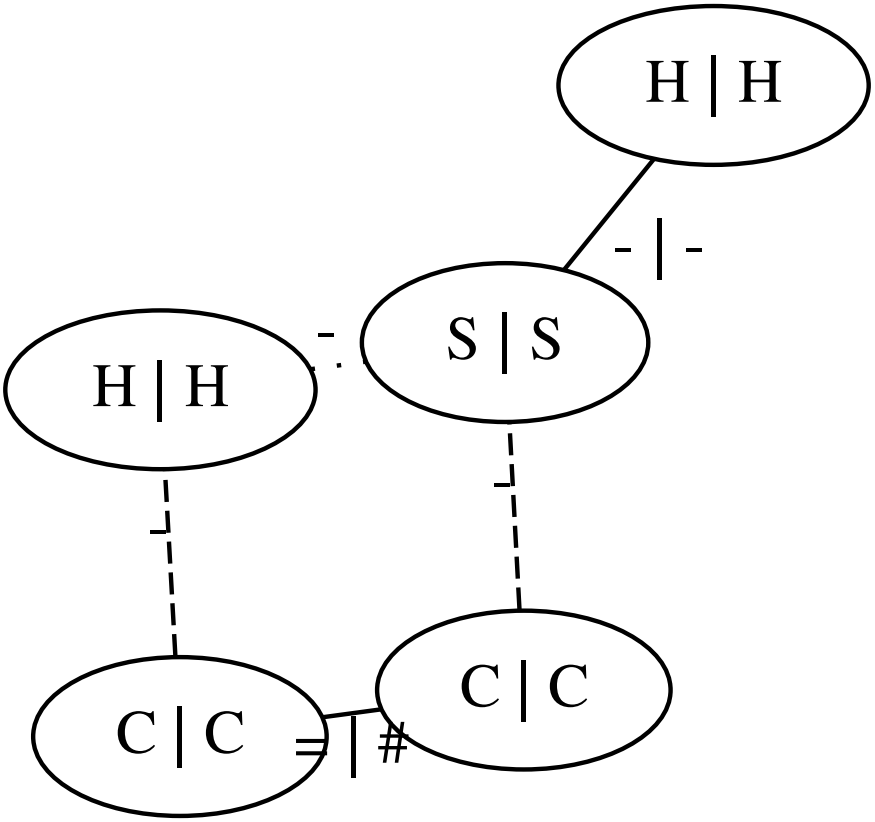
0.0.58 Alkyne Addition, S, H, inverse



Files: out/286_r_56_10300000_{L, K, R}

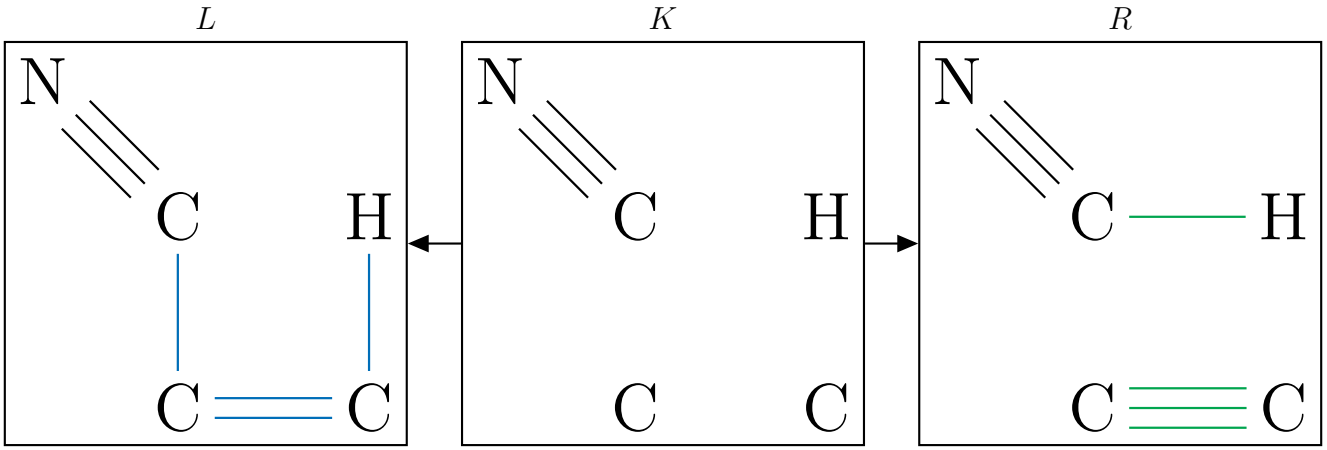


Files: out/287_r_56_11300100_{L, K, R}

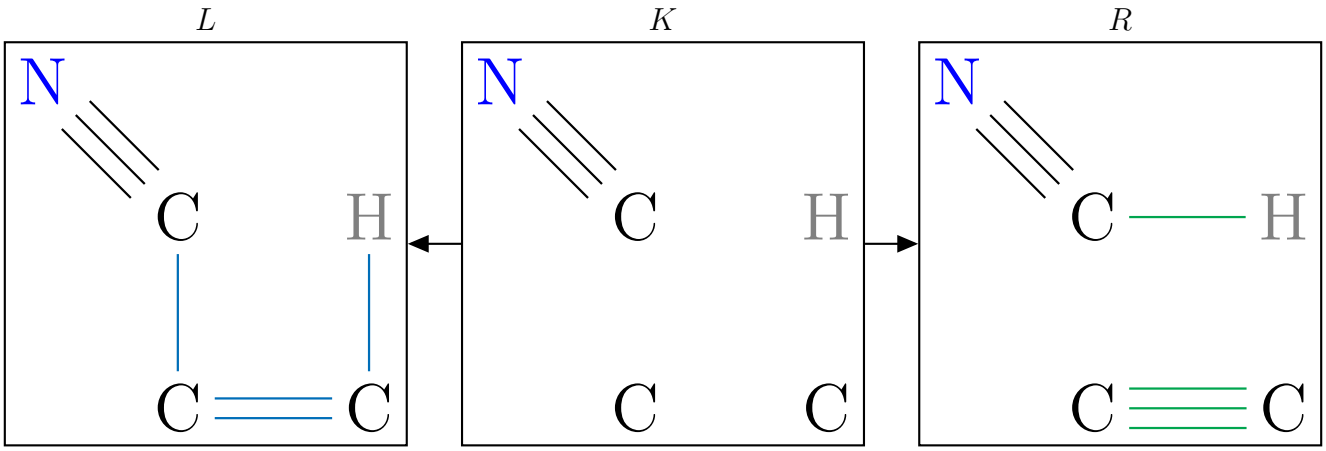


File: out/288_r_56_combined

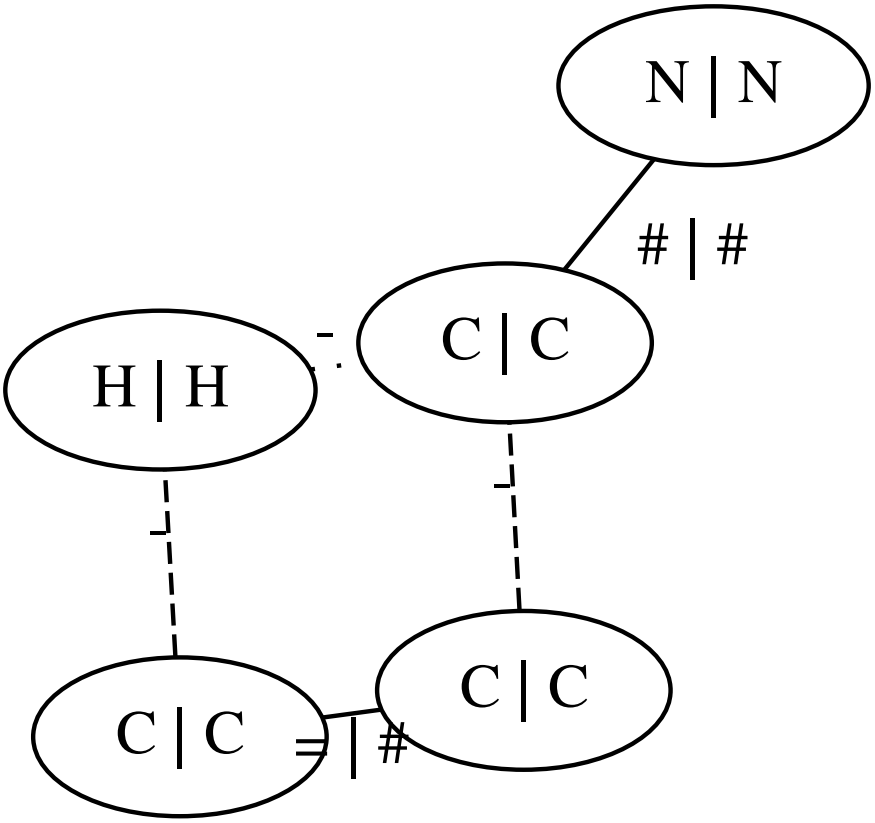
0.0.59 Alkyne Addition, C, inverse



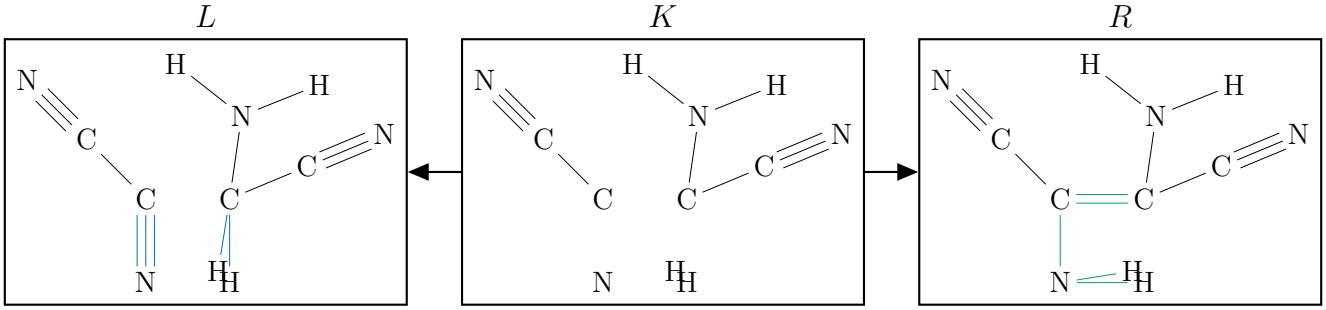
Files: out/291_r_57_10300000_{L, K, R}



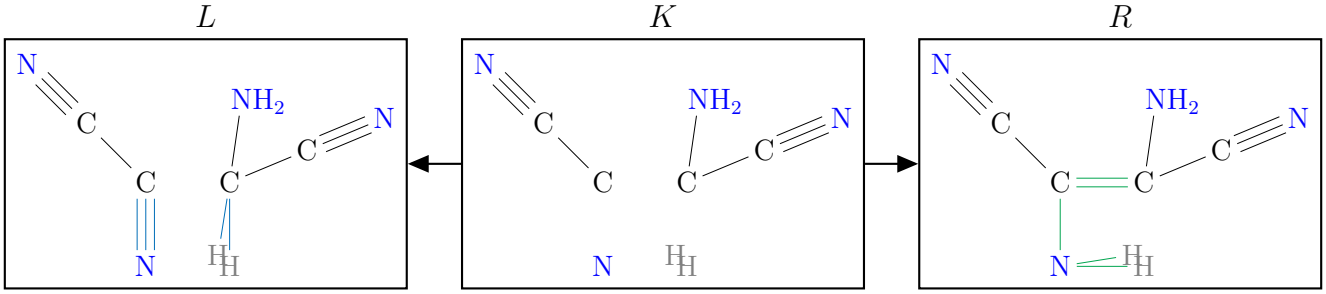
Files: out/292_r_57_11300100_{L, K, R}



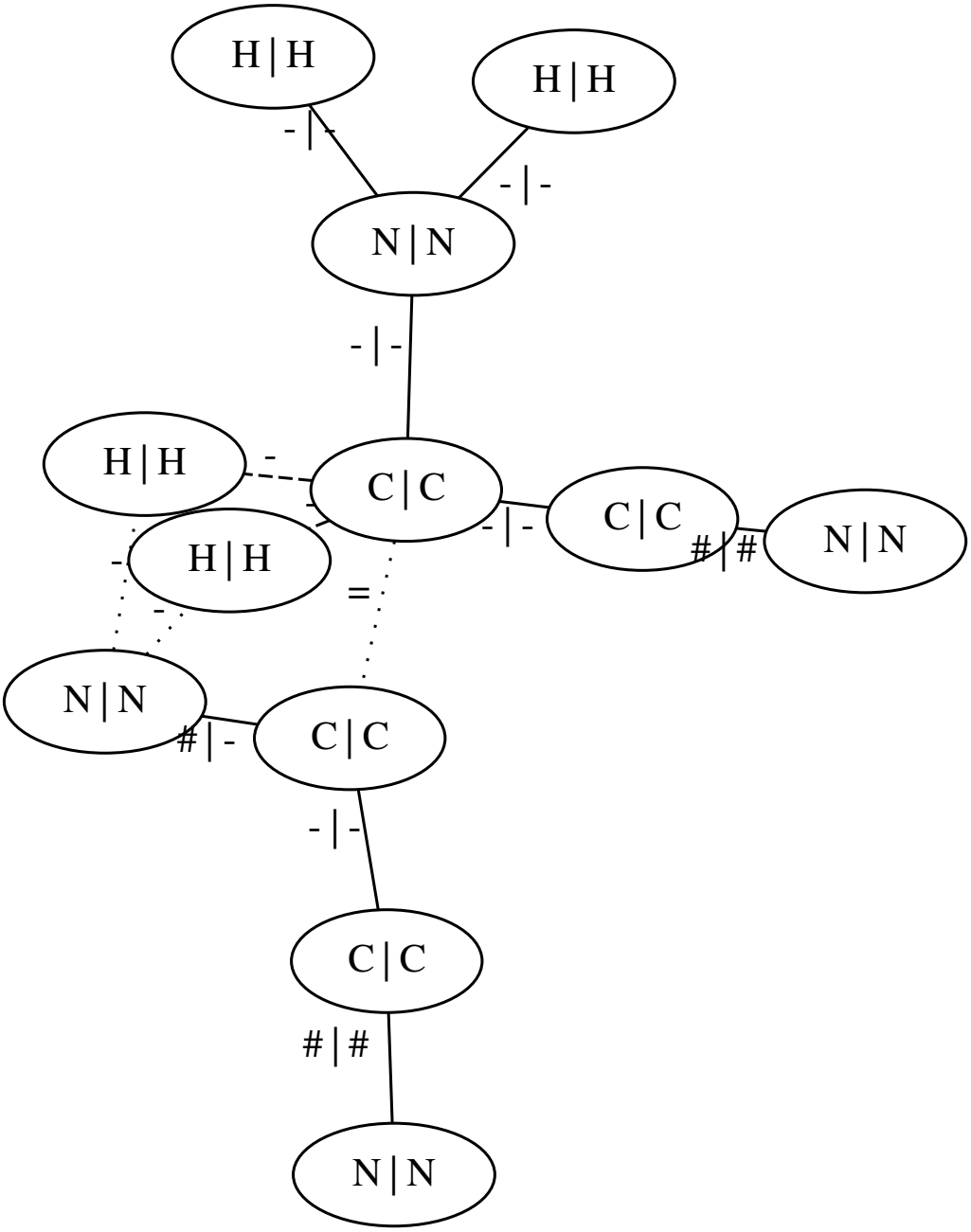
0.0.60 DAMN Scission, inverse



Files: out/296_r_58_10300000_{L, K, R}

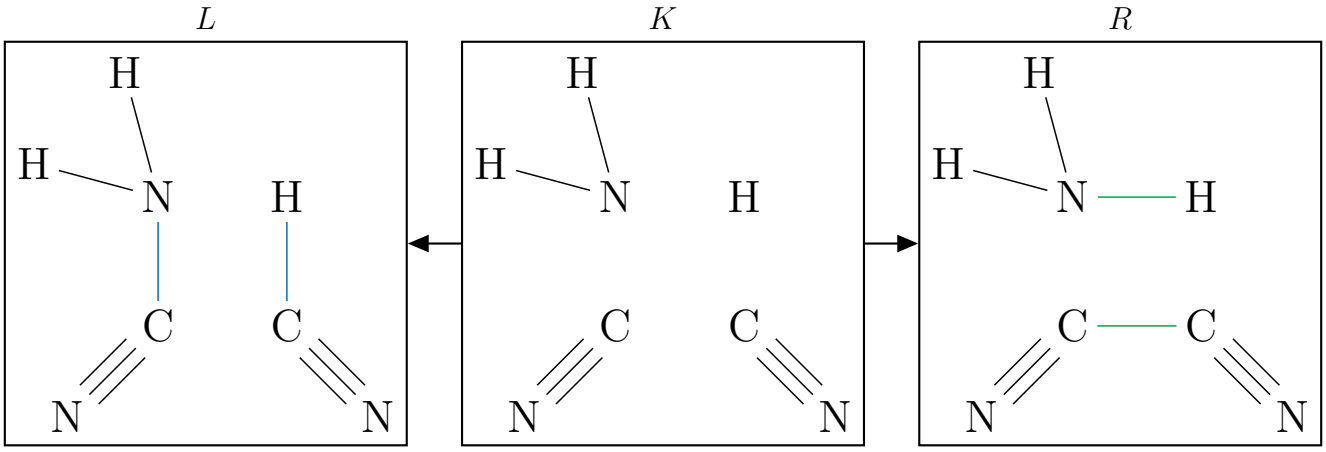


Files: out/297_r_58_11300100_{L, K, R}

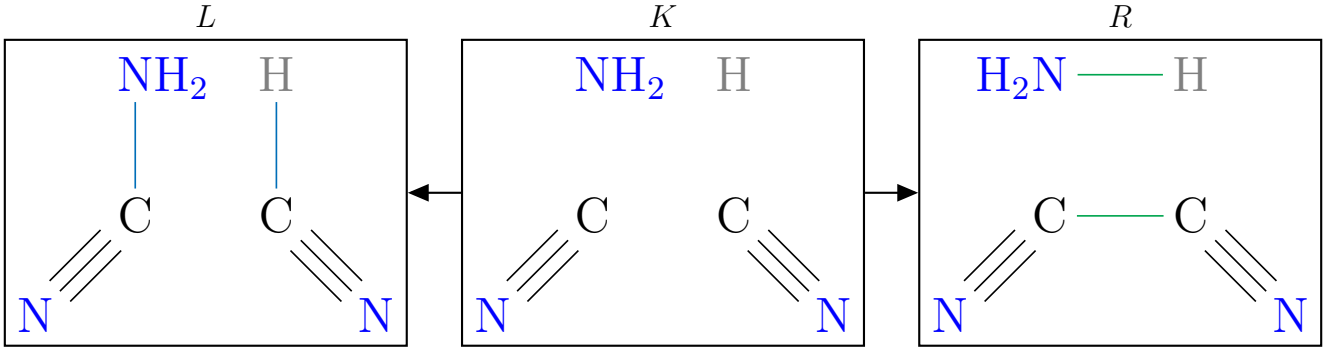


File: out/298_r_58_combined

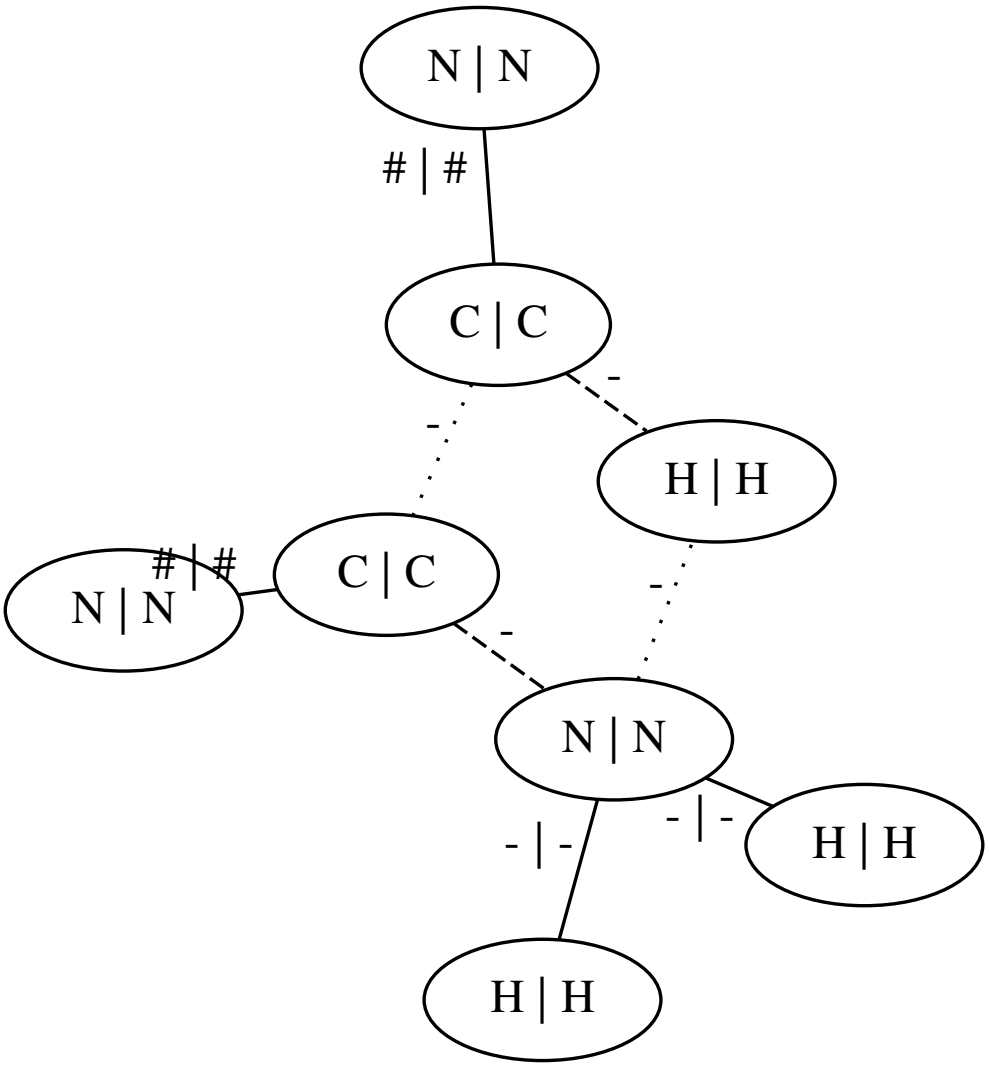
0.0.61 Cyanogen Ammonolysis, inverse



Files: out/301_r_59_10300000_{L, K, R}

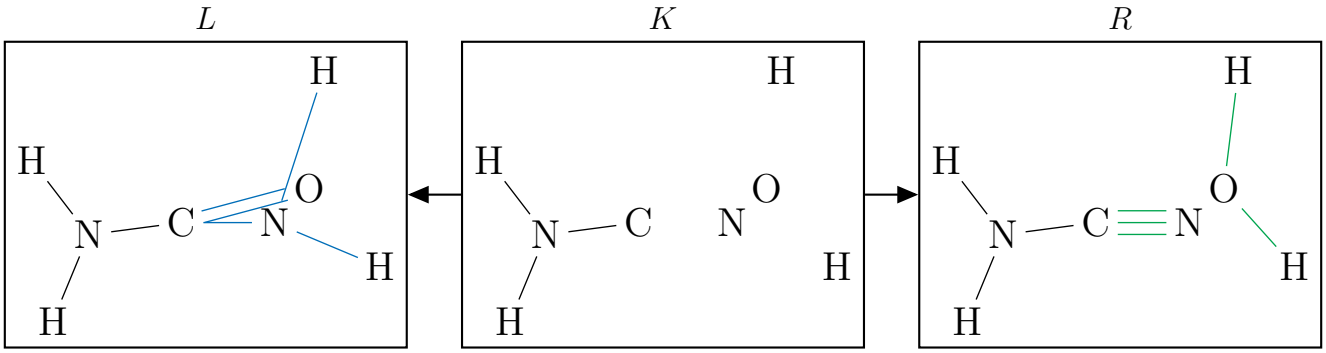


Files: out/302_r_59_11300100_{L, K, R}

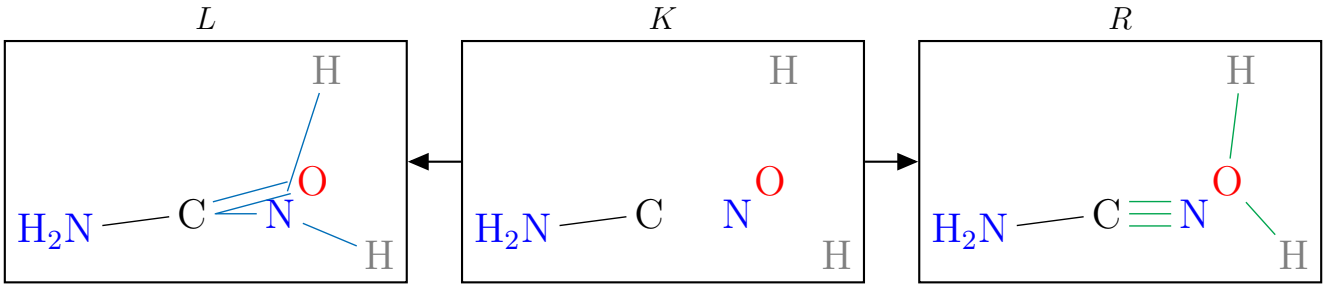


File: out/303_r_59_combined

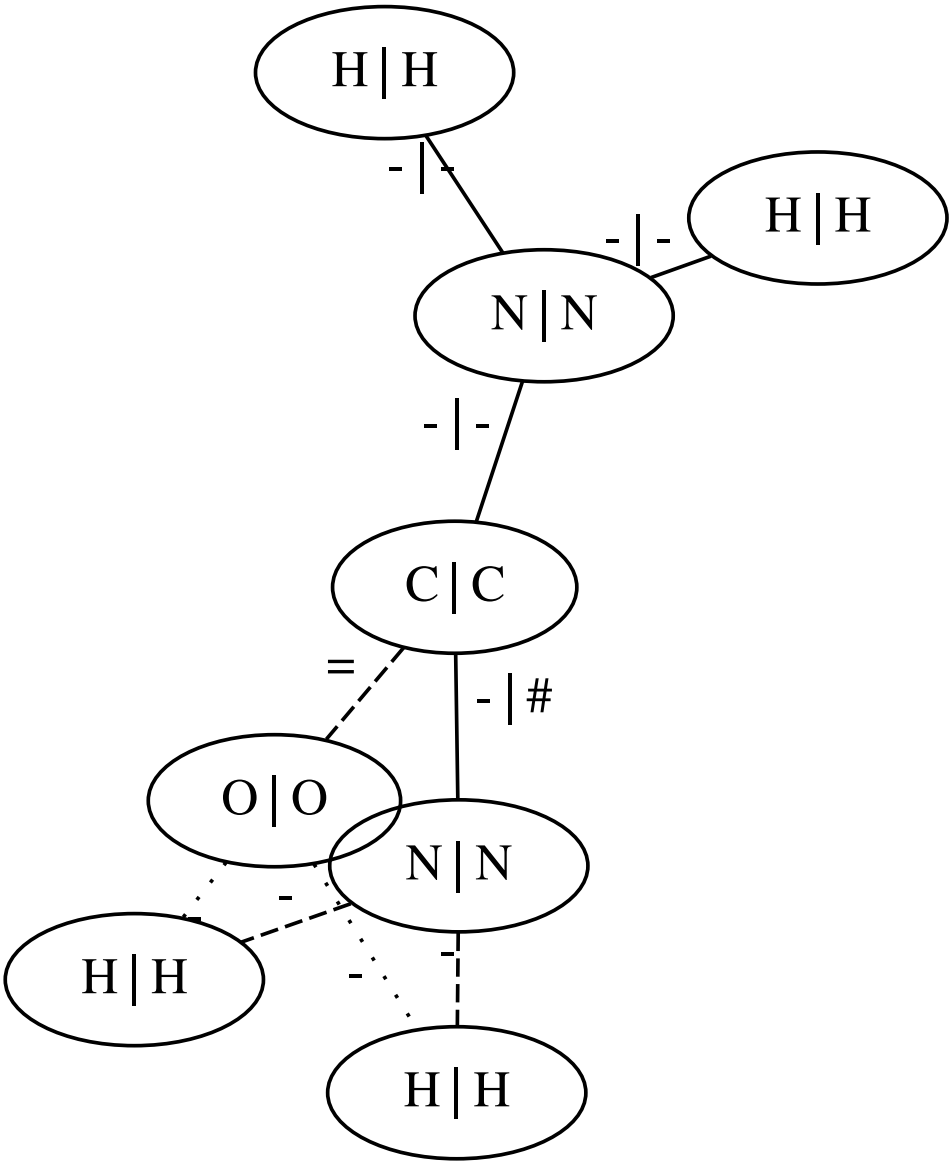
0.0.62 Cyanamide Hydration, inverse



Files: out/306_r_60_10300000_{L, K, R}

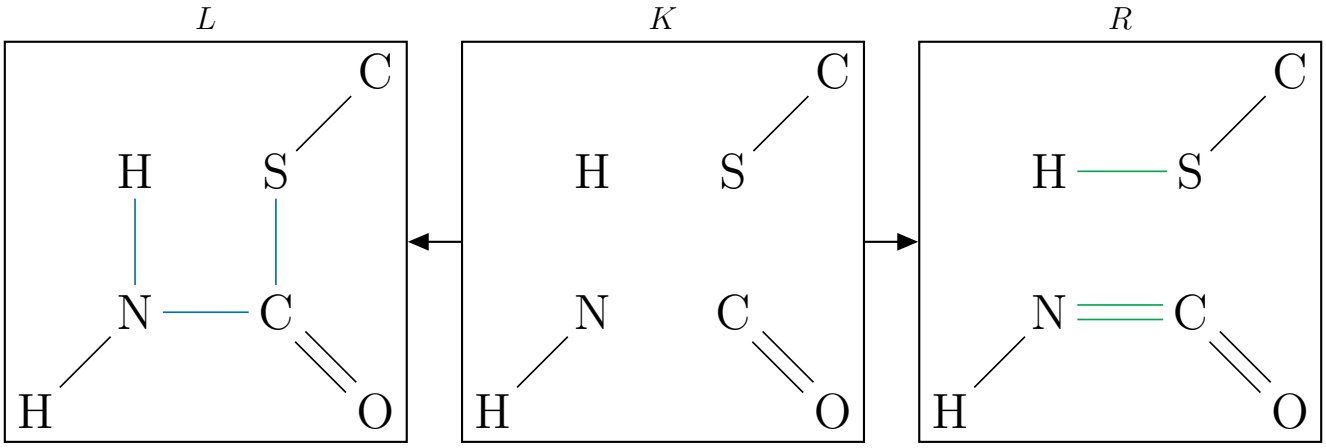


Files: out/307_r_60_11300100_{L, K, R}

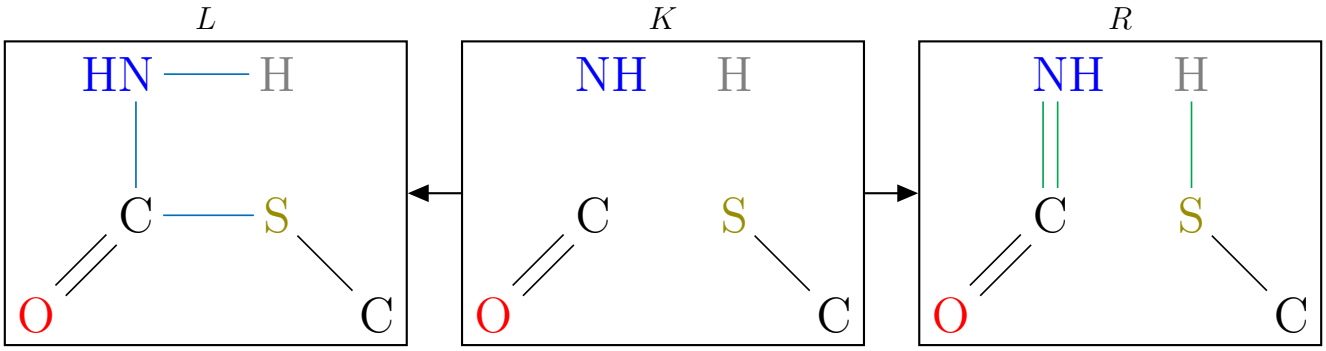


File: out/308_r_60_combined

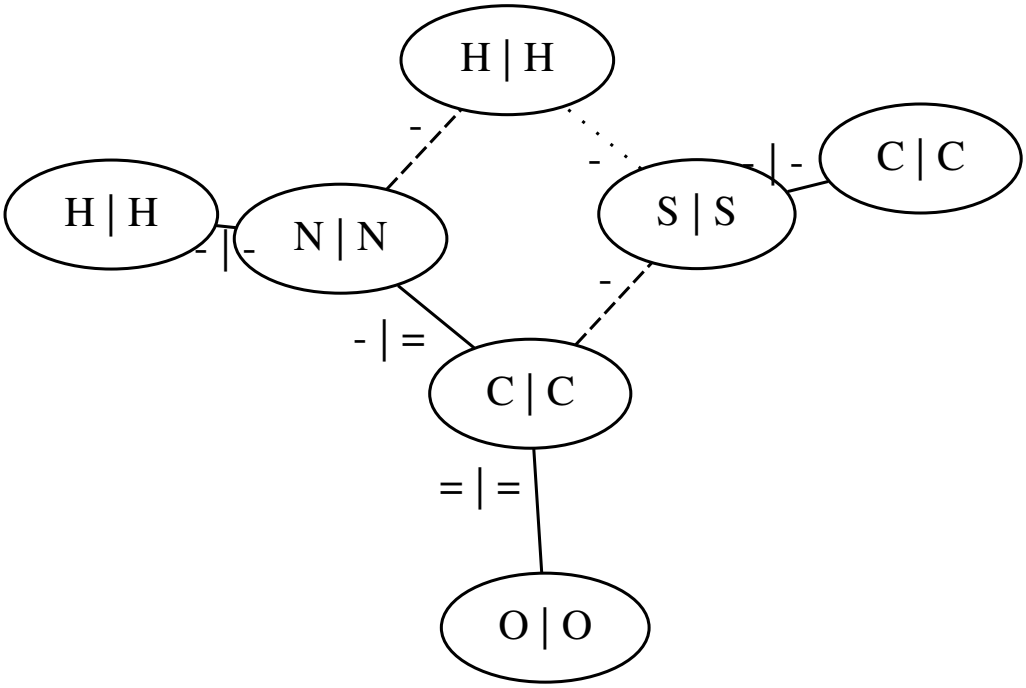
0.0.63 Carbamylation, SC, inverse



Files: out/311_r_61_10300000_{L, K, R}

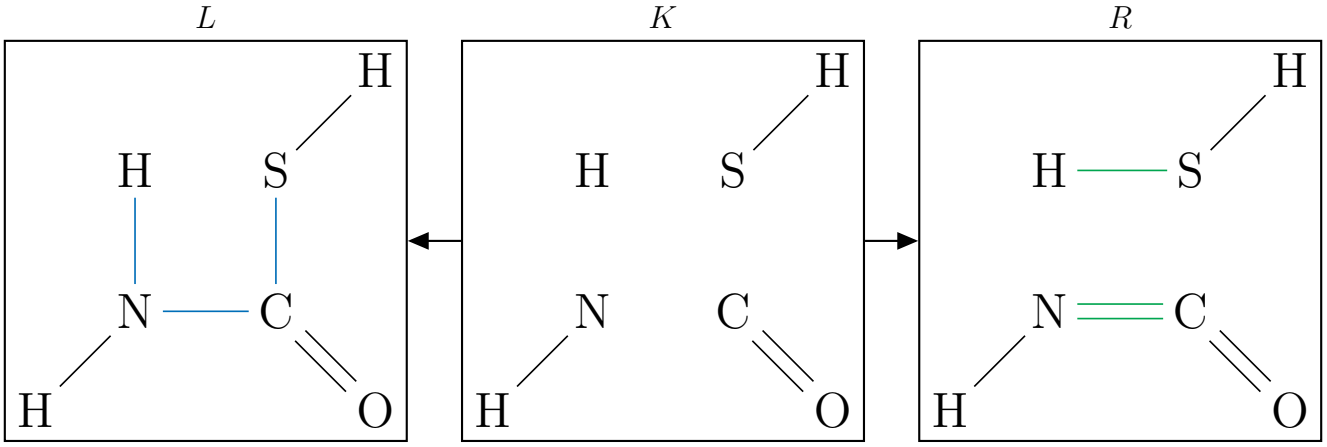


Files: out/312_r_61_11300100_{L, K, R}

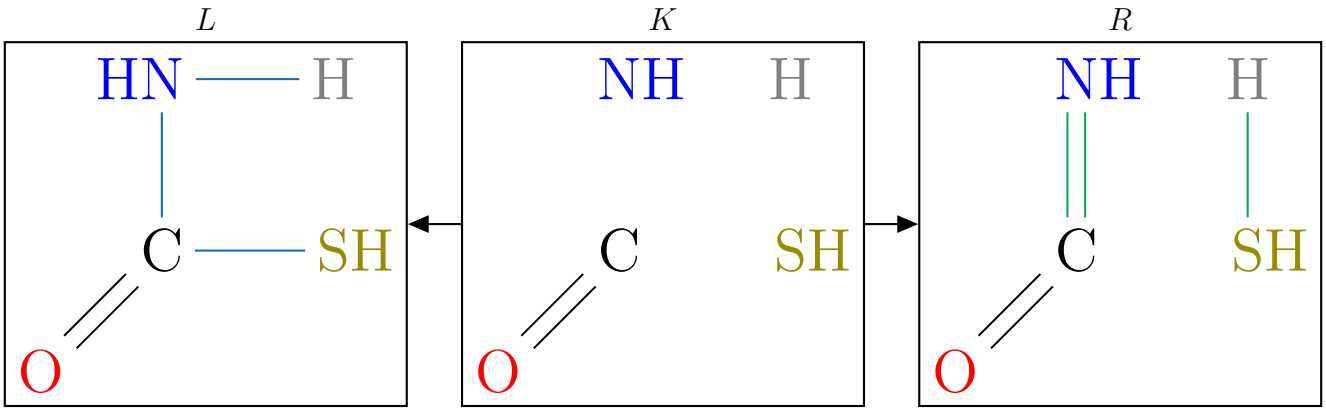


File: out/313_r_61_combined

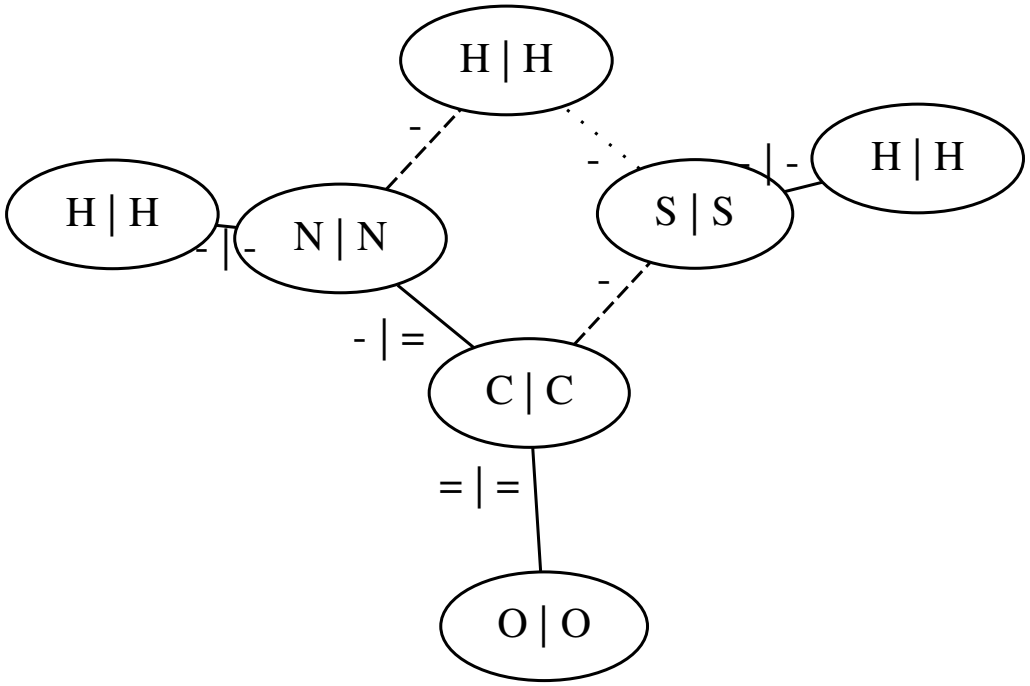
0.0.64 Carbamylation, SH, inverse



Files: out/316_r_62_10300000_{L, K, R}

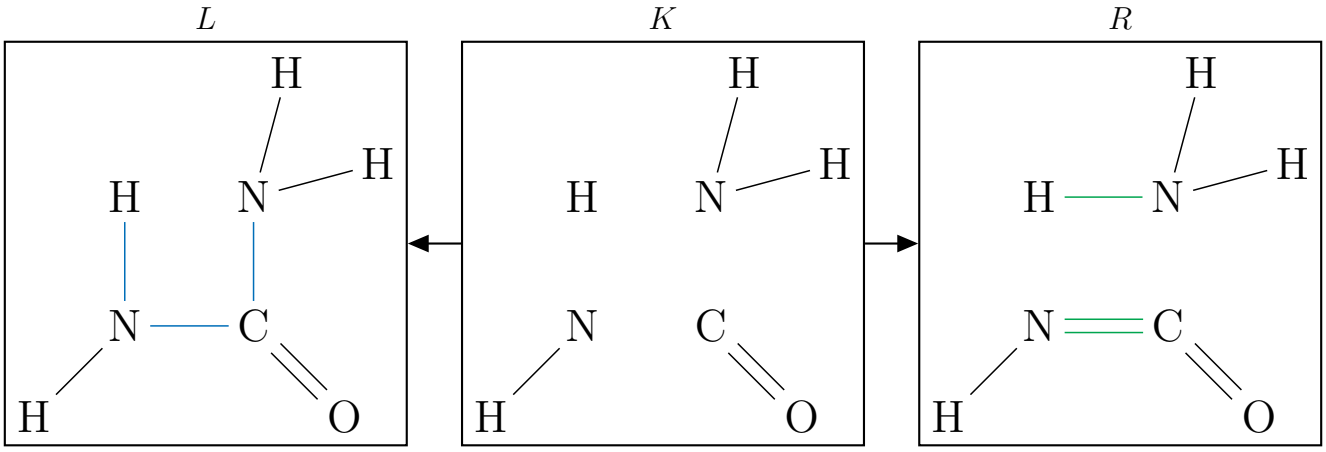


Files: out/317_r_62_11300100_{L, K, R}

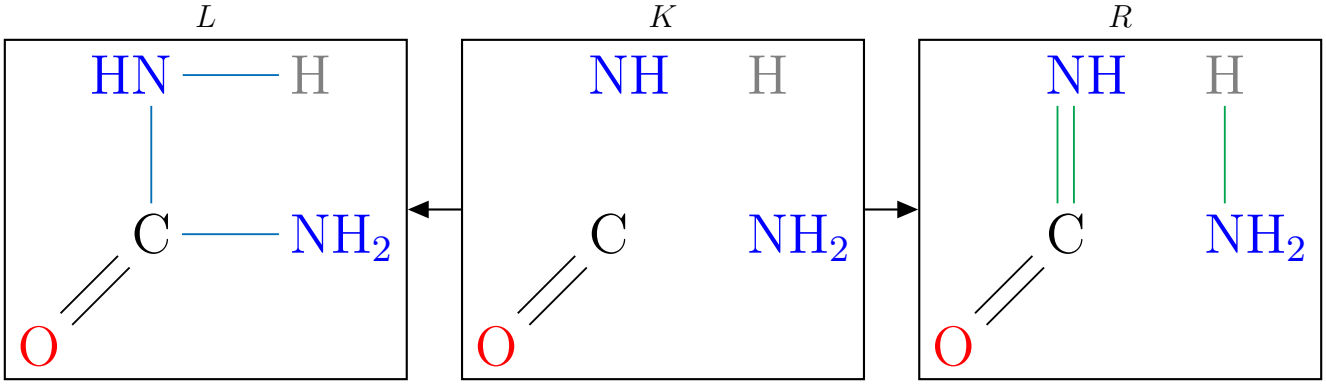


File: out/318_r_62_combined

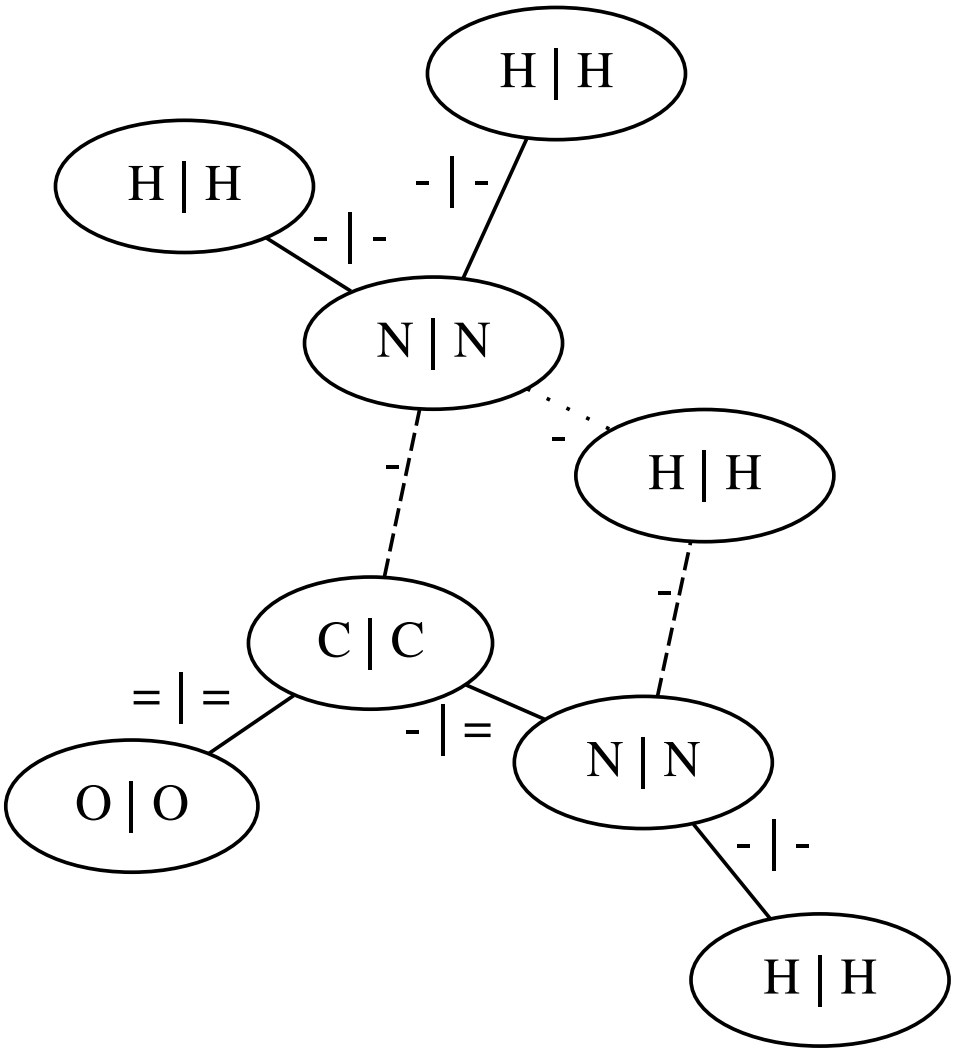
0.0.65 Carbamylation, N, HH, inverse



Files: out/321_r_63_10300000_{L, K, R}

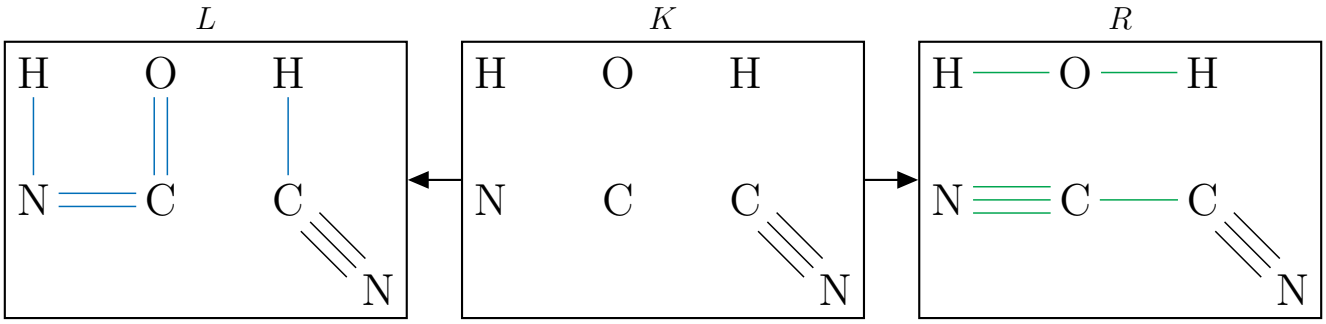


Files: out/322_r_63_11300100_{L, K, R}

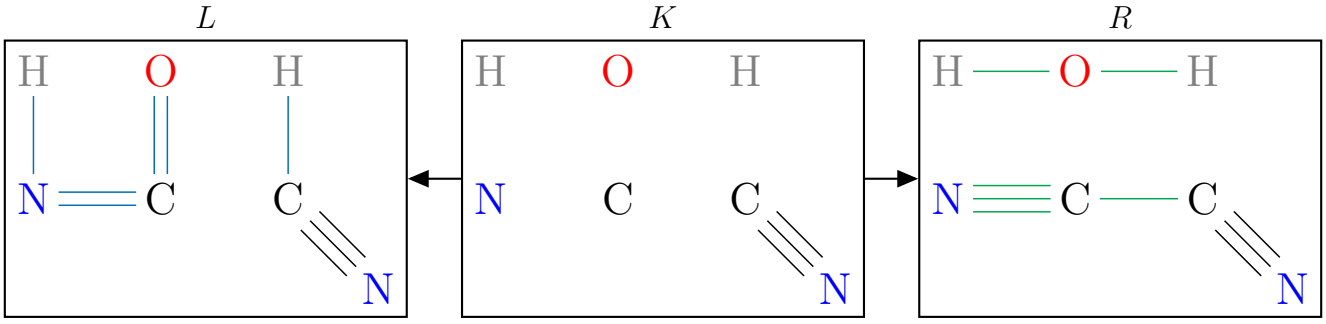


File: out/323_r_63_combined

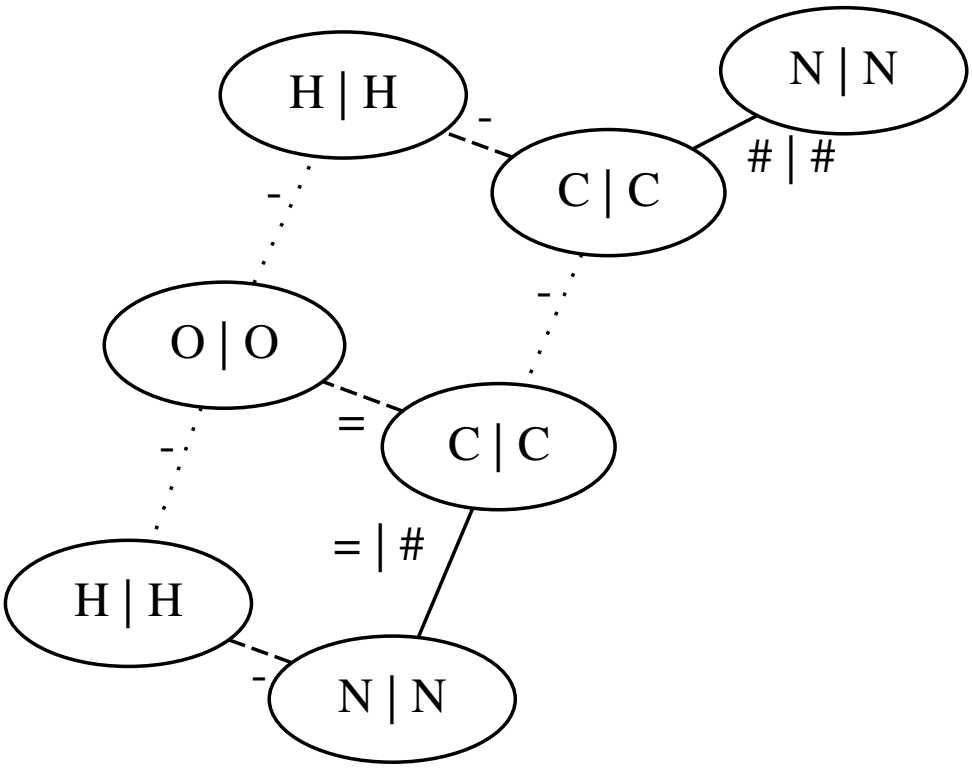
0.0.66 Cyanate from cyanogen, inverse



Files: out/326_r_64_10300000_{L, K, R}

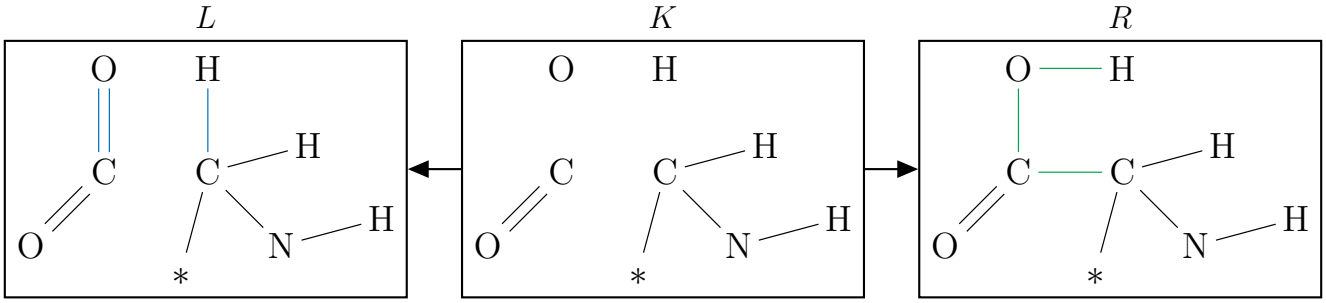


Files: out/327_r_64_11300100_{L, K, R}

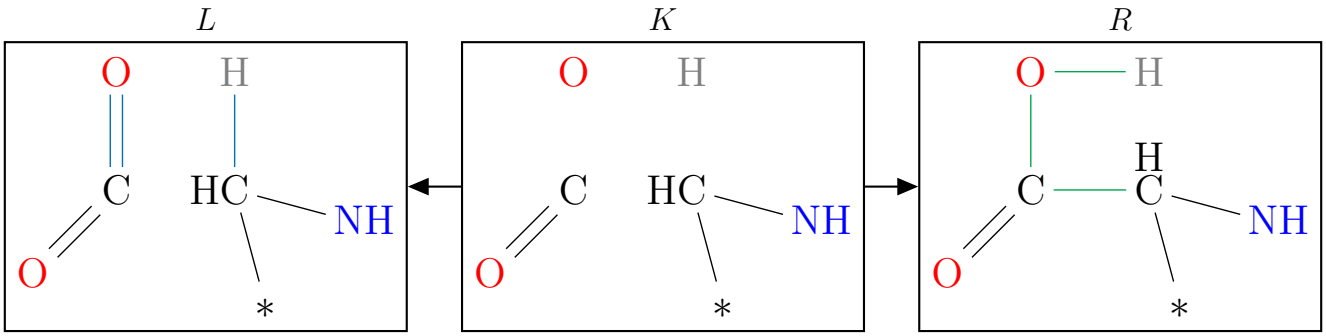


File: out/328_r_64_combined

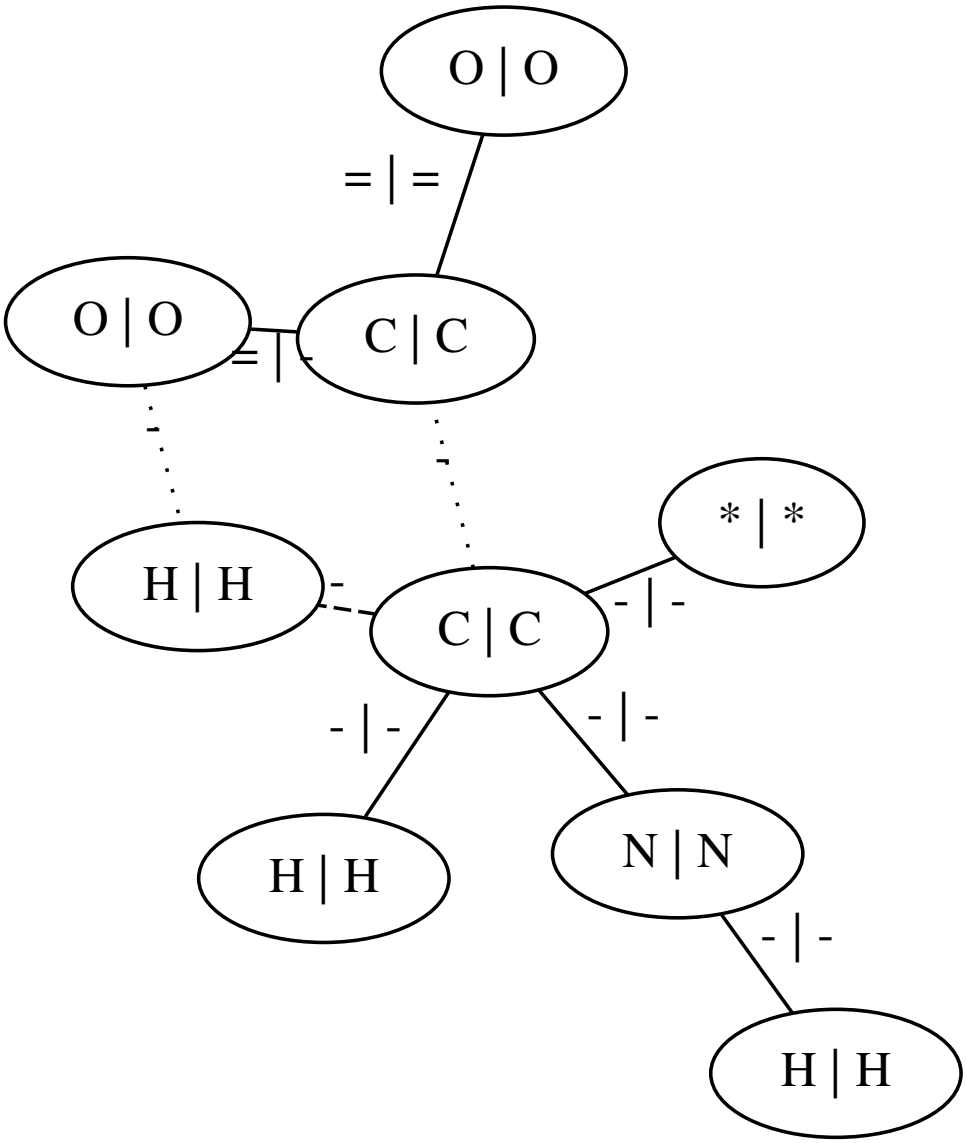
0.0.67 Ketone-Catalyzed Decarboxylation, inverse



Files: out/331_r_65_10300000_{L, K, R}

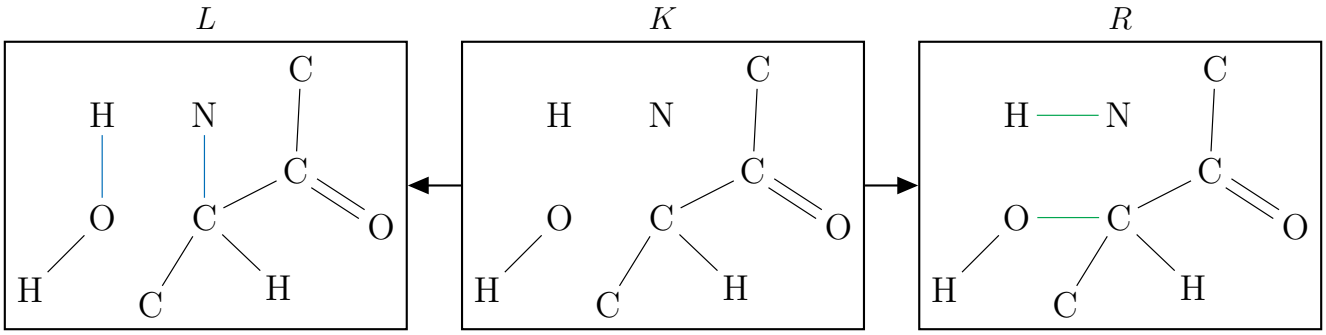


Files: out/332_r_65_11300100_{L, K, R}

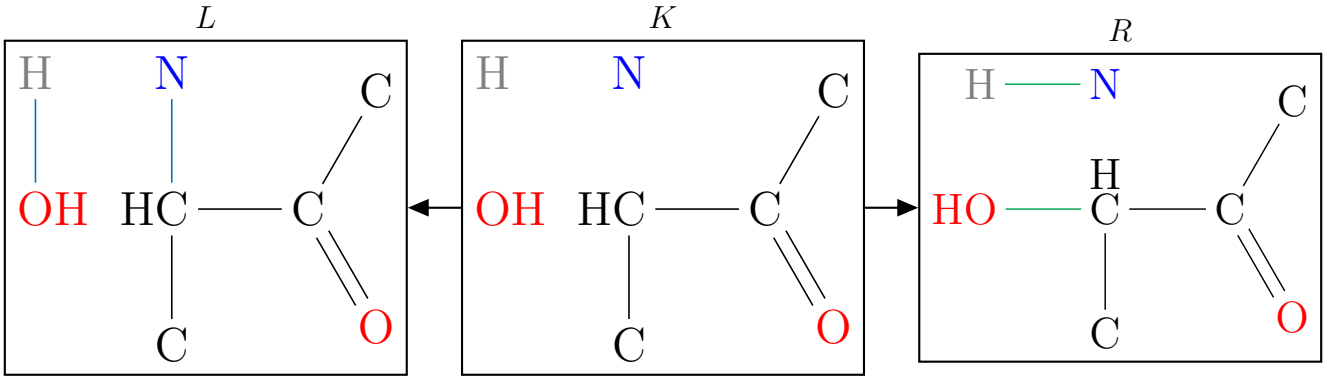


File: out/333_r_65_combined

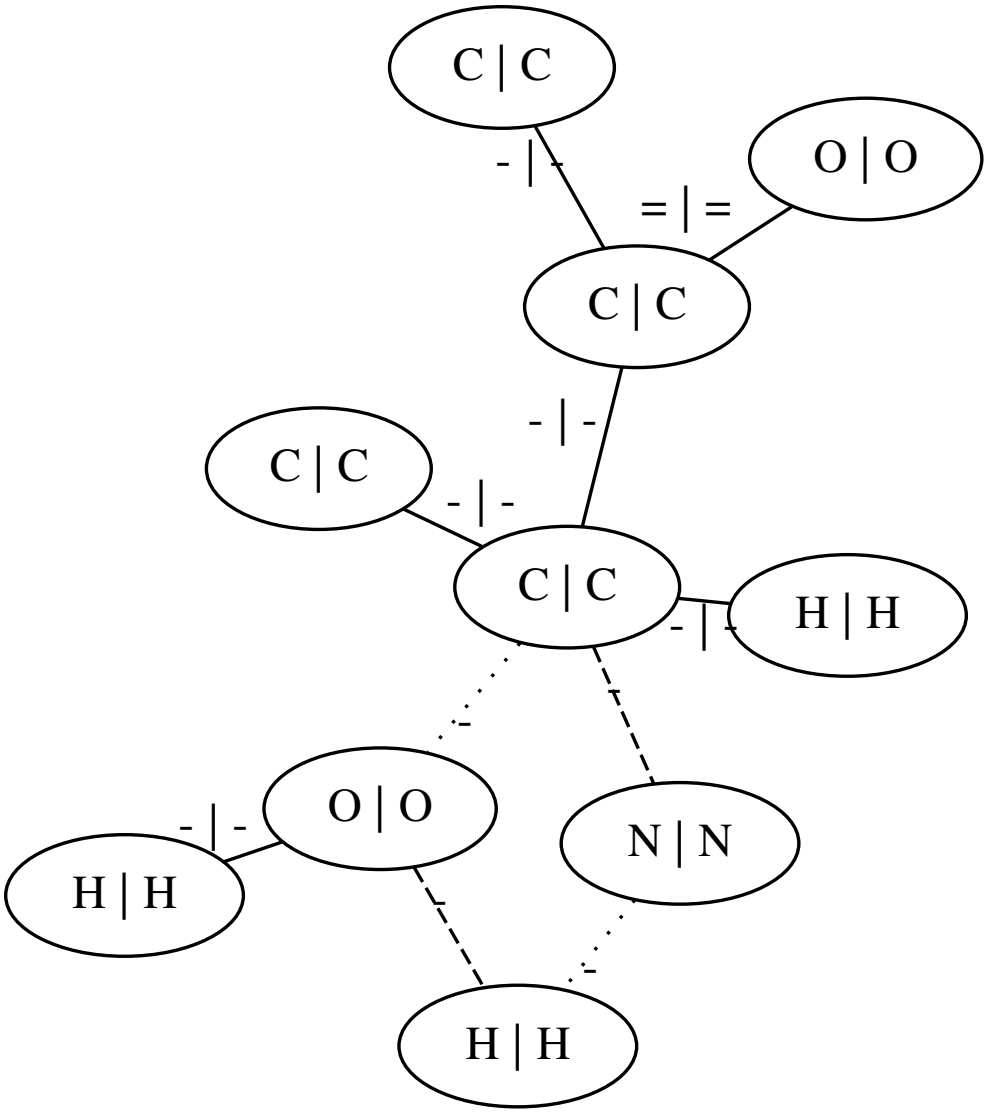
0.0.68 Amadori Rearrangement, inverse



Files: out/336_r_66_10300000_{L, K, R}

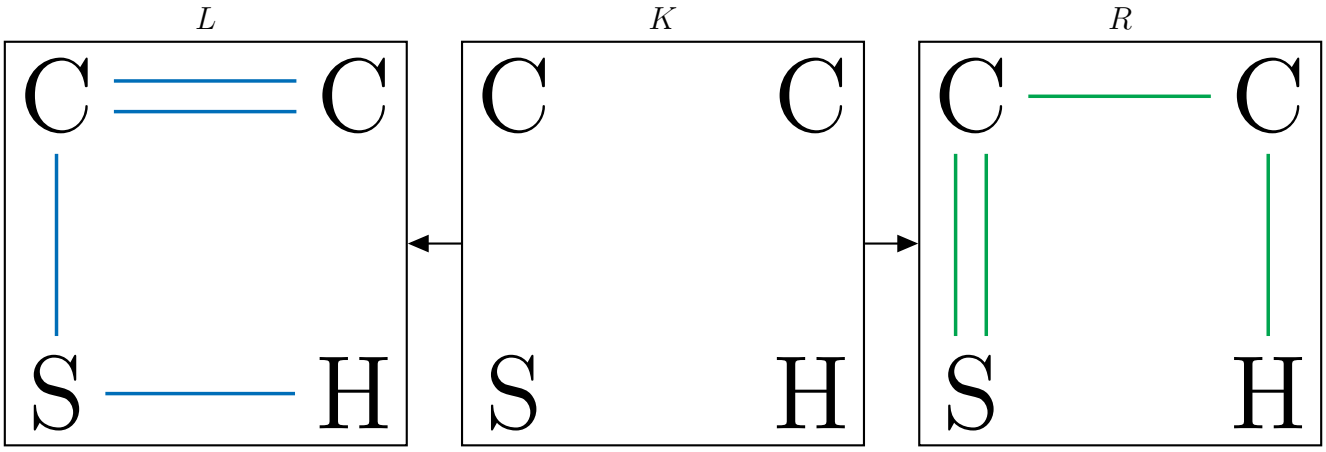


Files: out/337_r_66_11300100_{L, K, R}

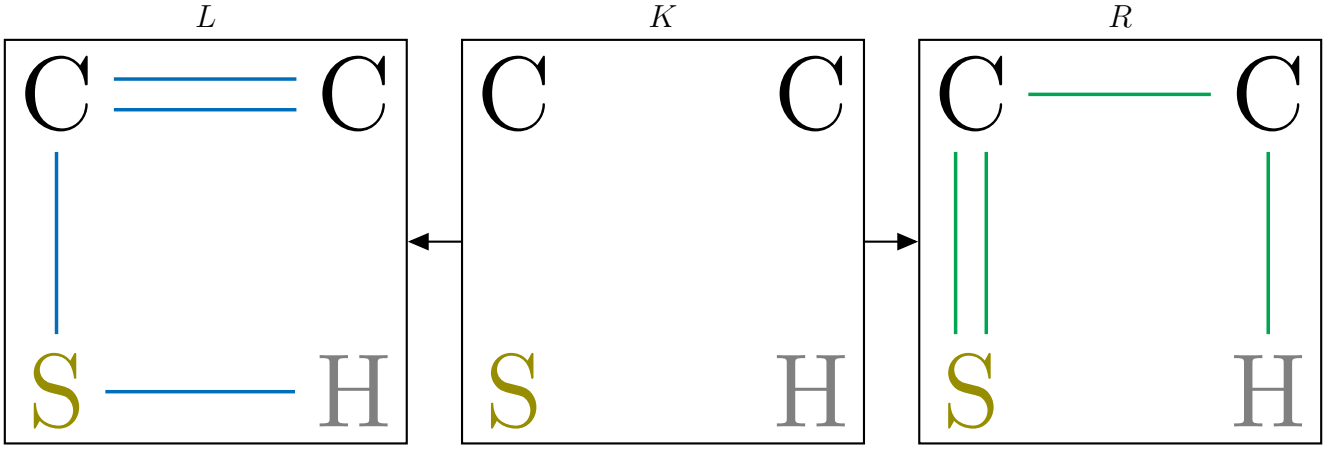


File: out/338_r_66_combined

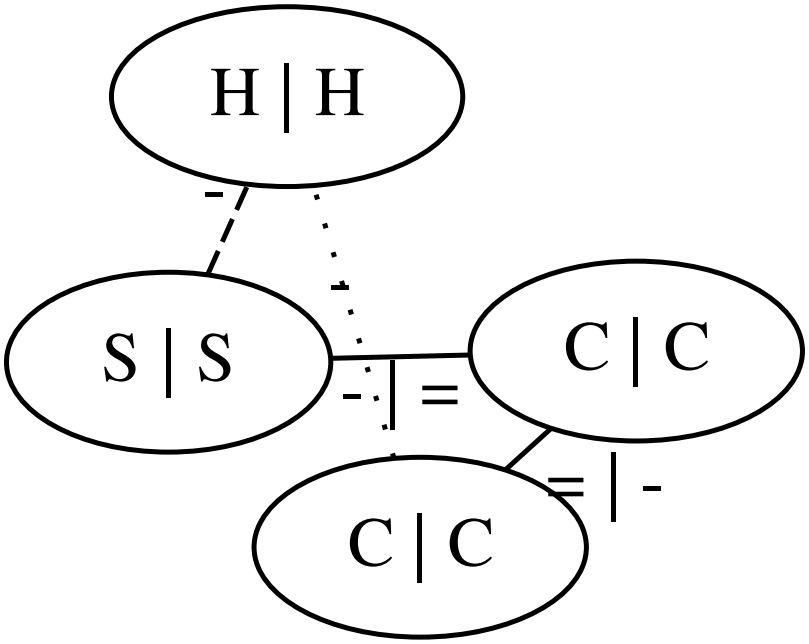
0.0.69 Thial -> Thiene, inverse



Files: out/341_r_67_10300000_{L, K, R}

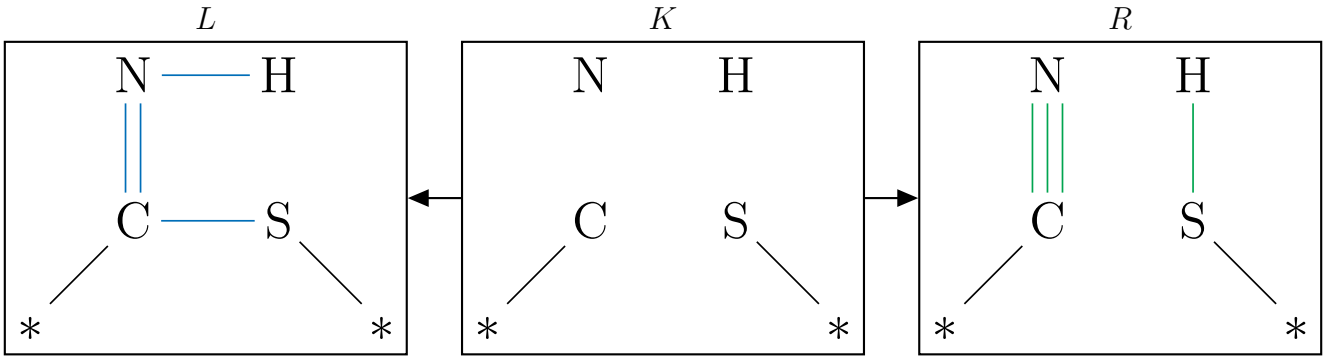


Files: out/342_r_67_11300100_{L, K, R}

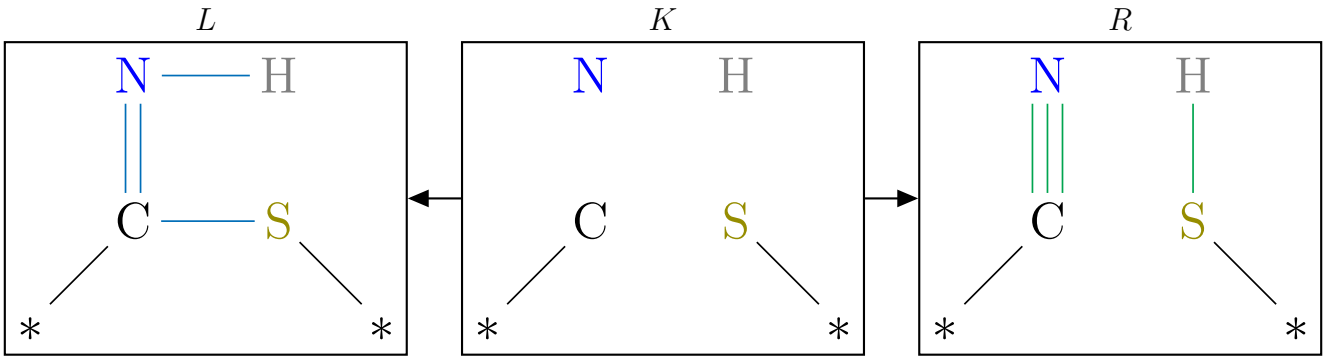


File: out/343_r_67_combined

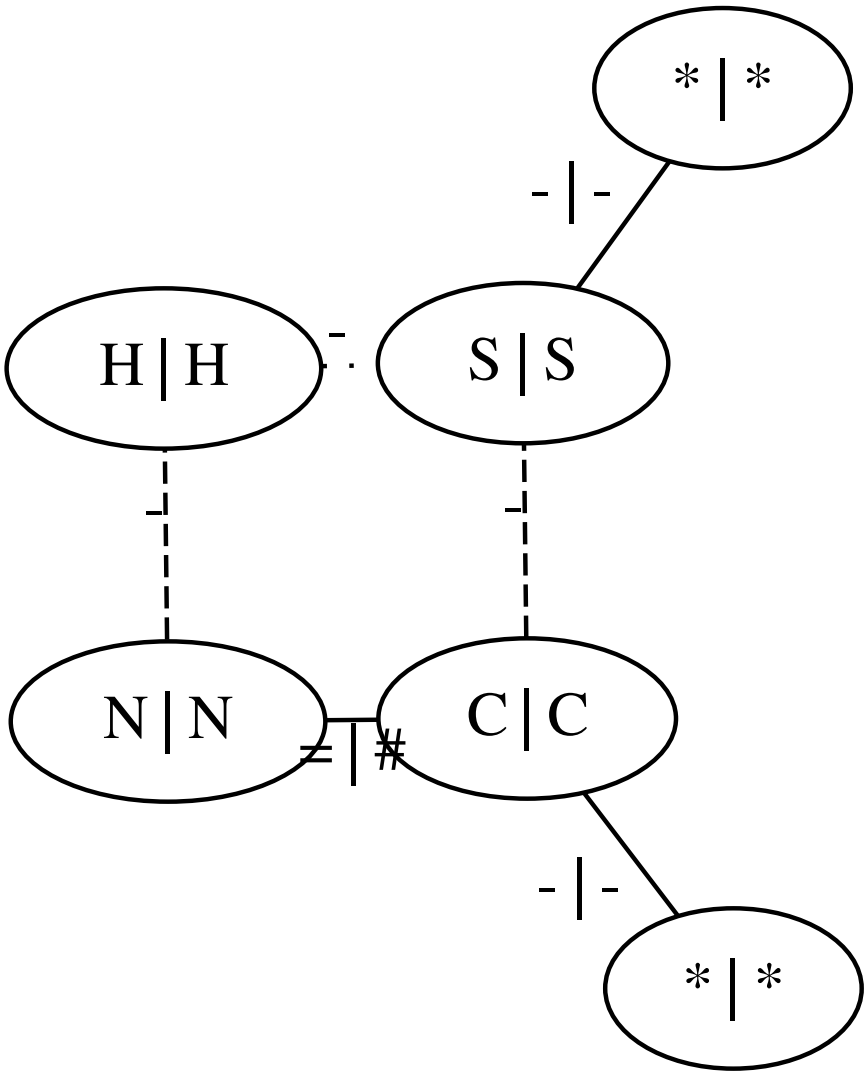
0.0.70 Sulfide to Nitrile Addition, inverse



Files: out/346_r_68_10300000_{L, K, R}

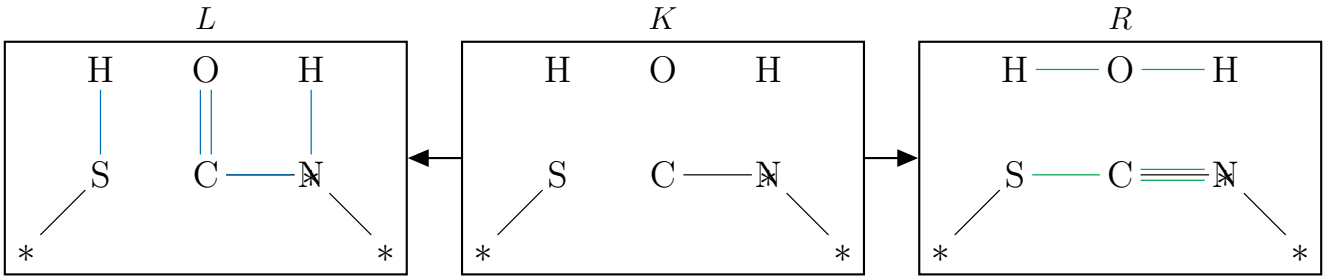


Files: out/347_r_68_11300100_{L, K, R}

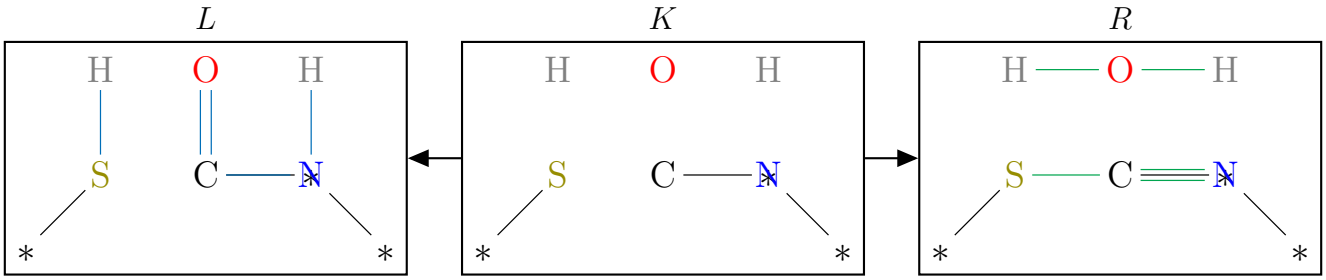


File: out/348_r_68_combined

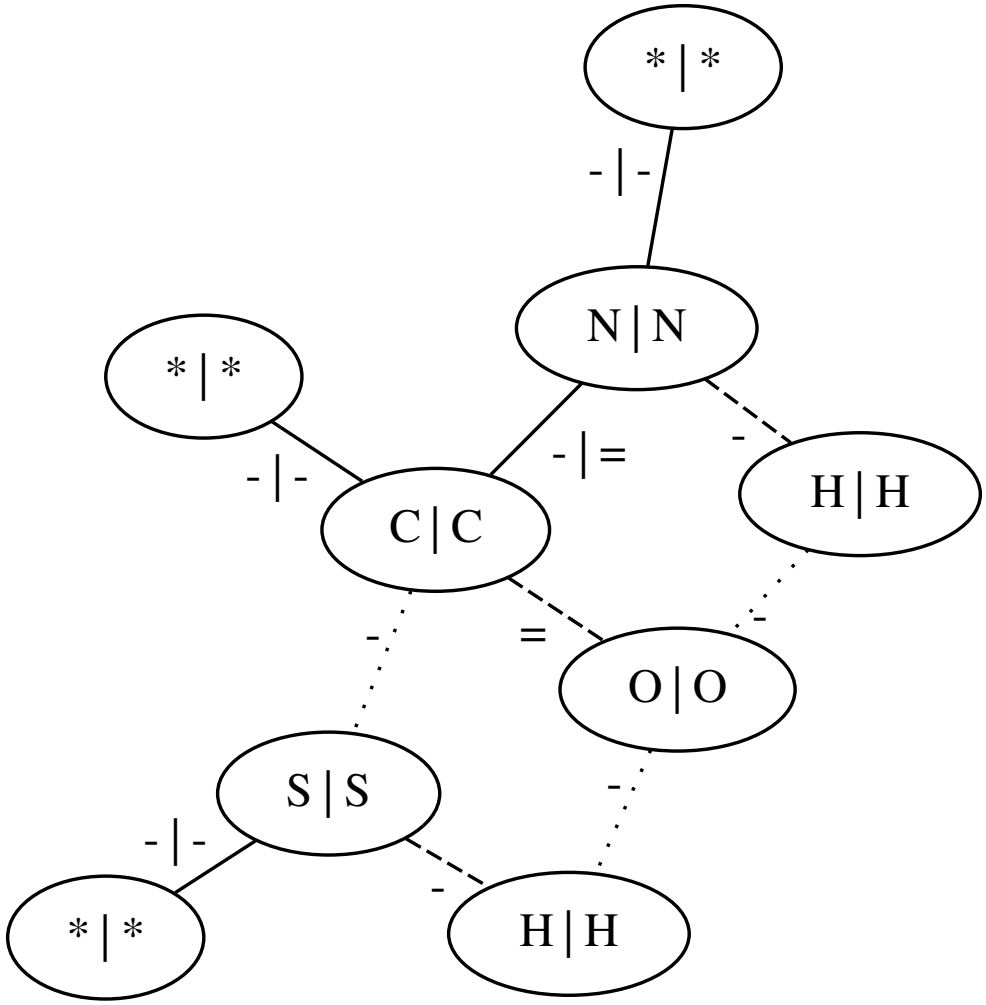
0.0.71 Thioamidine to Amide Hydrolysis, inverse



Files: out/351_r_69_10300000_{L, K, R}

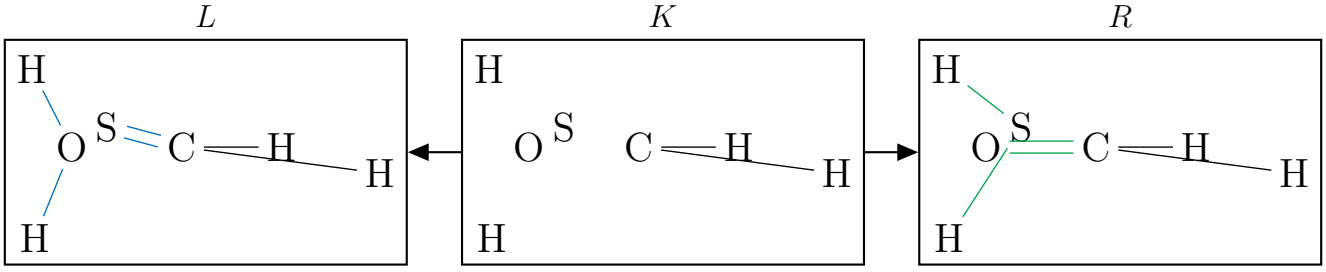


Files: out/352_r_69_11300100_{L, K, R}

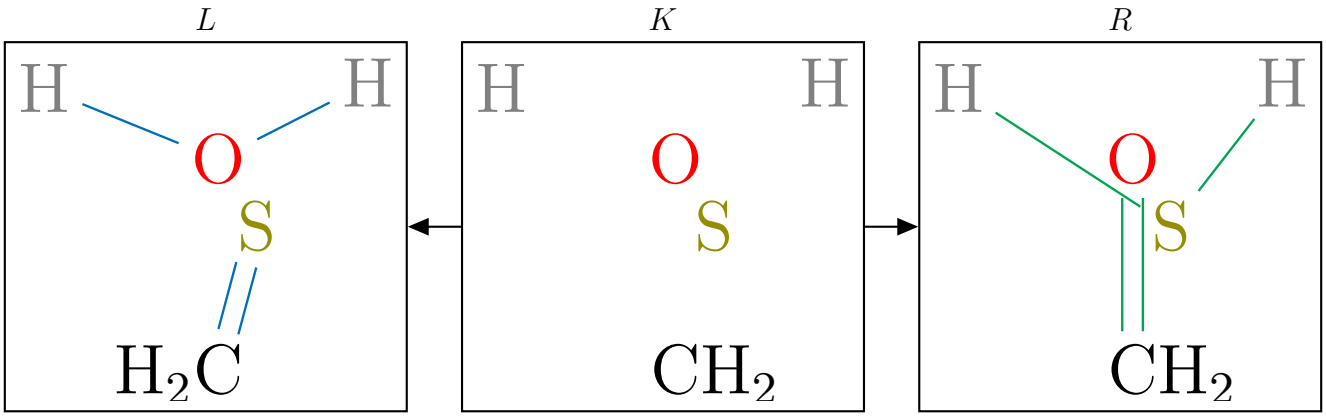


File: out/353_r_69_combined

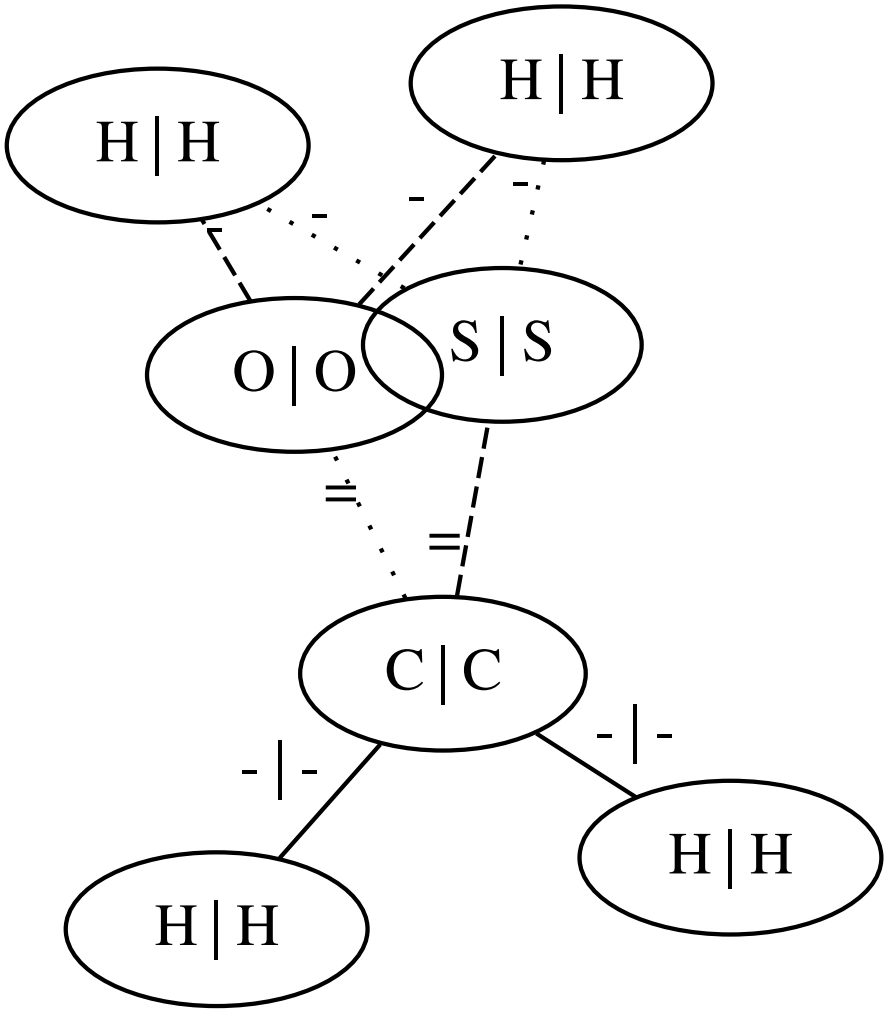
0.0.72 Ketone/Aldehyde to Thioketone/Thial, HH, inverse



Files: out/356_r_70_10300000_{L, K, R}

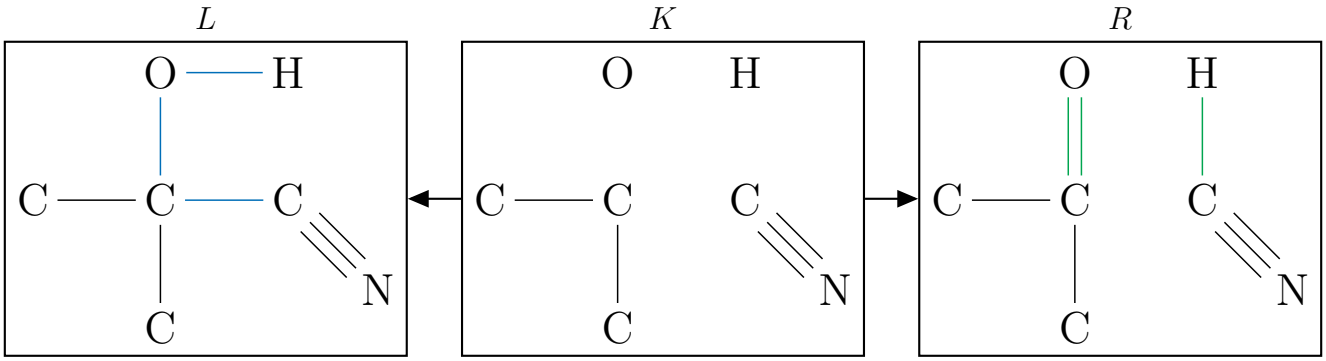


Files: out/357_r_70_11300100_{L, K, R}

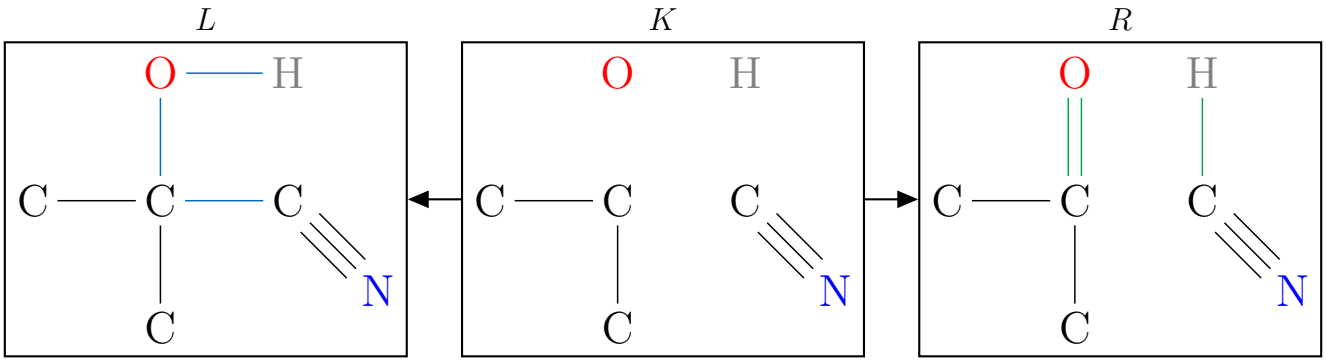


File: out/358_r_70_combined

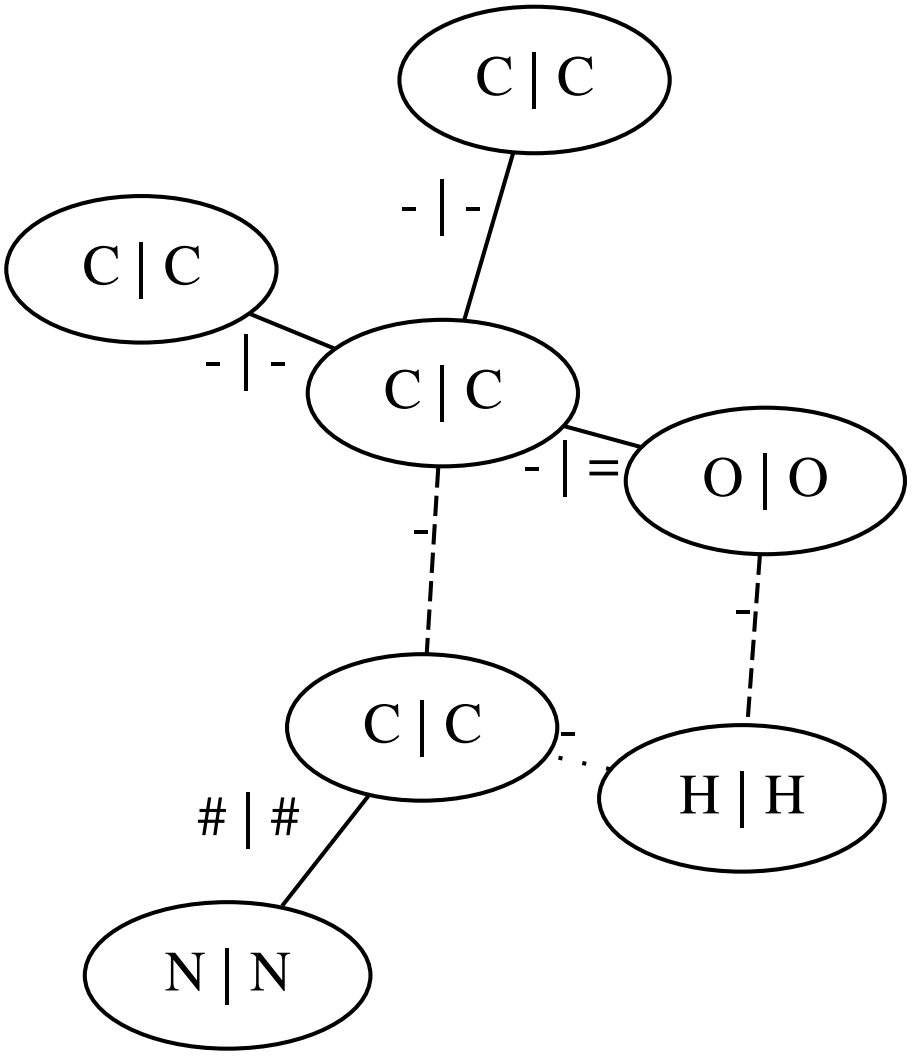
0.0.73 HCN to Ketone, inverse



Files: out/361_r_71_10300000_{L, K, R}

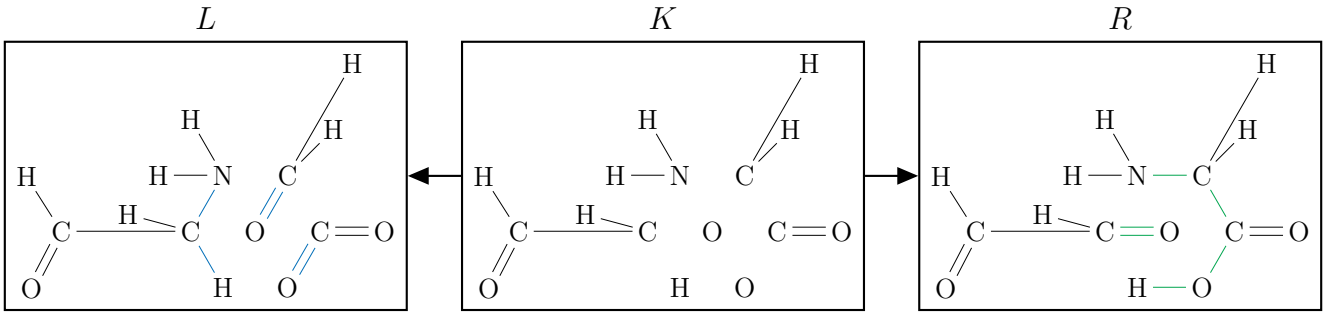


Files: out/362_r_71_11300100_{L, K, R}

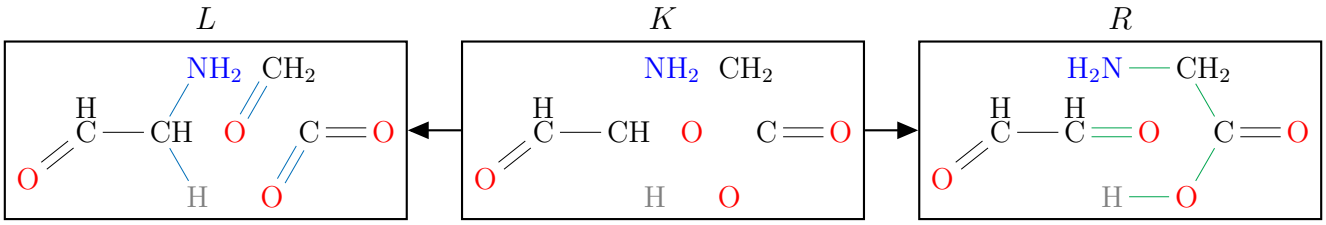


File: out/363_r_71_combined

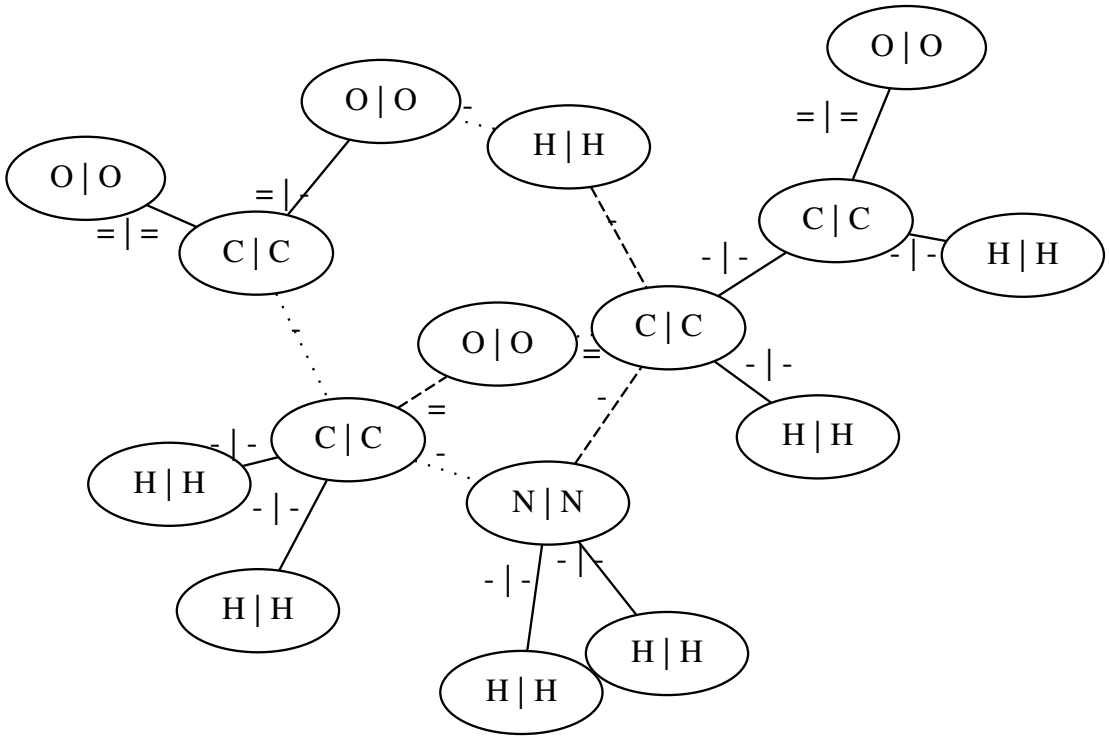
0.0.74 Strecker Degradation Dicarbonyl, H, H, H, H, inverse



Files: out/366_r_72_10300000_{L, K, R}

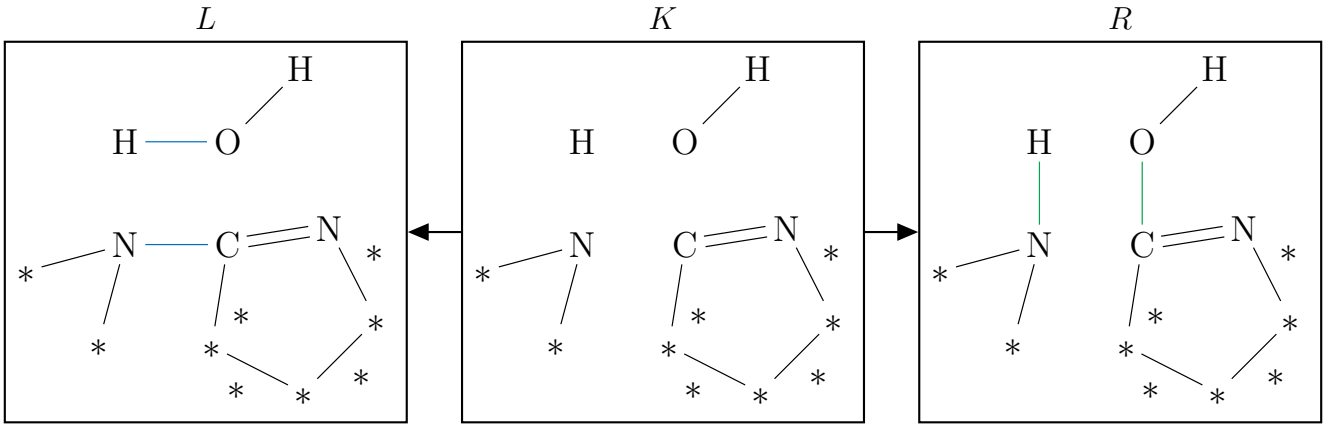


Files: out/367_r_72_11300100_{L, K, R}

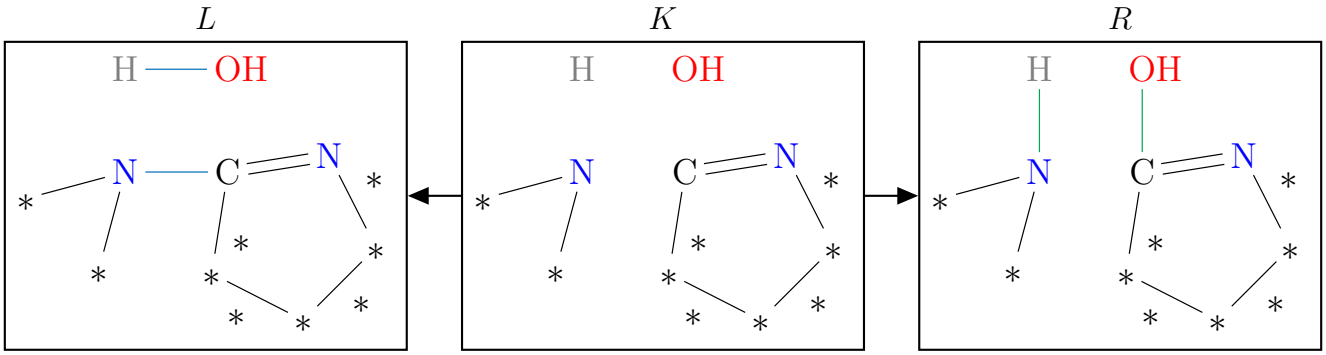


File: out/368_r_72_combined

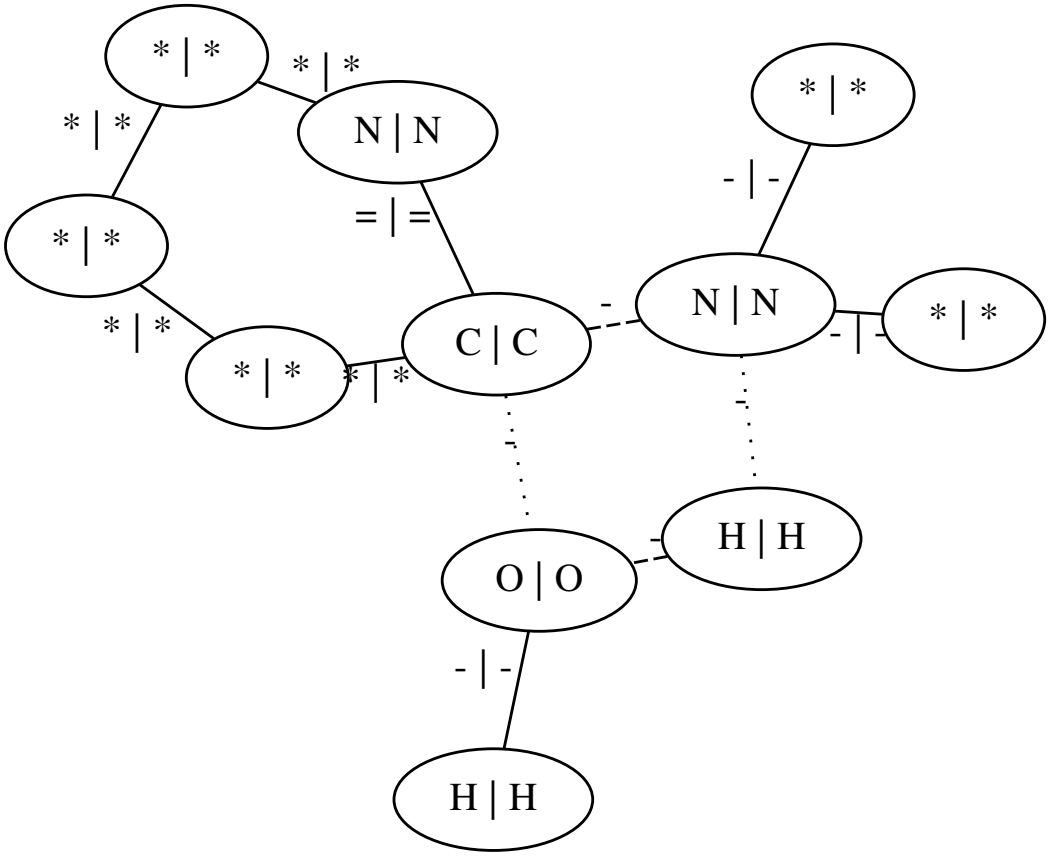
0.0.75 5 Membered Ring Exoamine Hydrolysis



Files: out/371_r_74_10300000_{L, K, R}

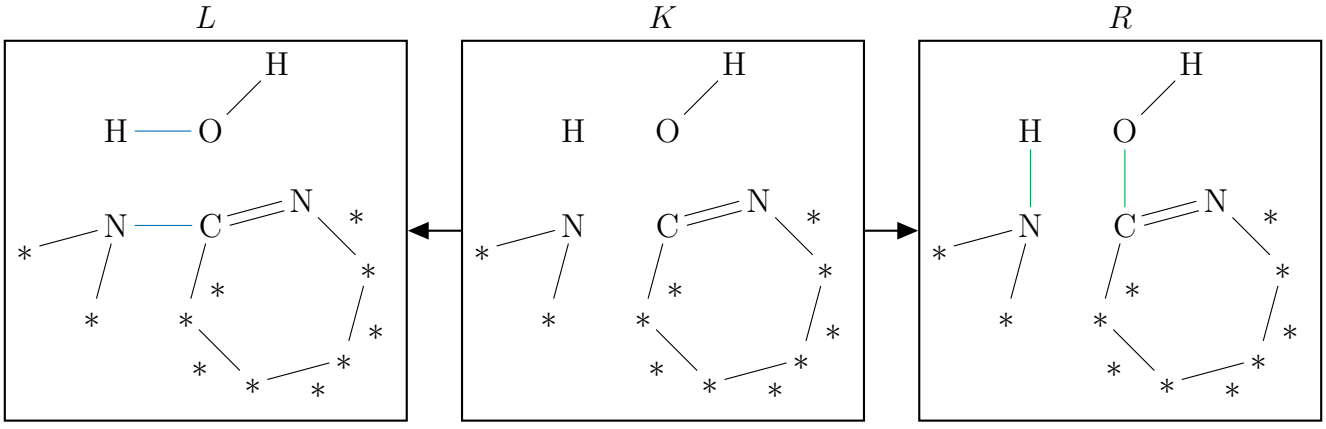


Files: out/372_r_74_11300100_{L, K, R}

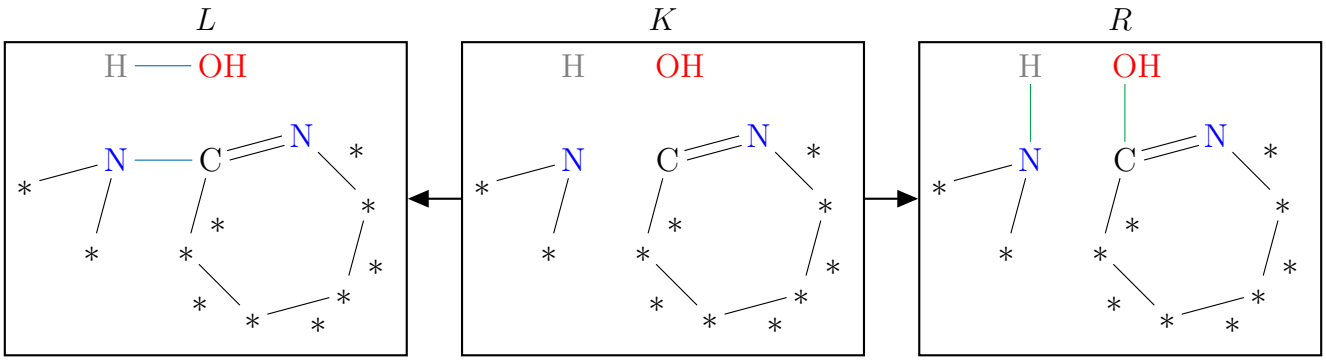


File: out/373_r_74_combined

0.0.76 6 Membered Ring Exoamine Hydrolysis



Files: out/376_r_75_10300000_{L, K, R}



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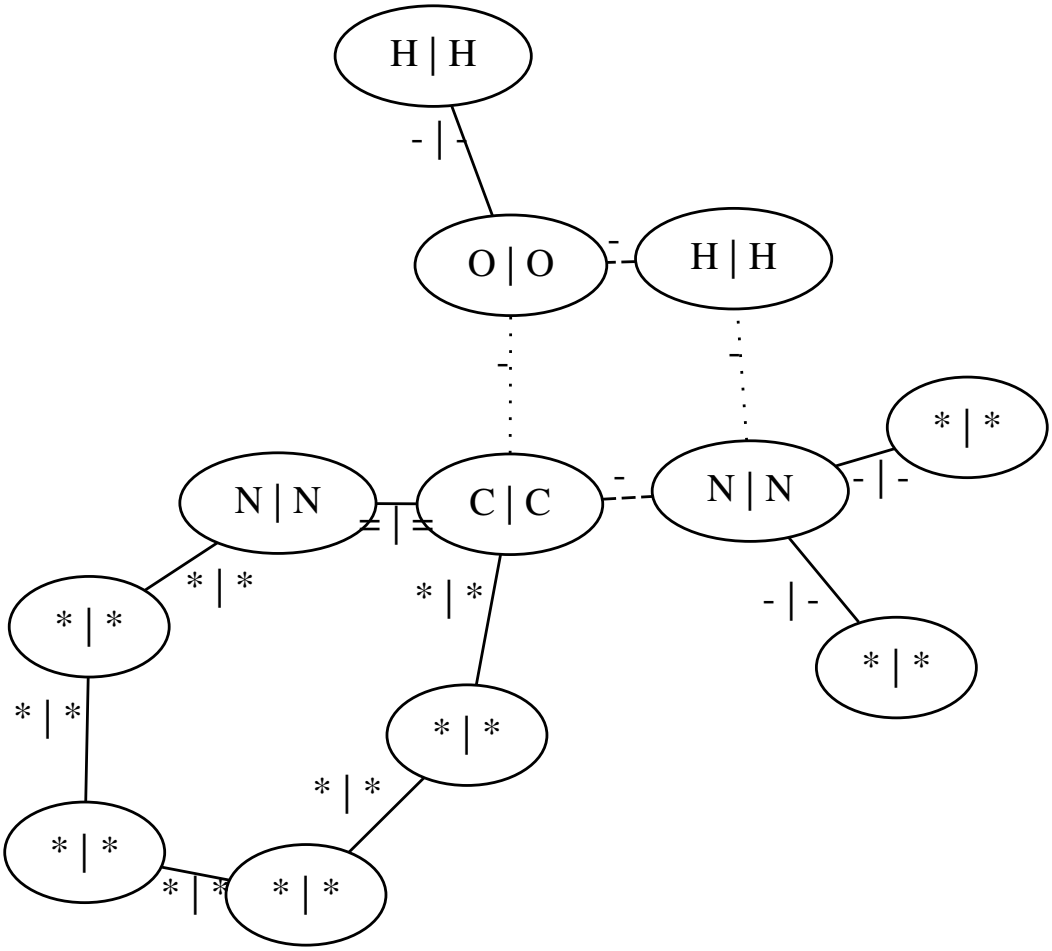
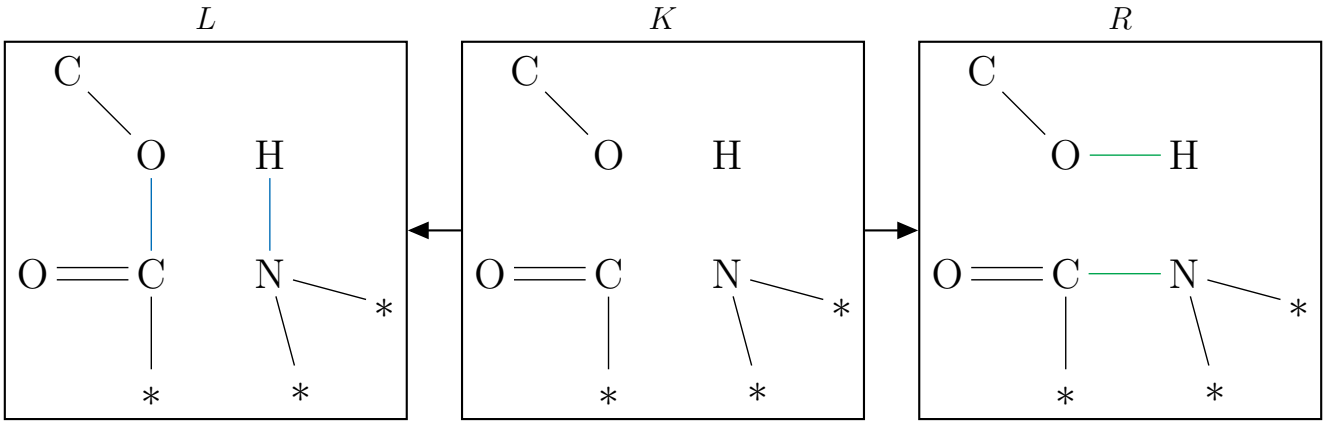


File: out/378_r_75_combined

0.0.77 Ammonolysis of Esters



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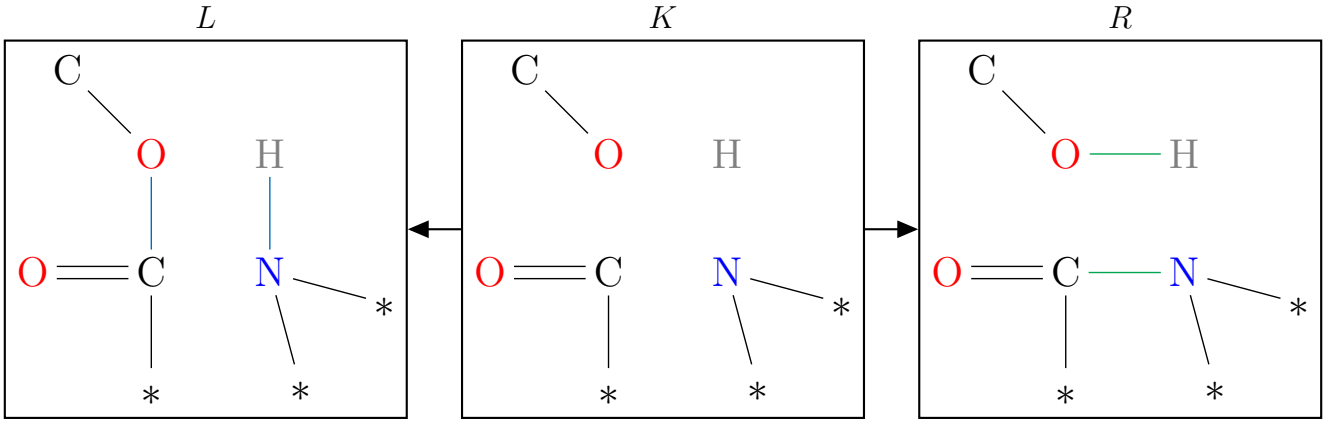
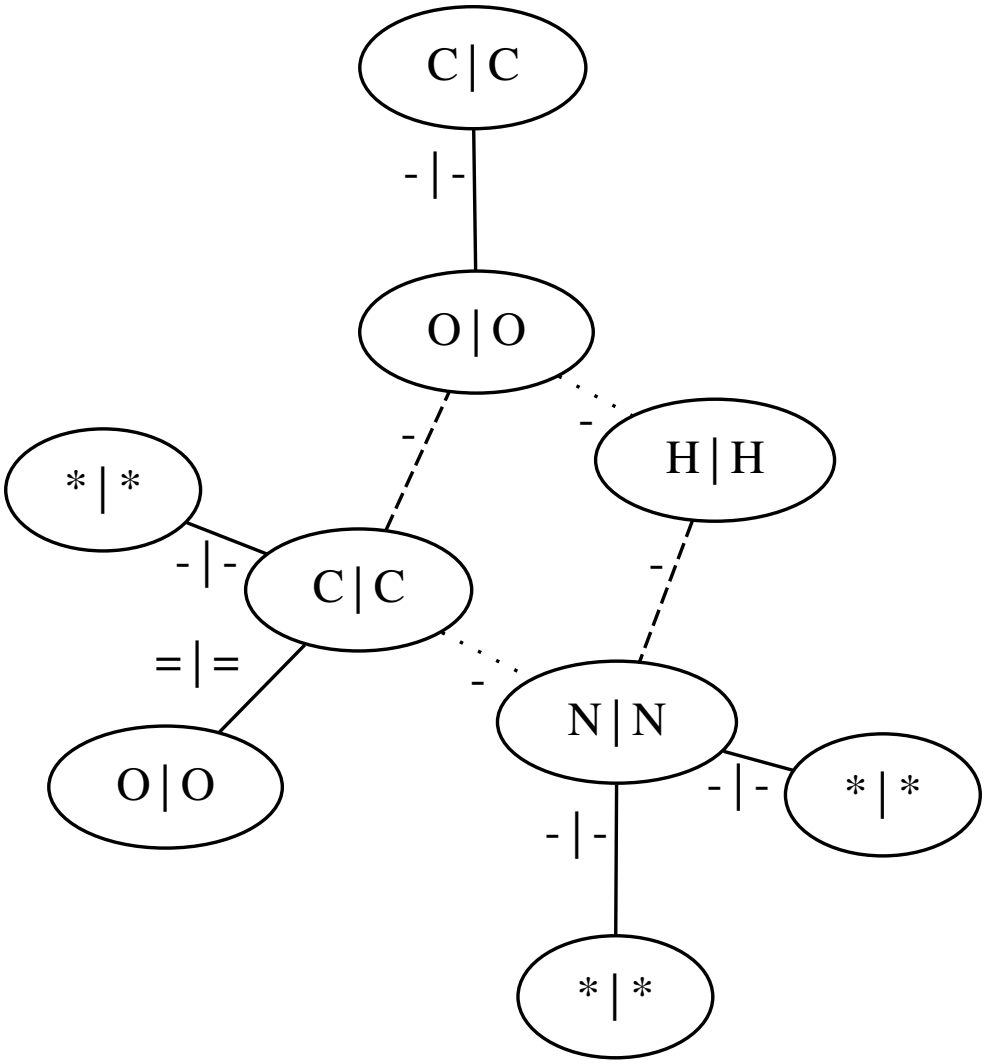
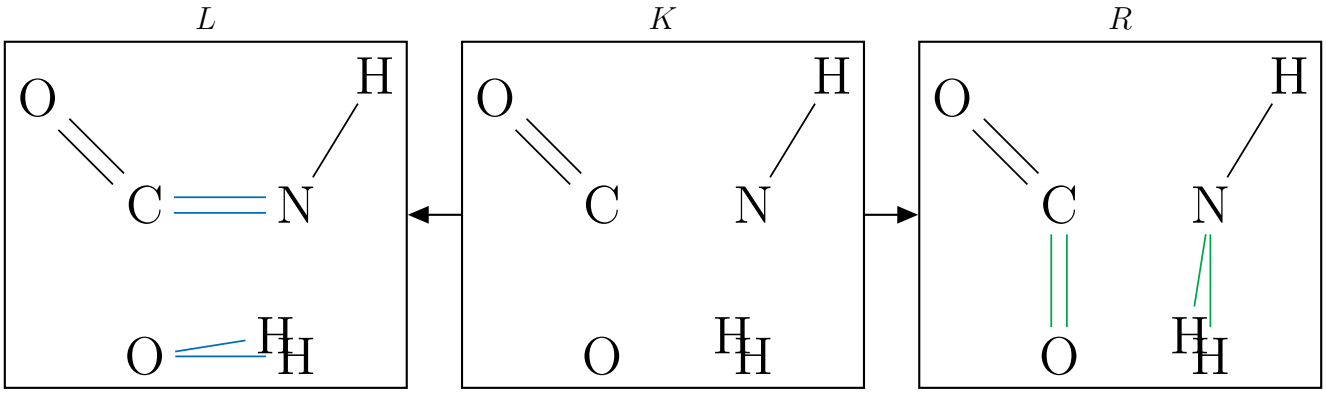


Files: out/382_r_76_11300100_{L, K, R}

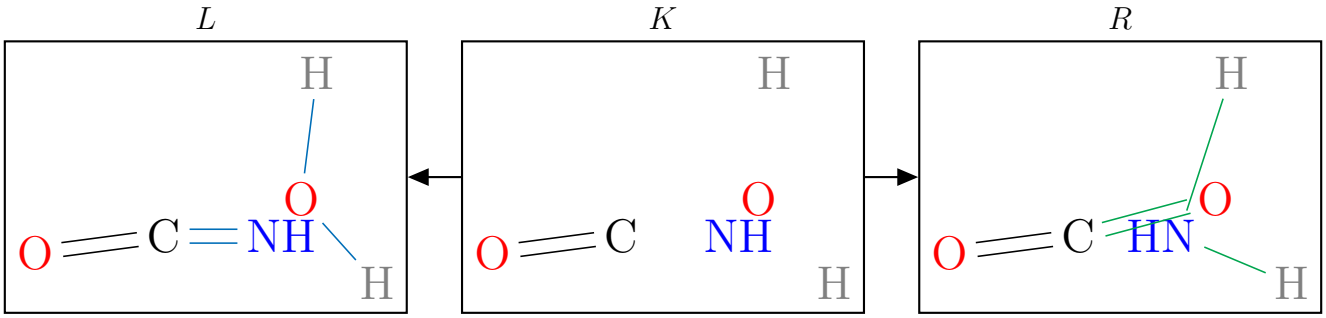


File: out/383_r_76_combined

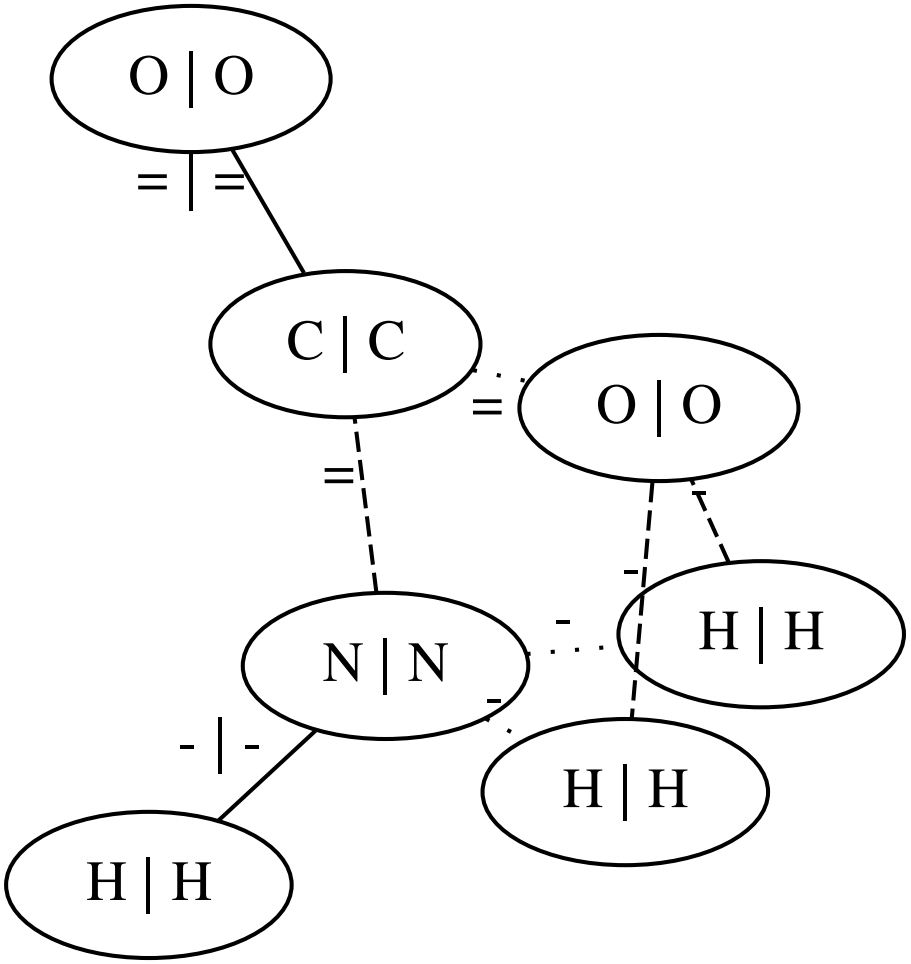
0.0.78 Isocyanate Hydrolysis



Files: out/386_r_77_10300000_{L, K, R}

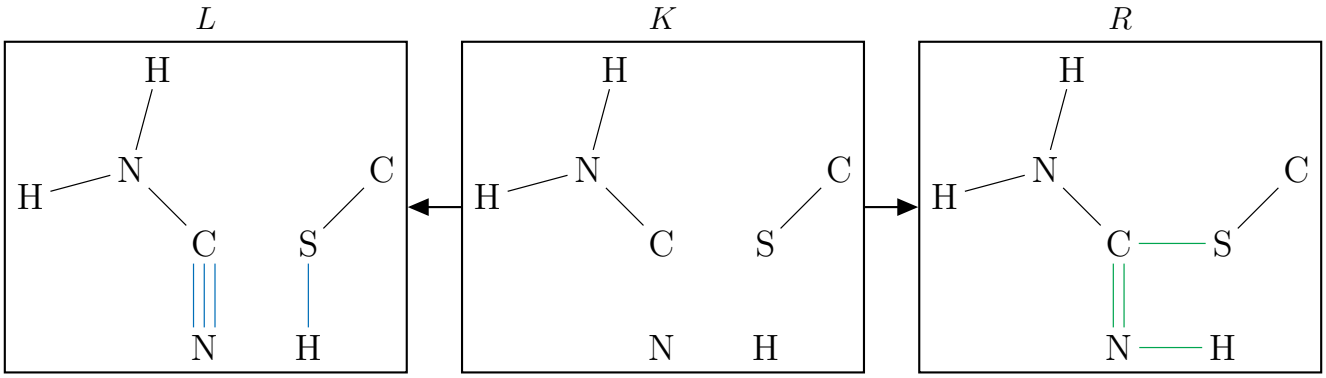


Files: out/387_r_77_11300100_{L, K, R}

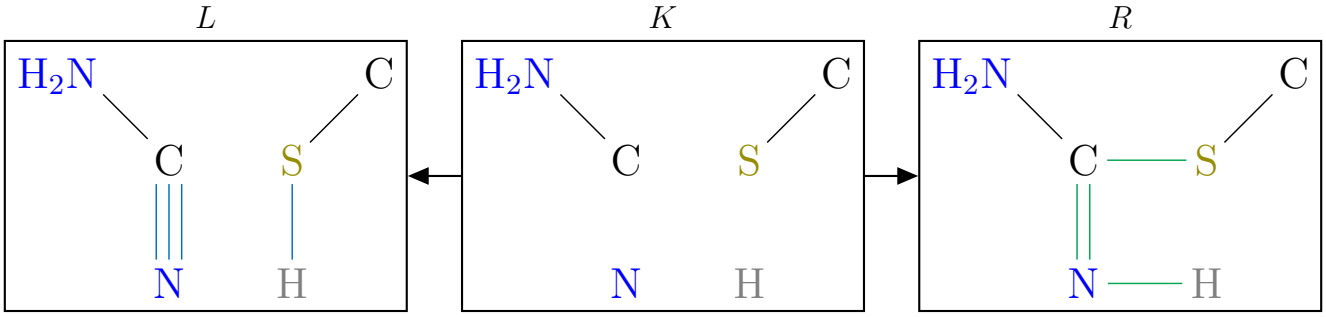


File: out/388_r_77_combined

0.0.79 Cyanamidation, SC



Files: out/391_r_78_10300000_{L, K, R}



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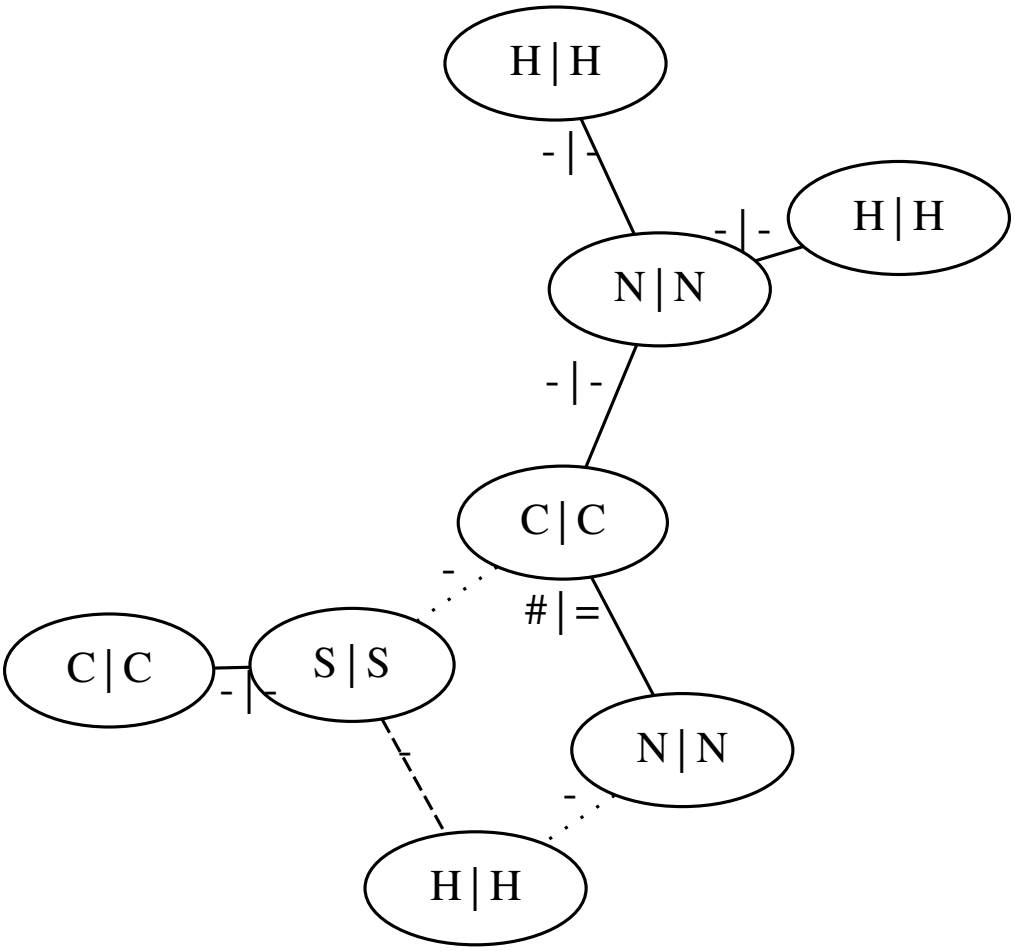
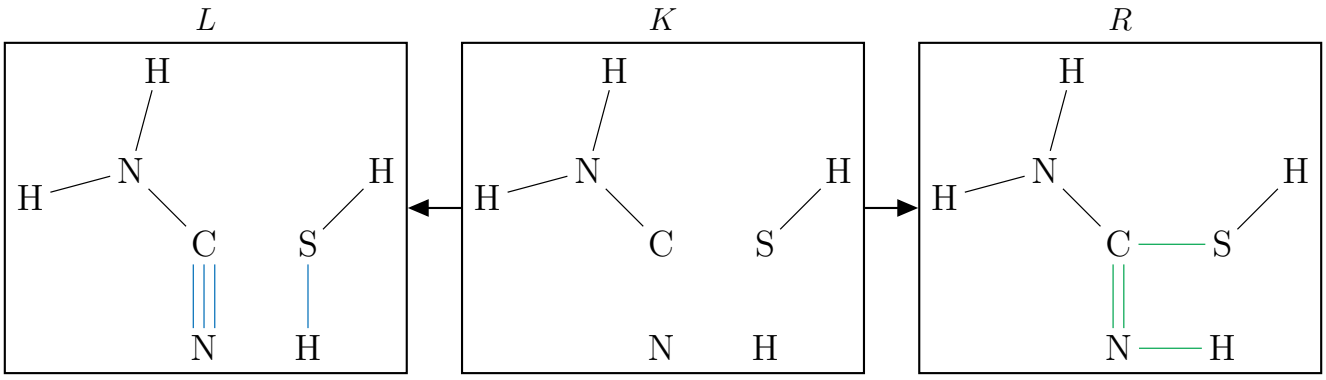
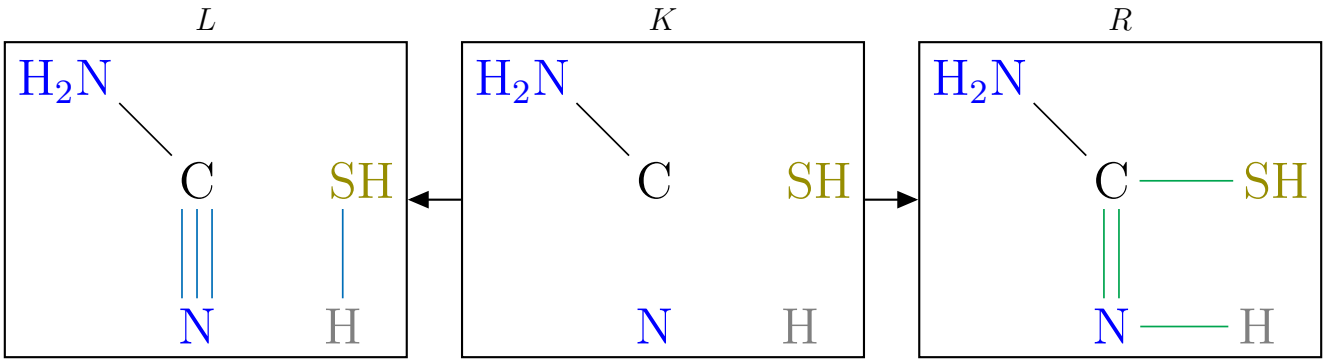


File: out/393_r_78_combined

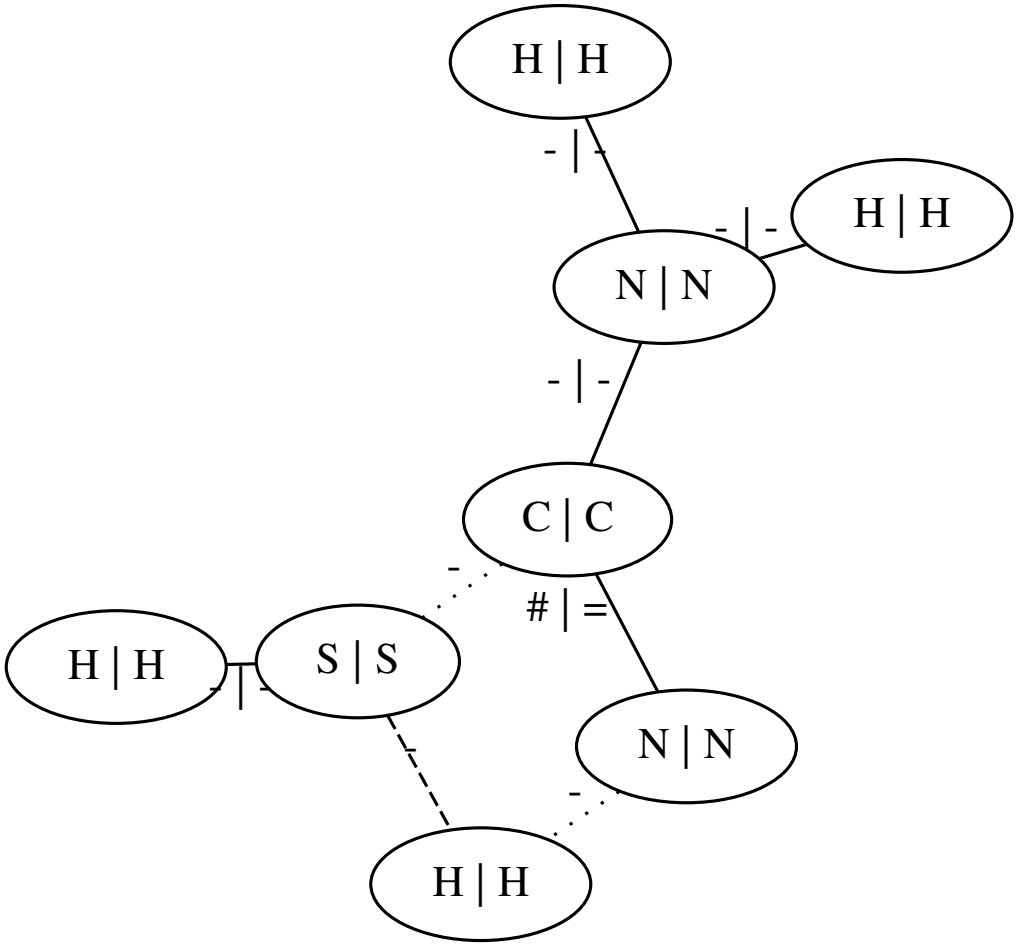
0.0.80 Cyanamidation, SH



Files: out/396_r_79_10300000_{L, K, R}

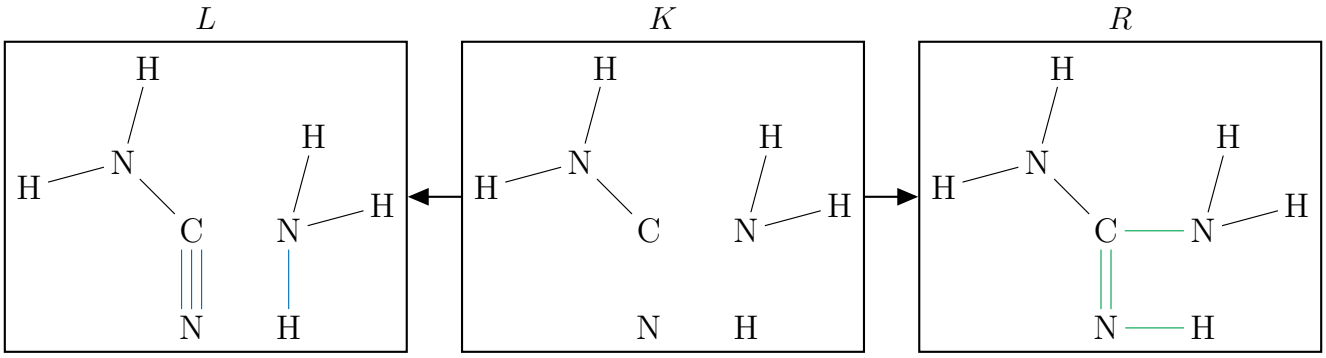


Files: out/397_r_79_11300100_{L, K, R}

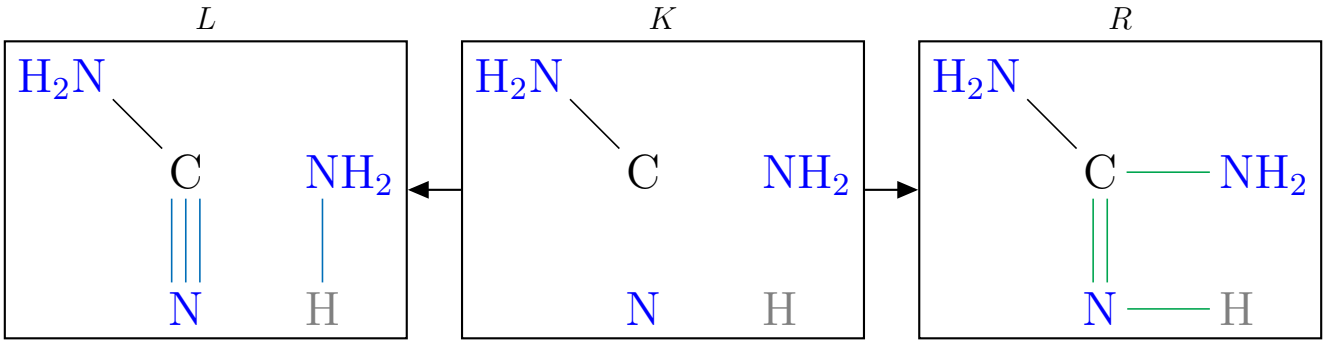


File: out/398_r_79_combined

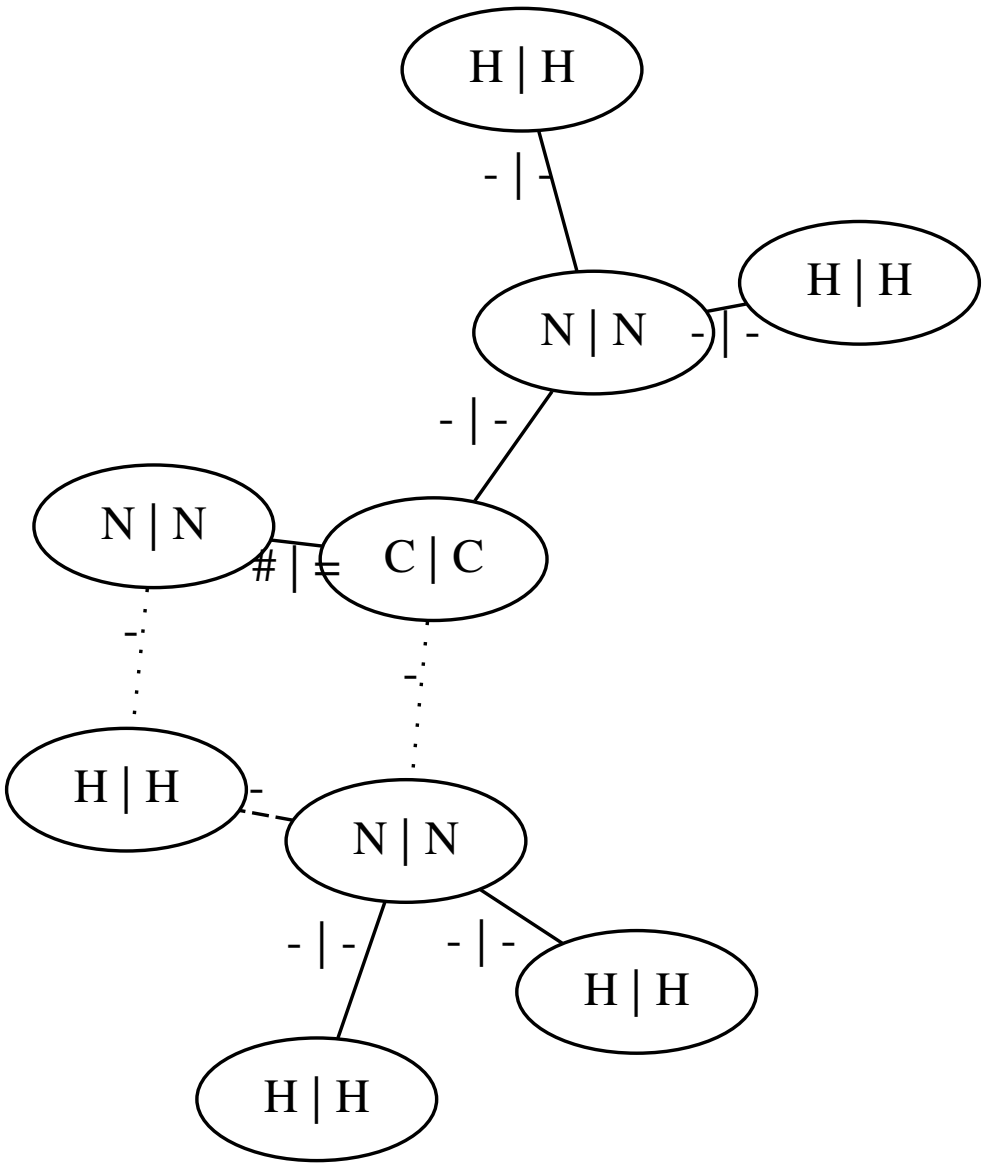
0.0.81 Cyanamidation, N, HH



Files: out/401_r_80_10300000_{L, K, R}

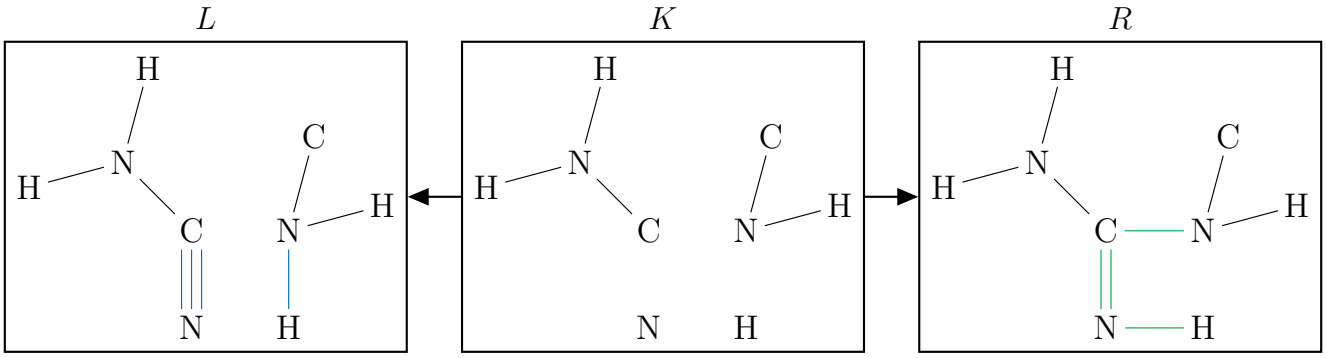


Files: out/402_r_80_11300100_{L, K, R}

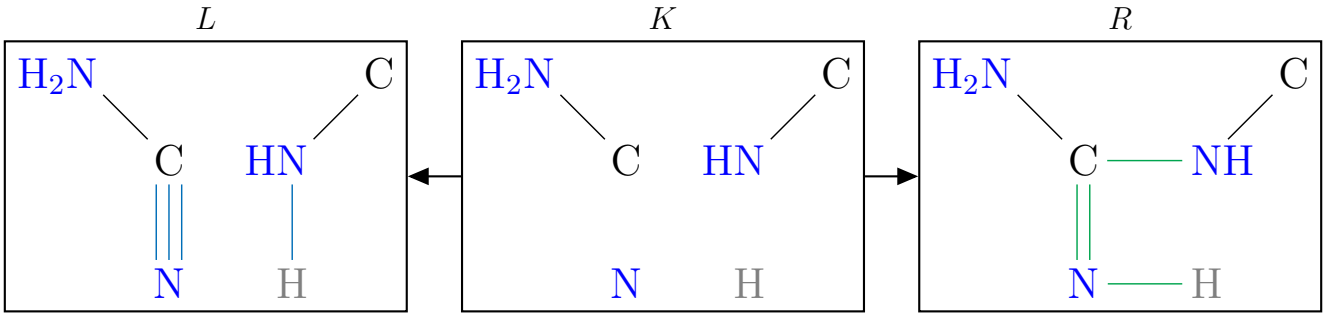


File: out/403_r_80_combined

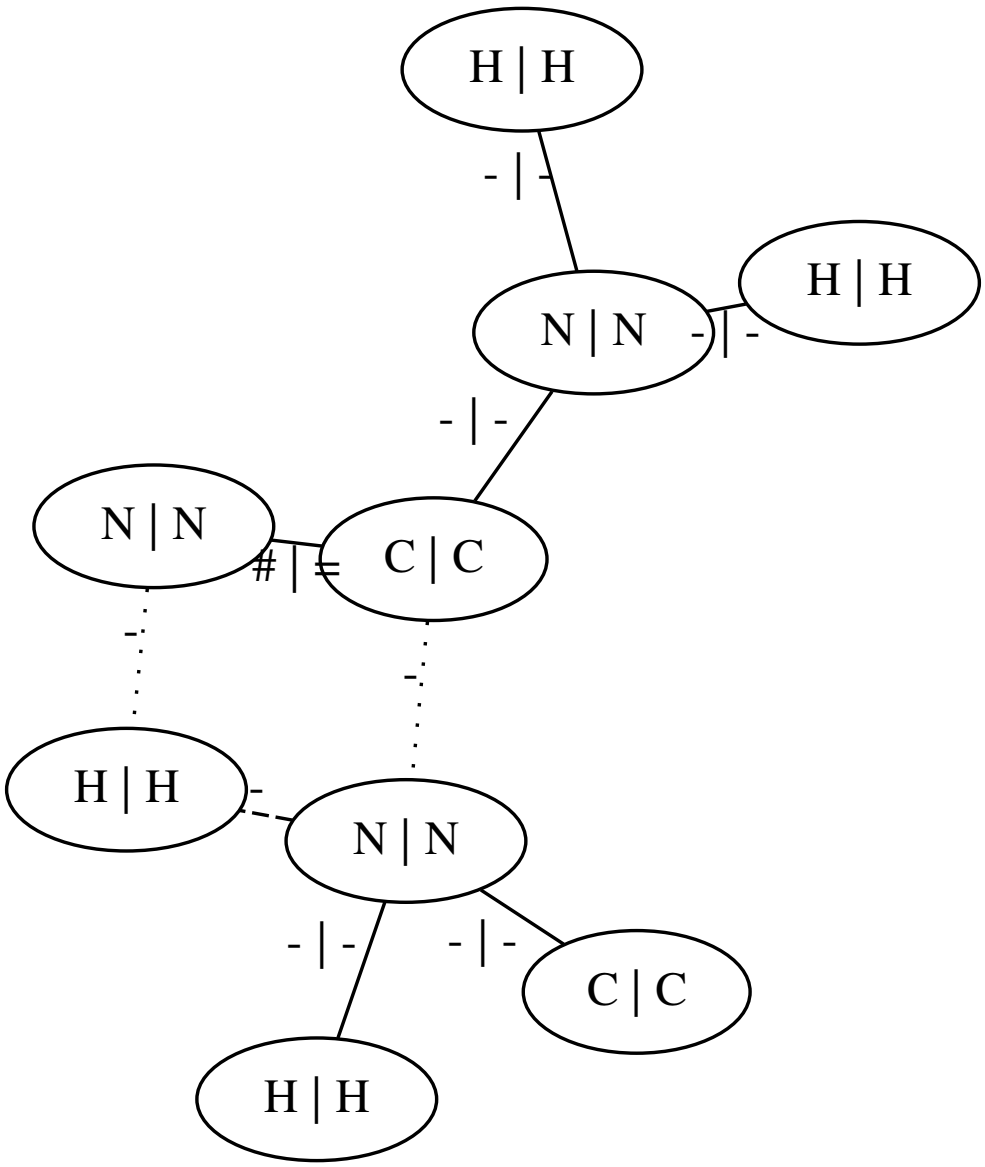
0.0.82 Cyanamidation, N, HC



Files: out/406_r_81_10300000_{L, K, R}



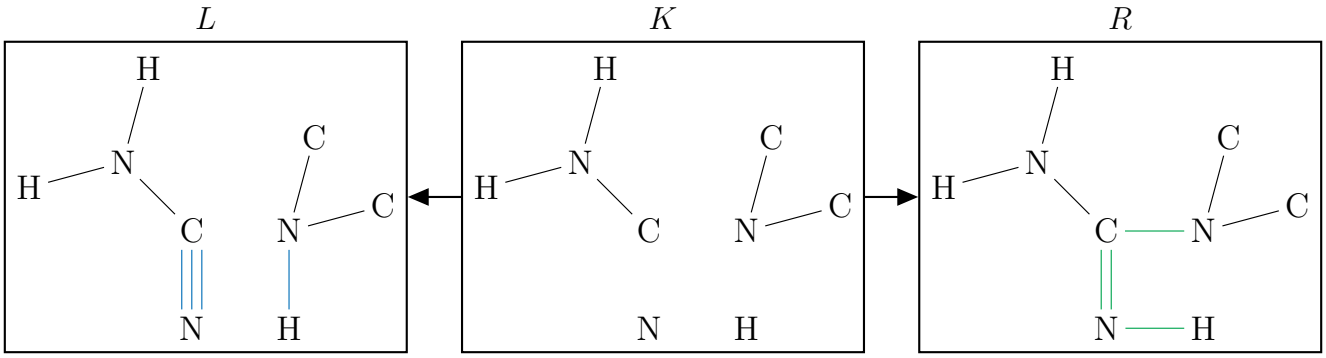
Files: out/407_r_81_11300100_{L, K, R}



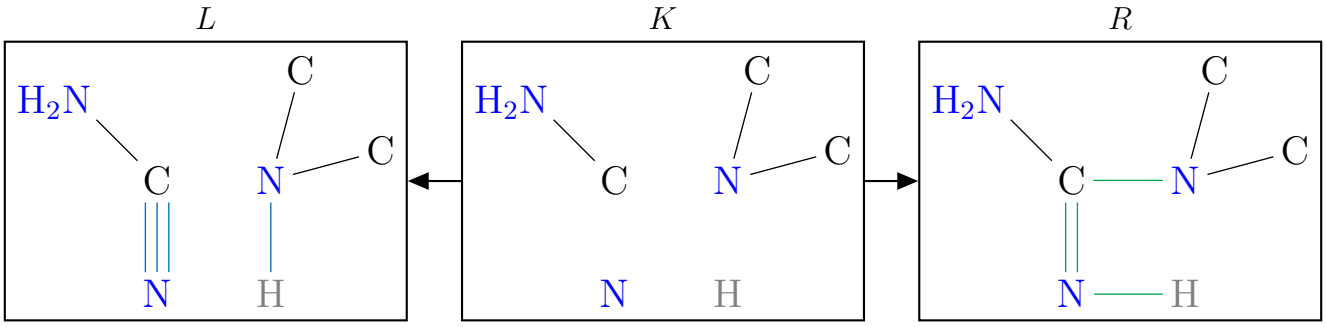
File: out/408_r_81_combined

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

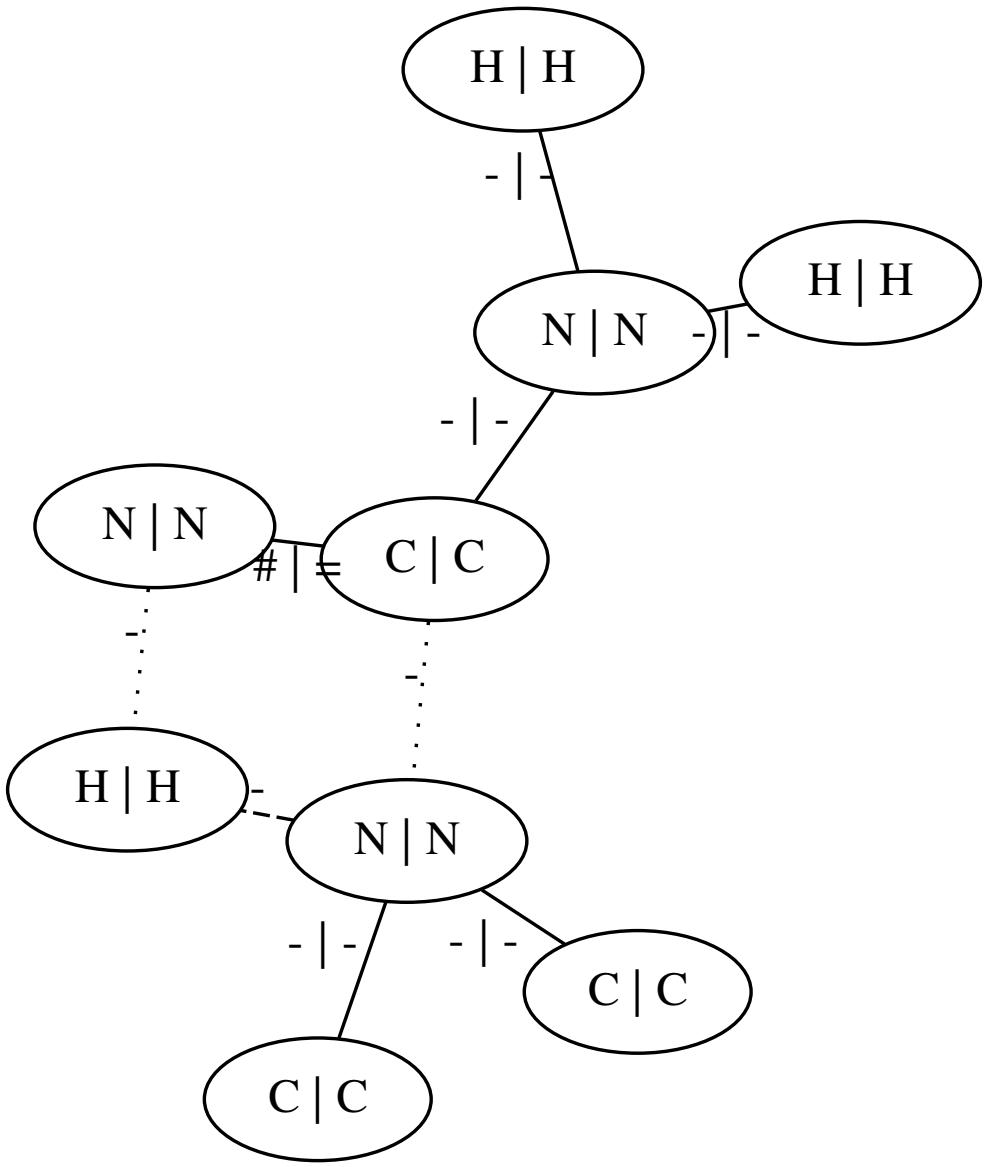
0.0.83 Cyanamidation, N, CC



Files: out/411_r_82_10300000_{L, K, R}



Files: out/412_r_82_11300100_{L, K, R}

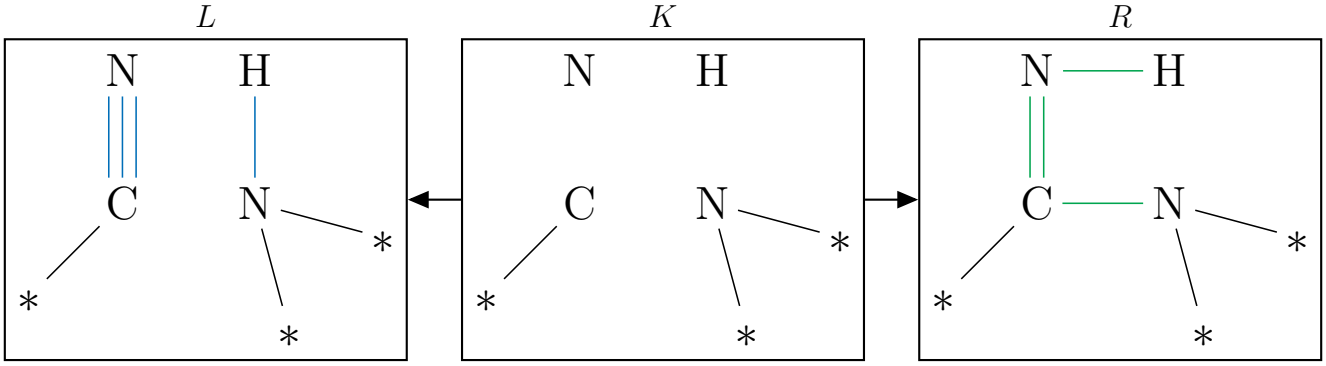


File: out/413_r_82_combined

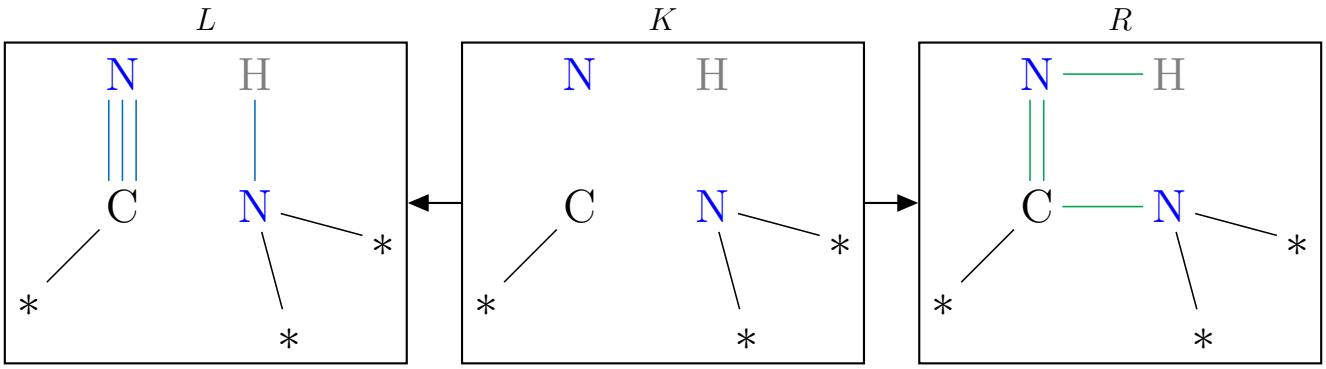
$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

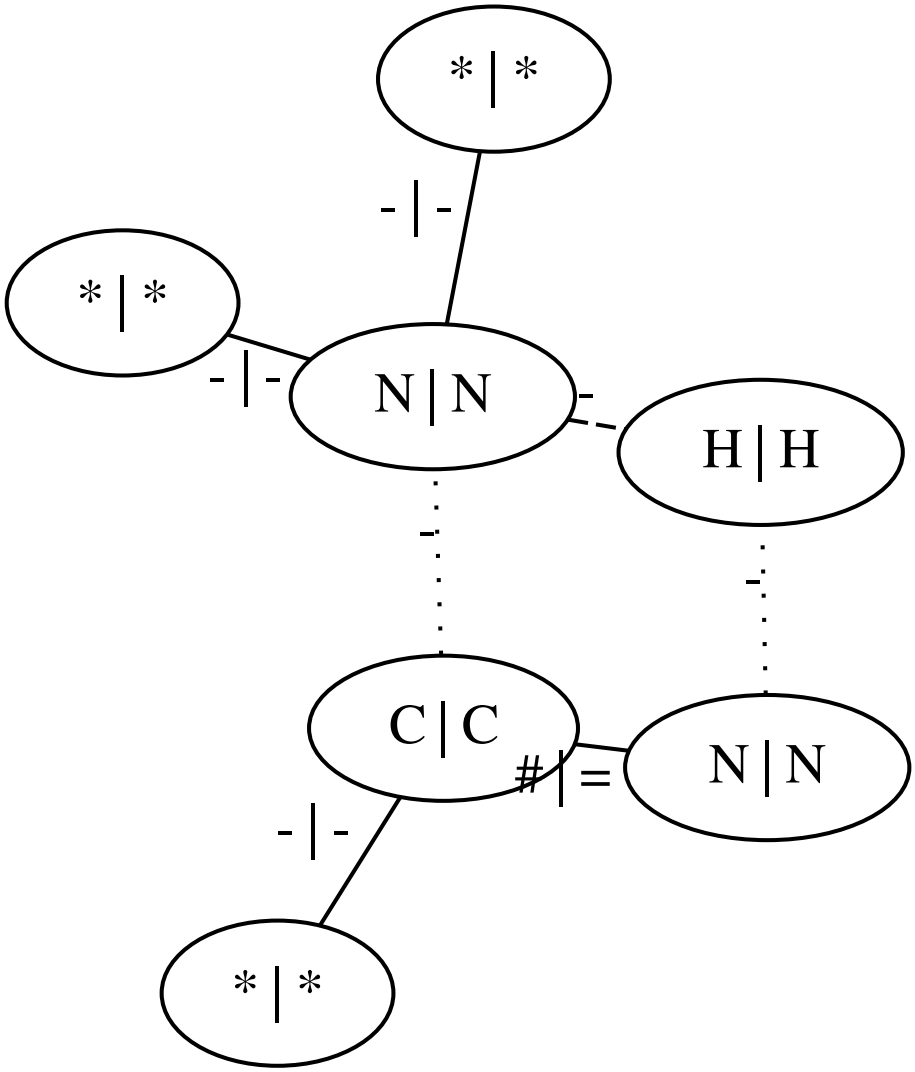
0.0.84 Nitrile Amination



Files: out/416_r_83_10300000_{L, K, R}



Files: out/417_r_83_11300100_{L, K, R}



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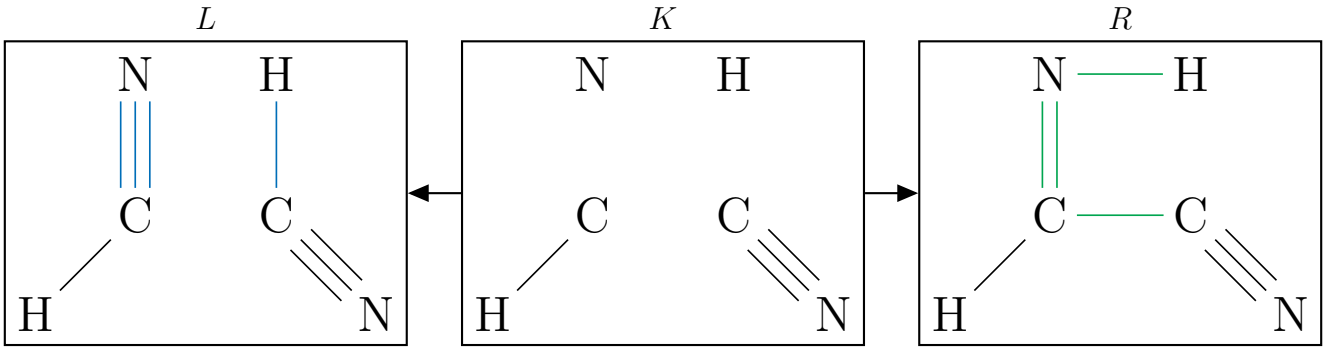
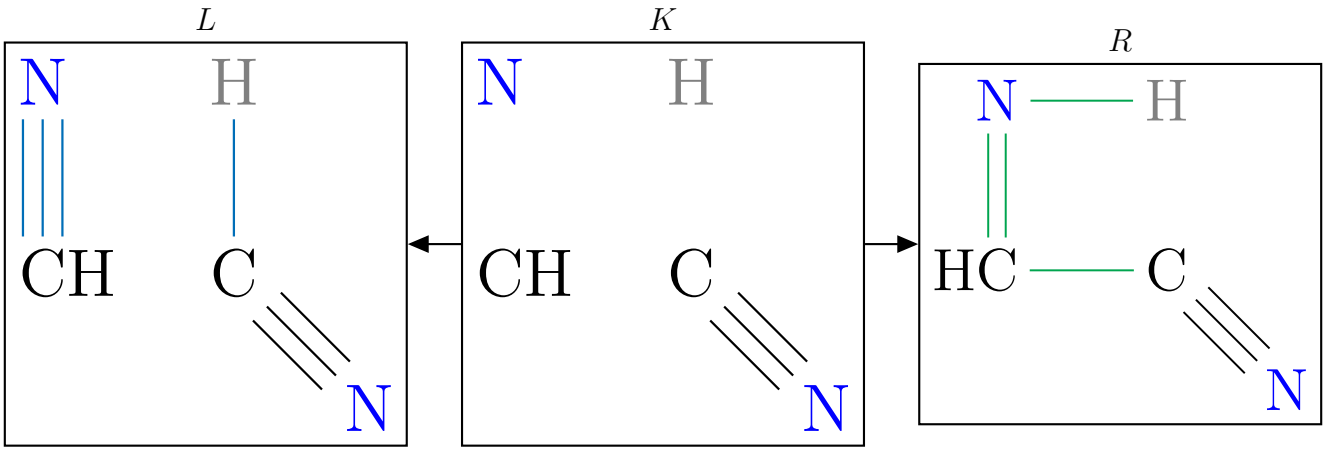
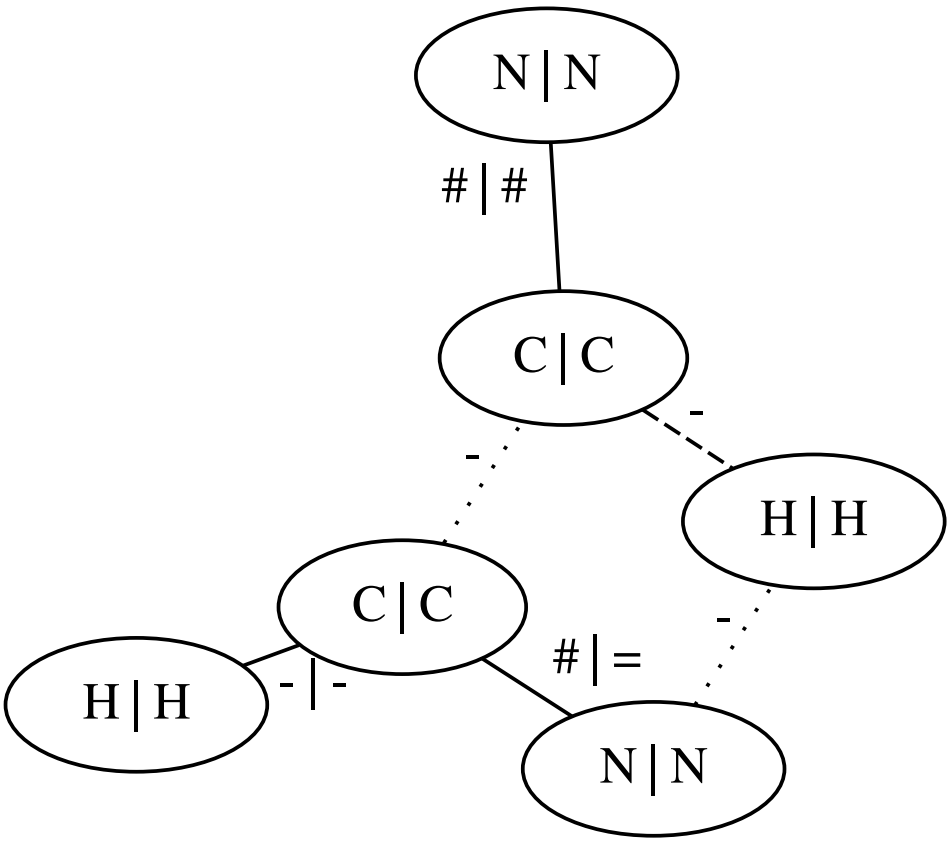
0.0.85 HCN Addition to Nitriles



Files: out/421_r_84_10300000_{L, K, R}

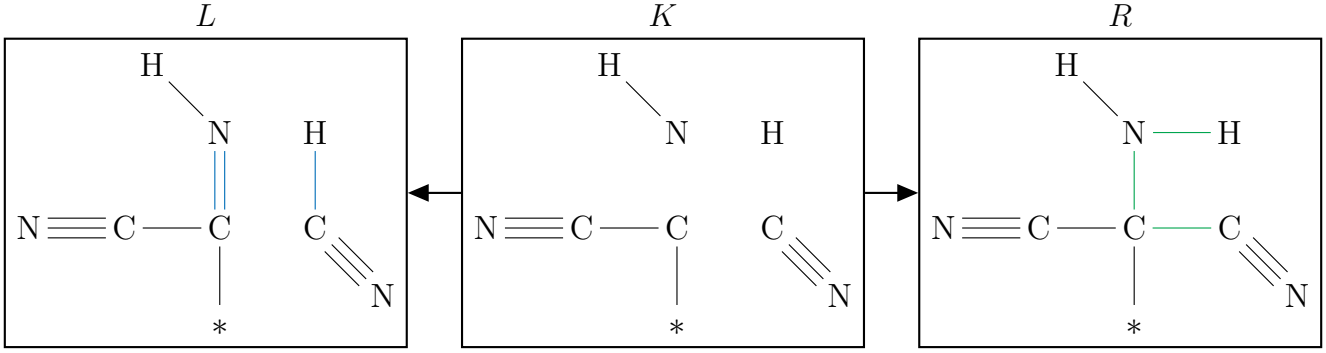


Files: out/422_r_84_11300100_{L, K, R}

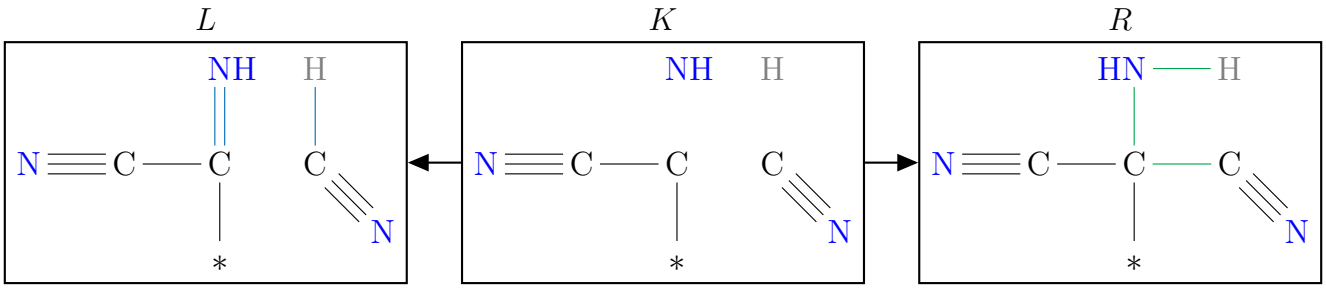


File: out/423_r_84_combined

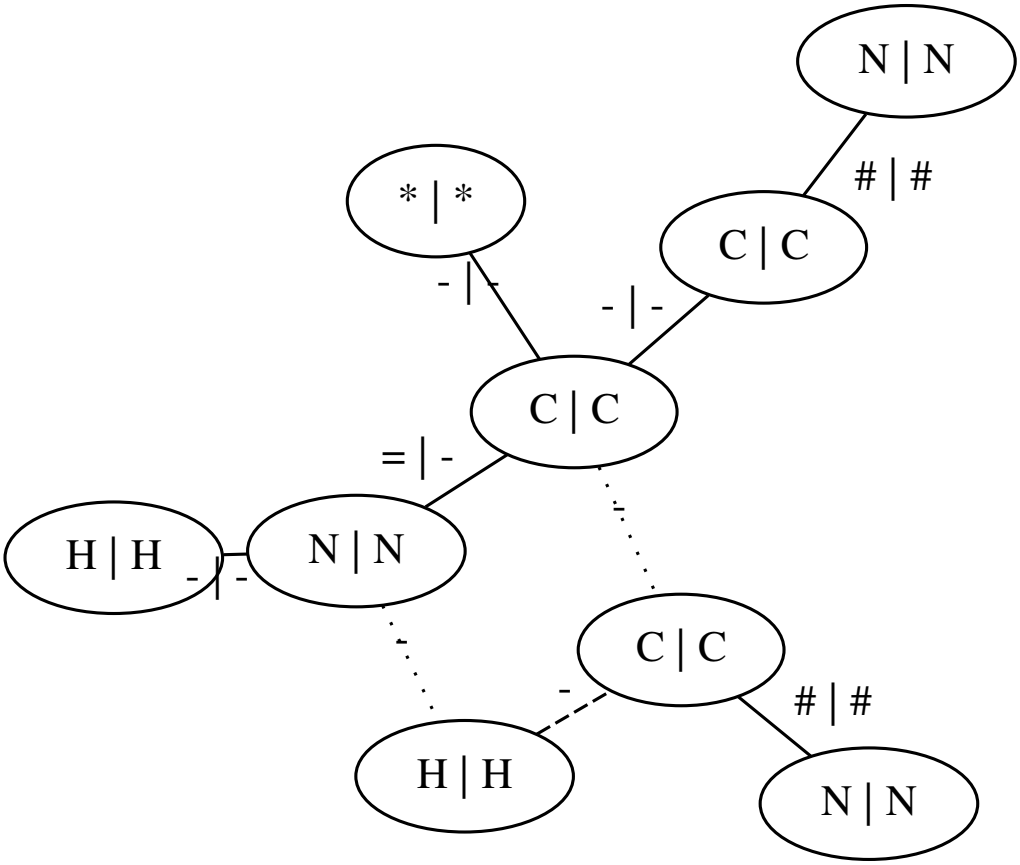
0.0.86 CN addition to iminonitriles



Files: out/426_r_86_10300000_{L, K, R}

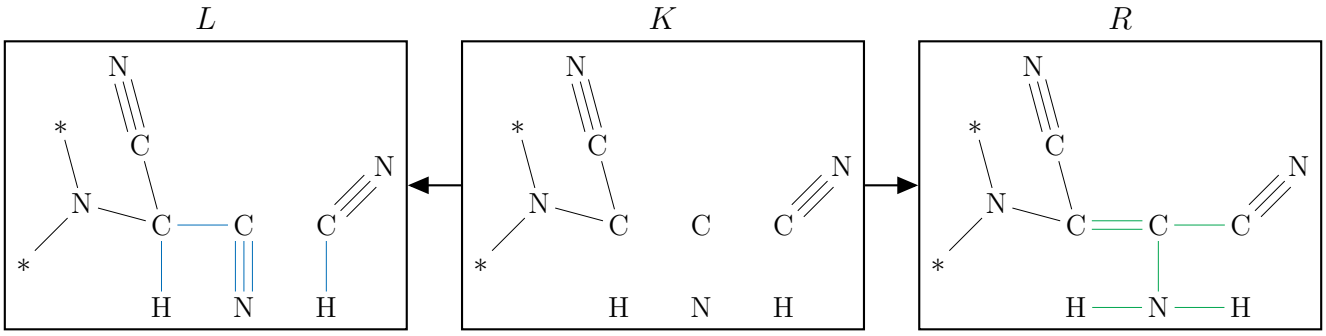


Files: out/427_r_86_11300100_{L, K, R}

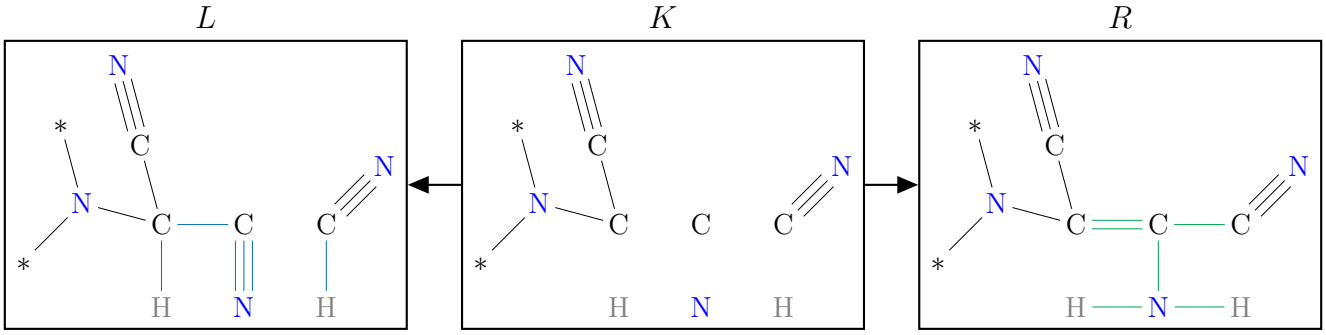


File: out/428_r_86_combined

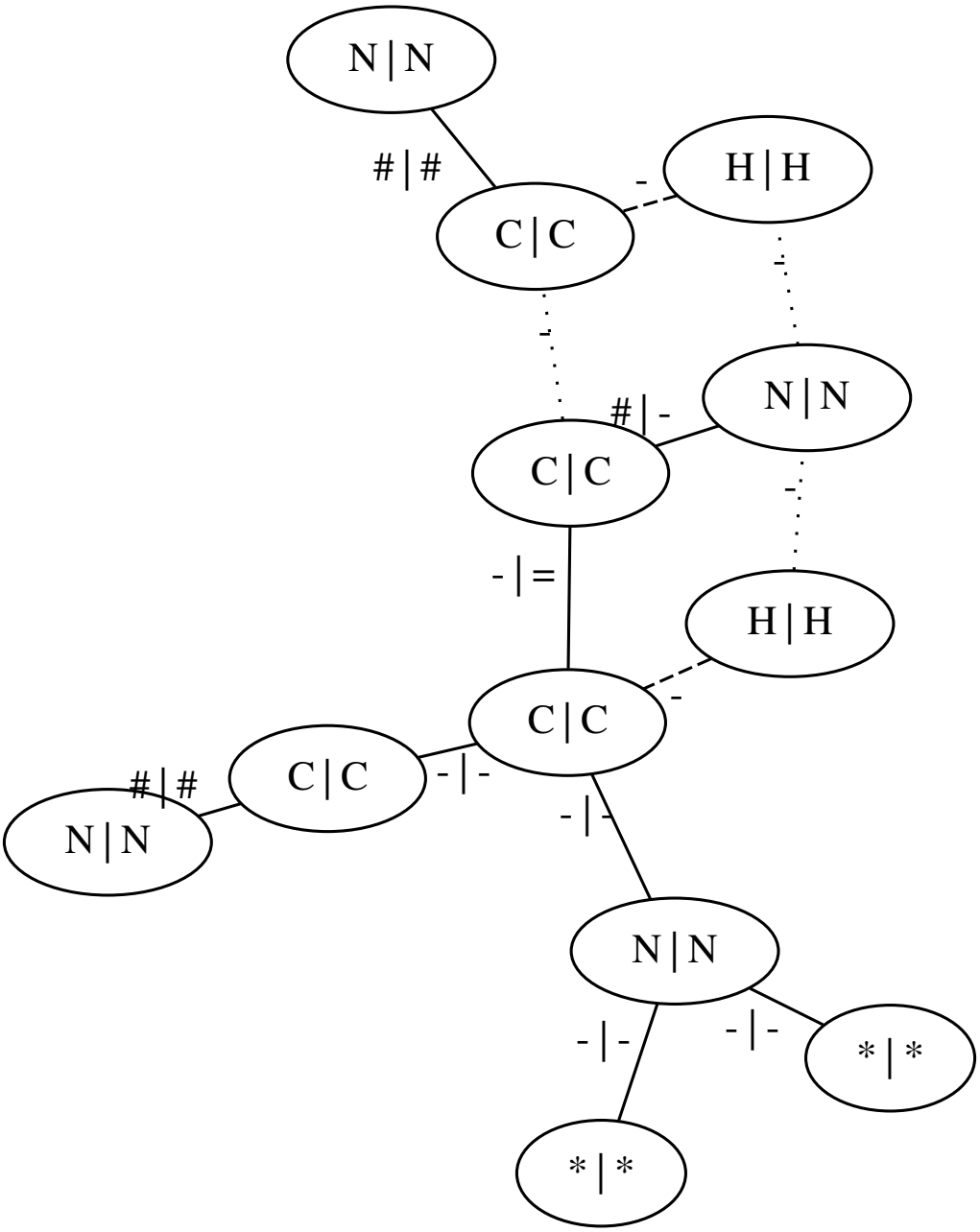
0.0.87 CN addition to aminodinitriles



Files: out/431_r_88_10300000_{L, K, R}

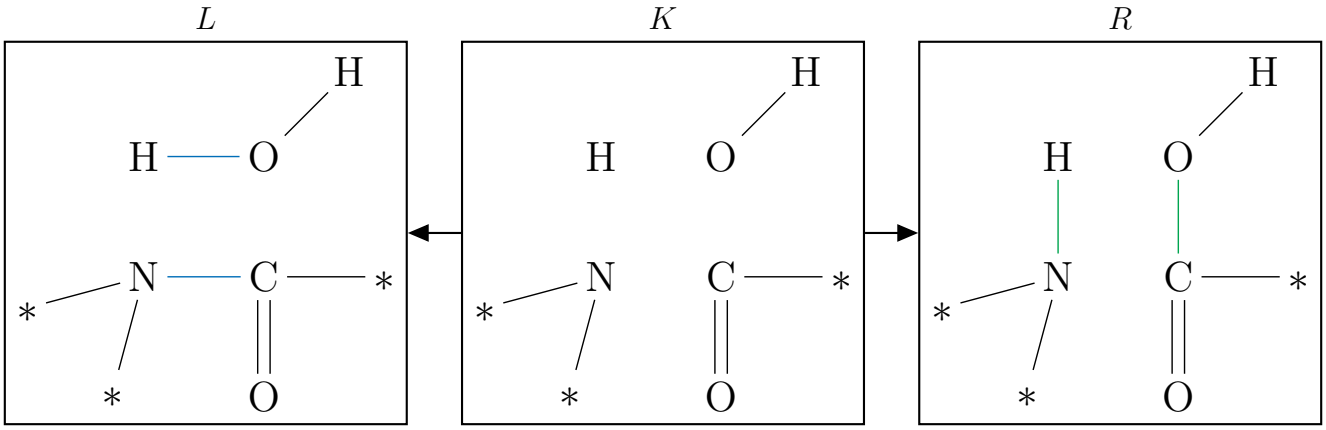


Files: out/432_r_88_11300100_{L, K, R}

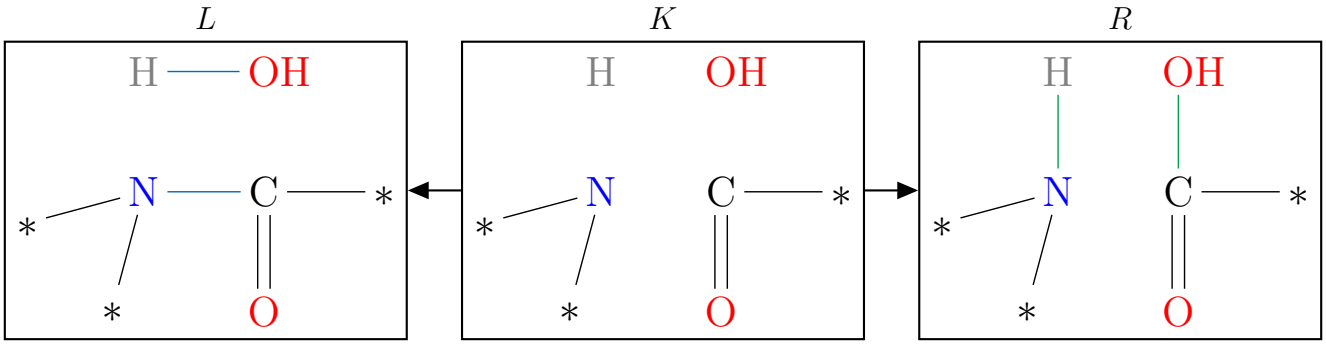


File: out/433_r_88_combined

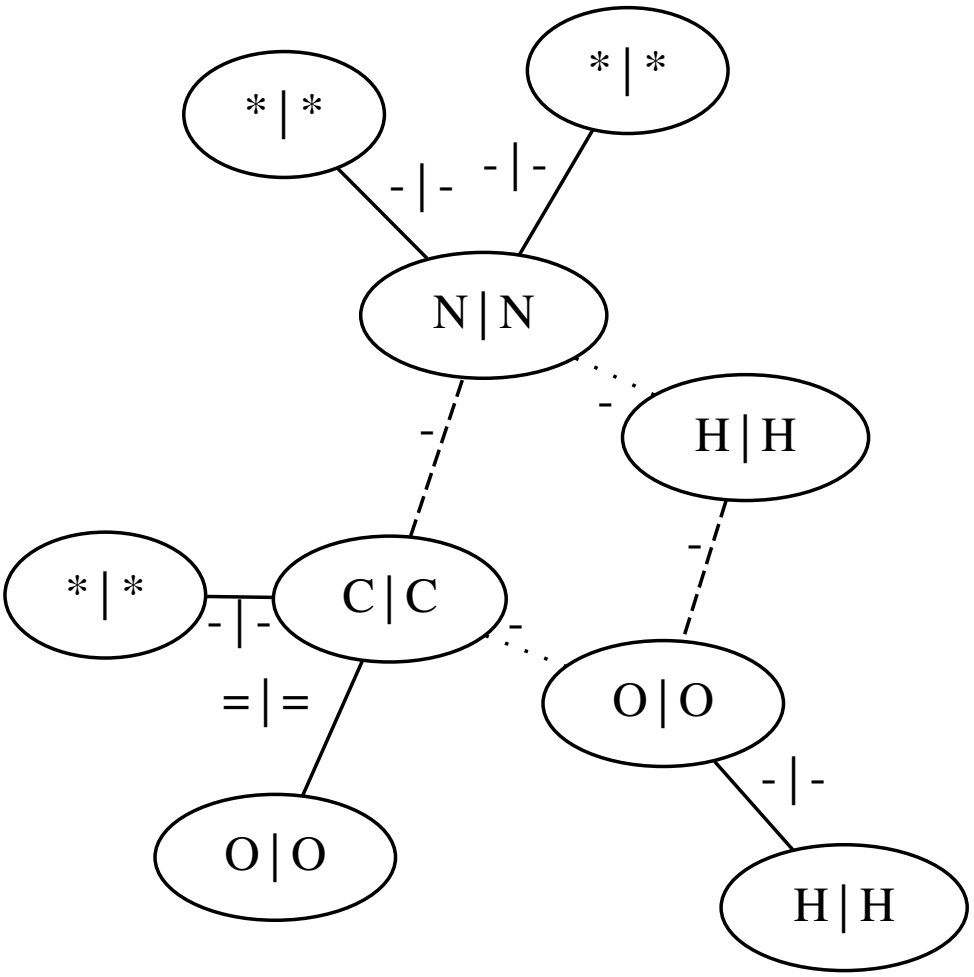
0.0.88 Amide Hydrolysis



Files: out/436_r_90_10300000_{L, K, R}



Files: out/437_r_90_11300100_{L, K, R}



File: out/438_r_90_combined

$$
\begin{aligned}
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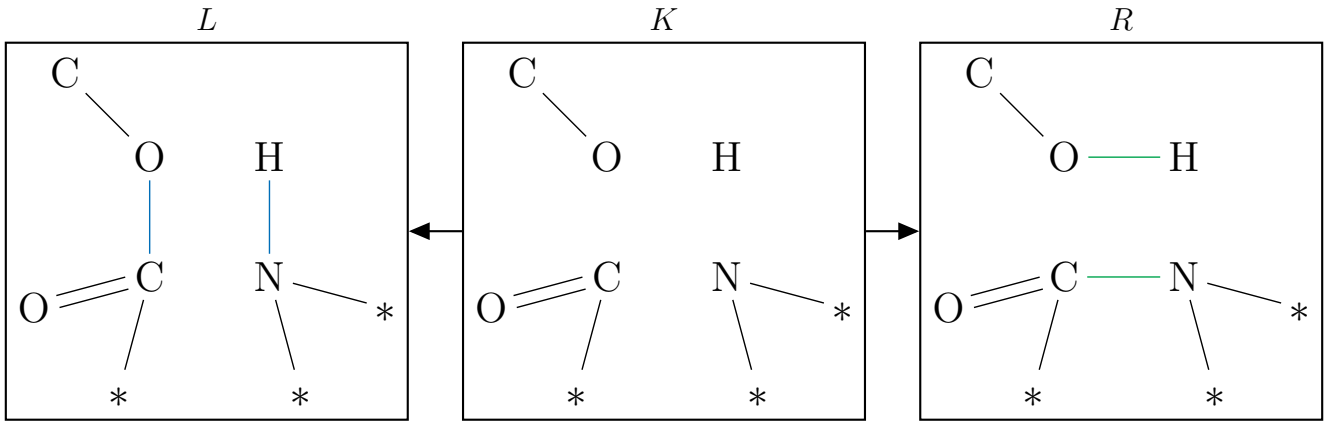
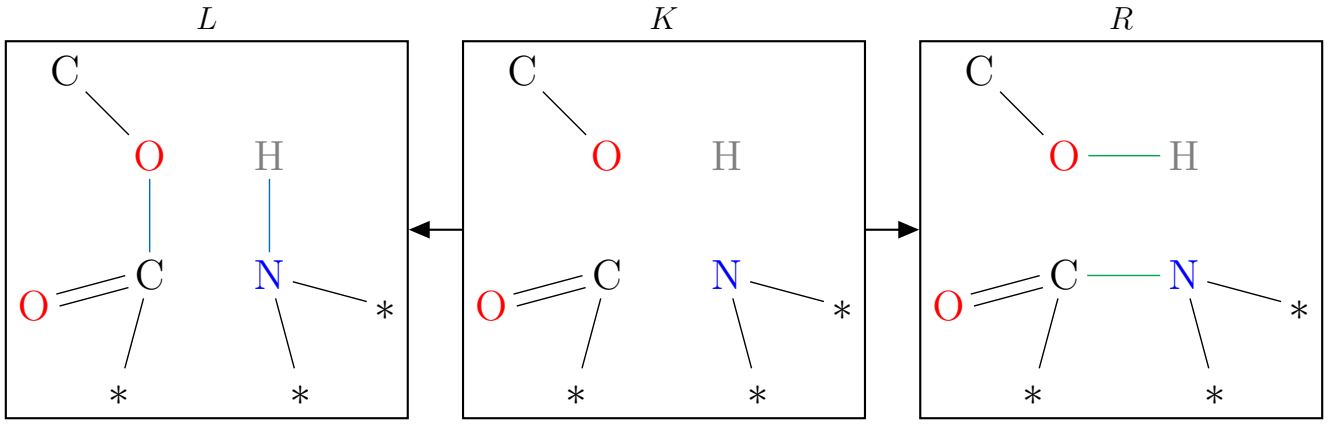
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

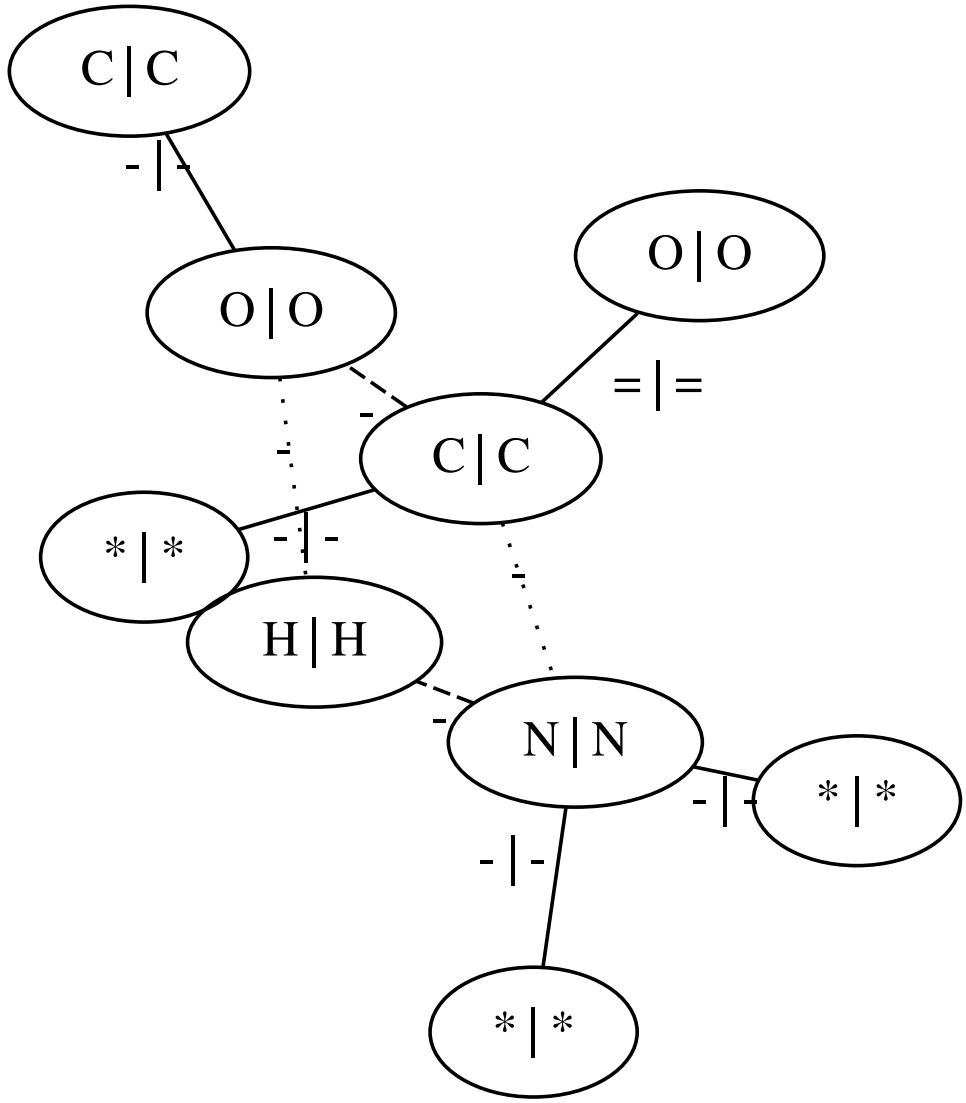
0.0.89 Amide Formation Hydrolysis, C



Files: out/441_r_91_10300000_{L, K, R}



Files: out/442_r_91_11300100_{L, K, R}

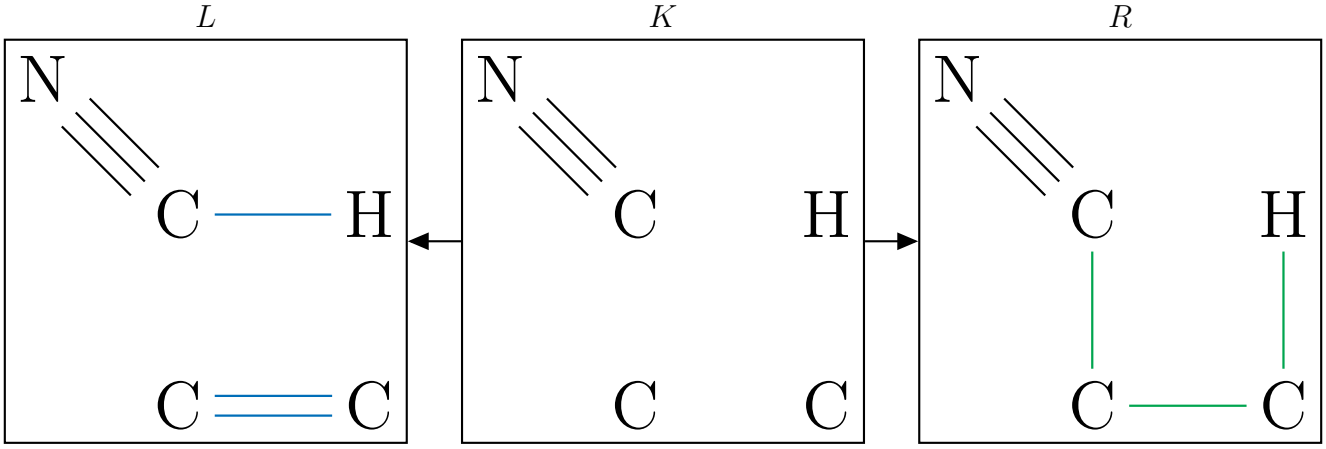


File: out/443_r_91_combined

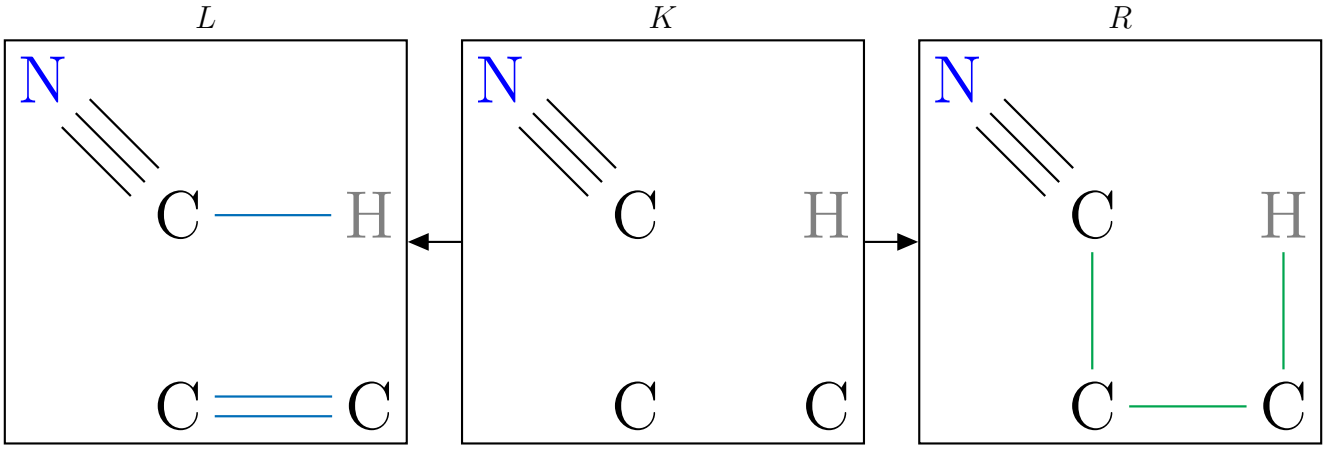
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

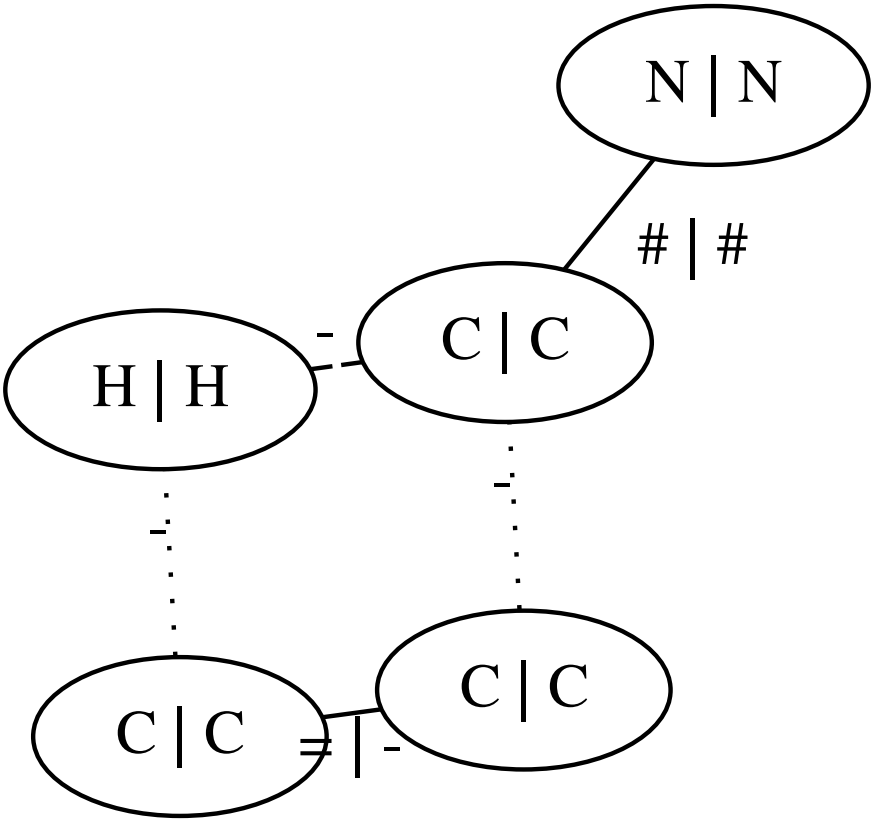
0.0.90 Alkene Addition, CN



Files: out/446_r_92_10300000_{L, K, R}

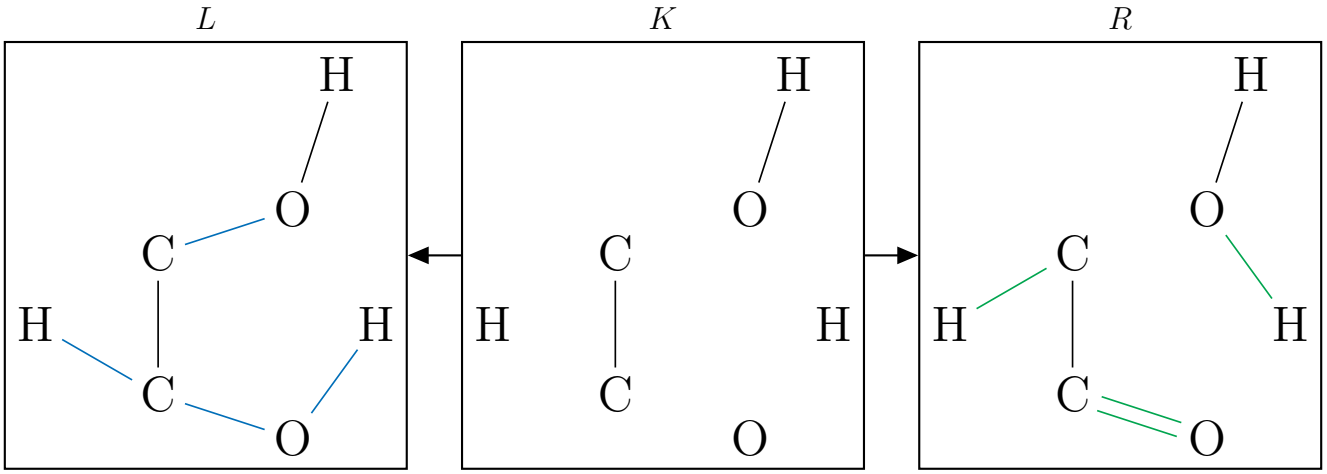


Files: out/447_r_92_11300100_{L, K, R}

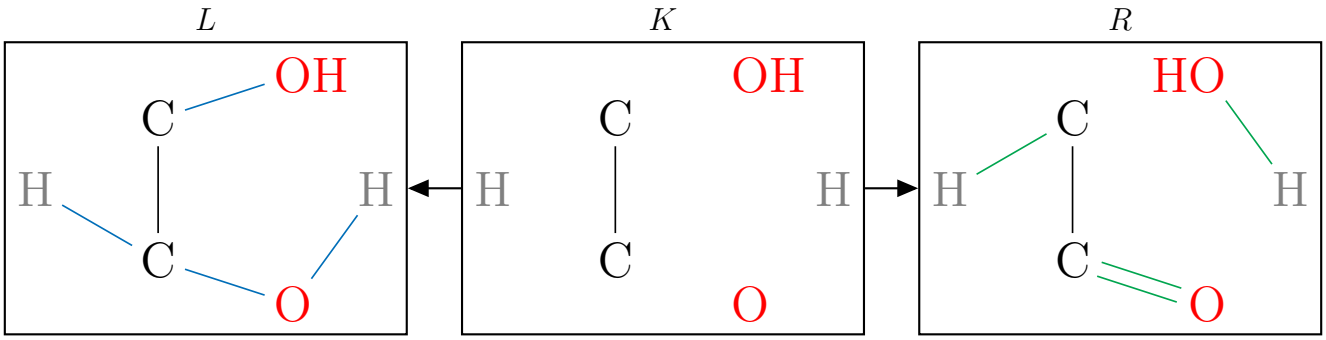


File: out/448_r_92_combined

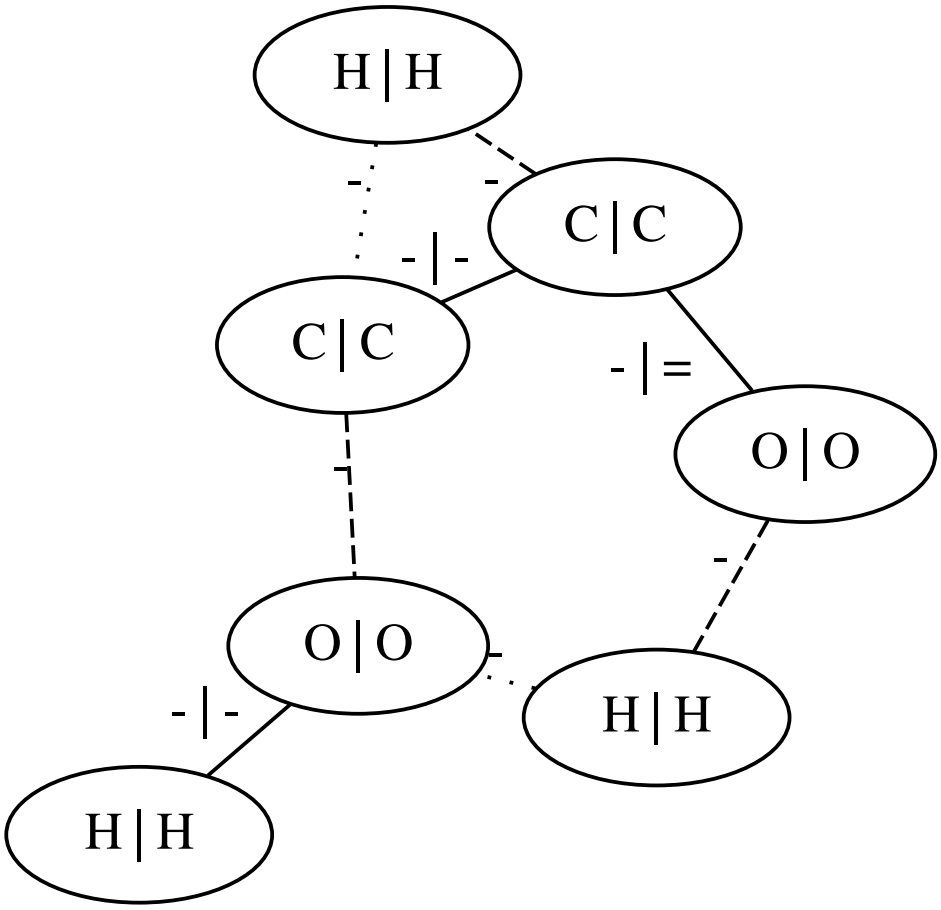
0.0.91 Elimination + enol to keto



Files: out/451_r_93_10300000_{L, K, R}



Files: out/452_r_93_11300100_{L, K, R}



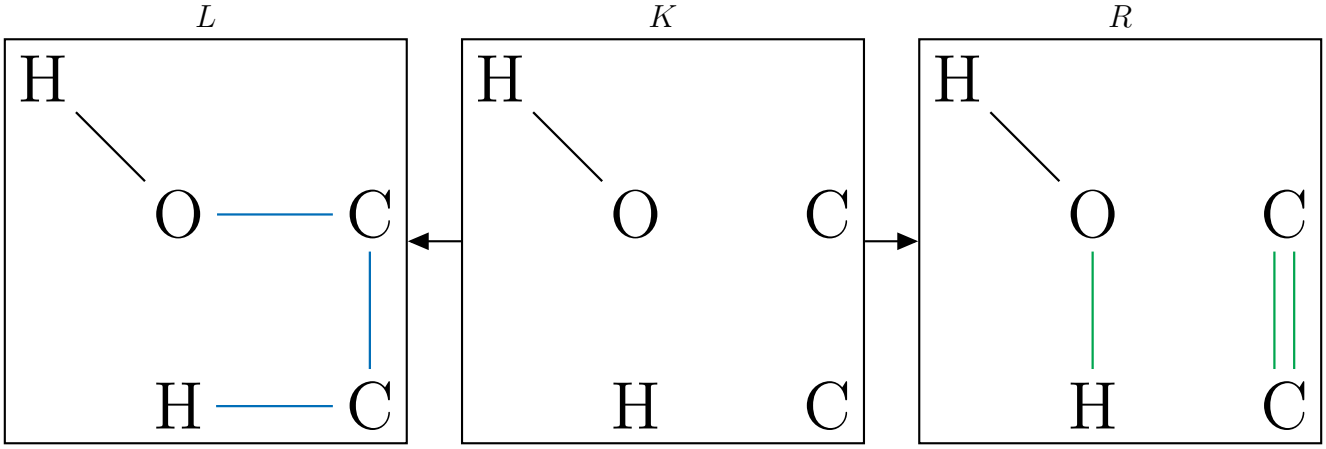
File: out/453_r_93_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

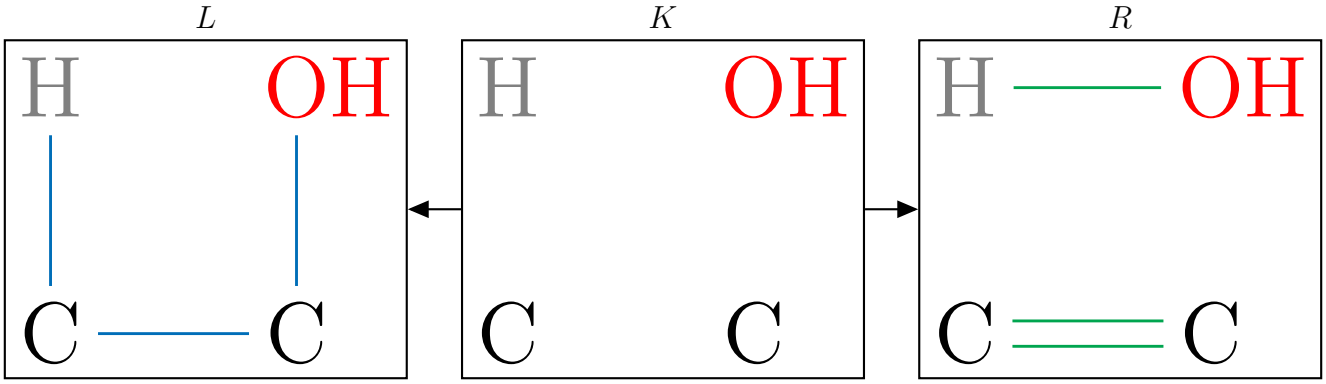
$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

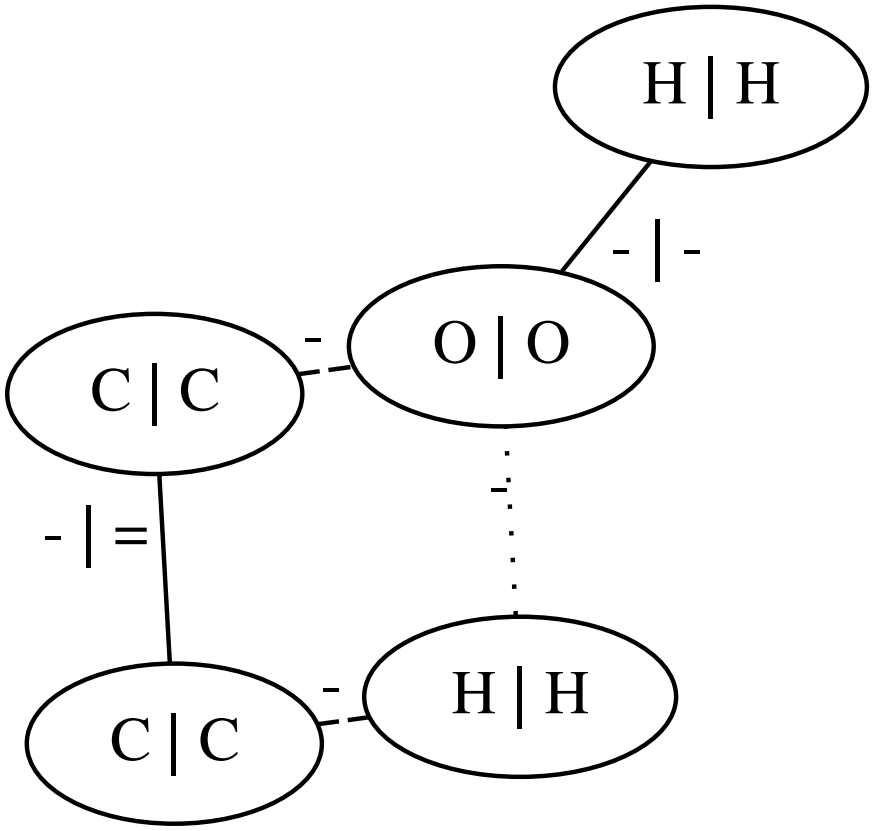
0.0.92 Elimination2



Files: out/456_r_94_10300000_{L, K, R}



Files: out/457_r_94_11300100_{L, K, R}



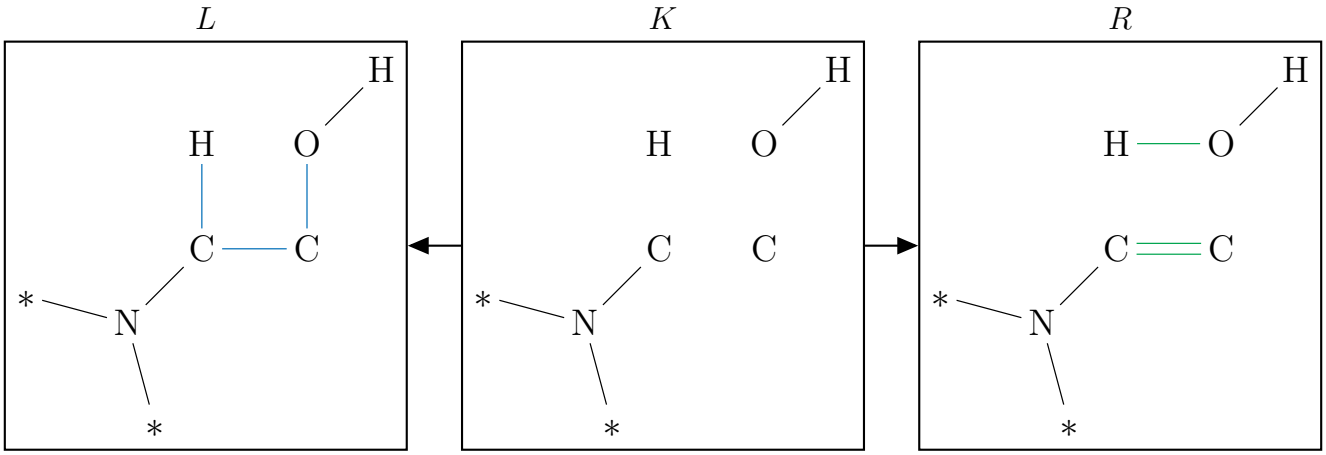
File: out/458_r_94_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

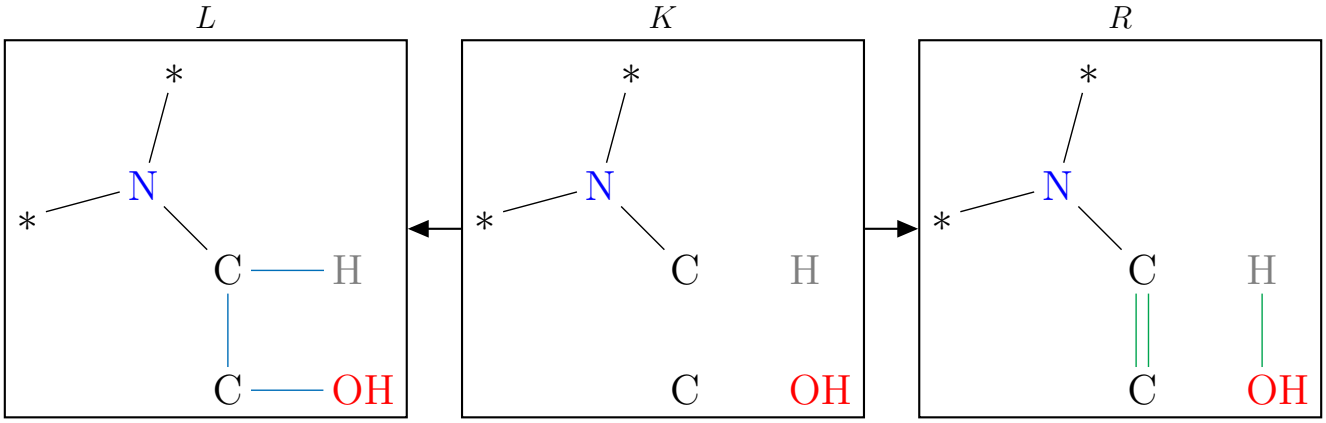
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

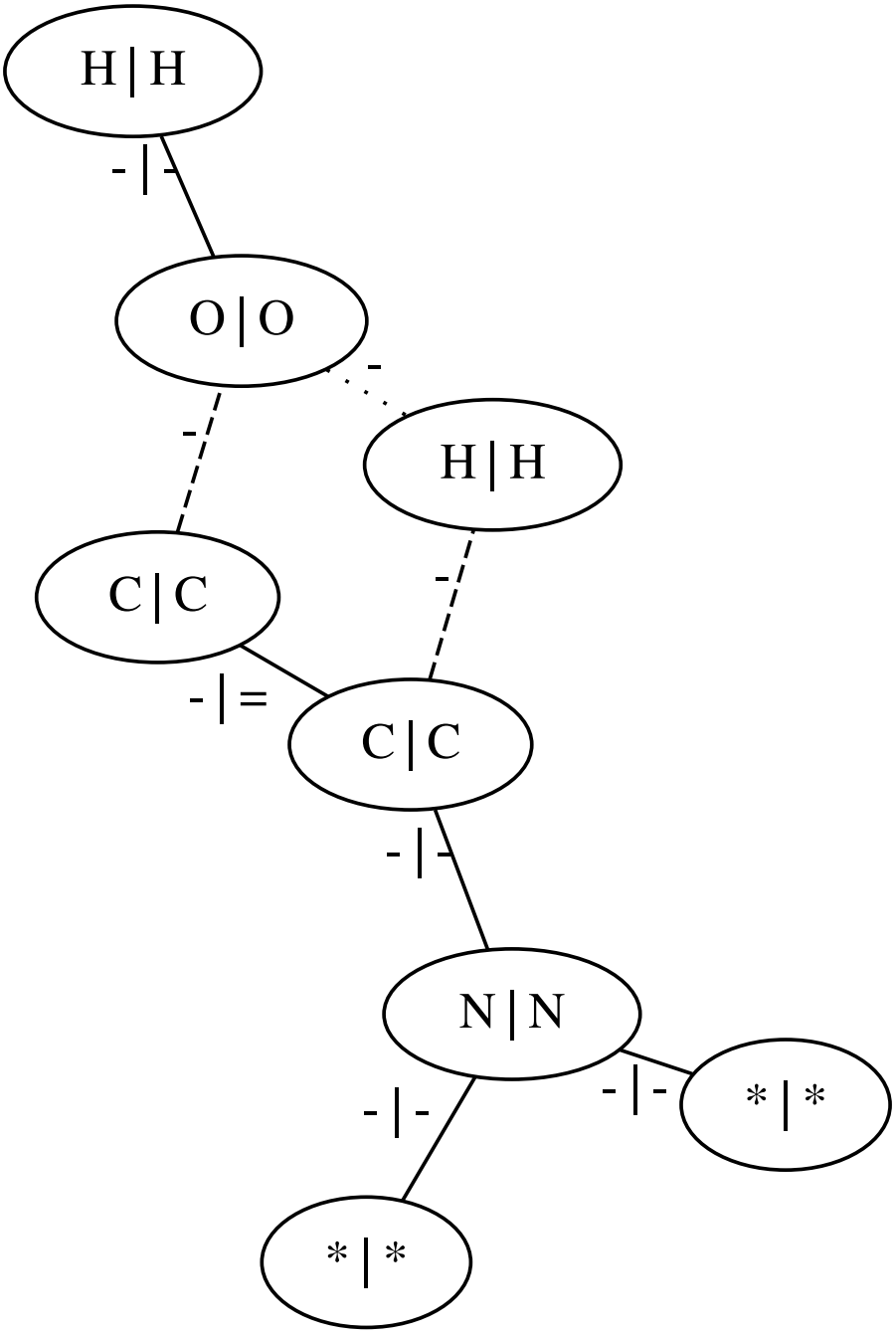
0.0.93 Dehydration of Amines



Files: out/461_r_95_10300000_{L, K, R}



Files: out/462_r_95_11300100_{L, K, R}

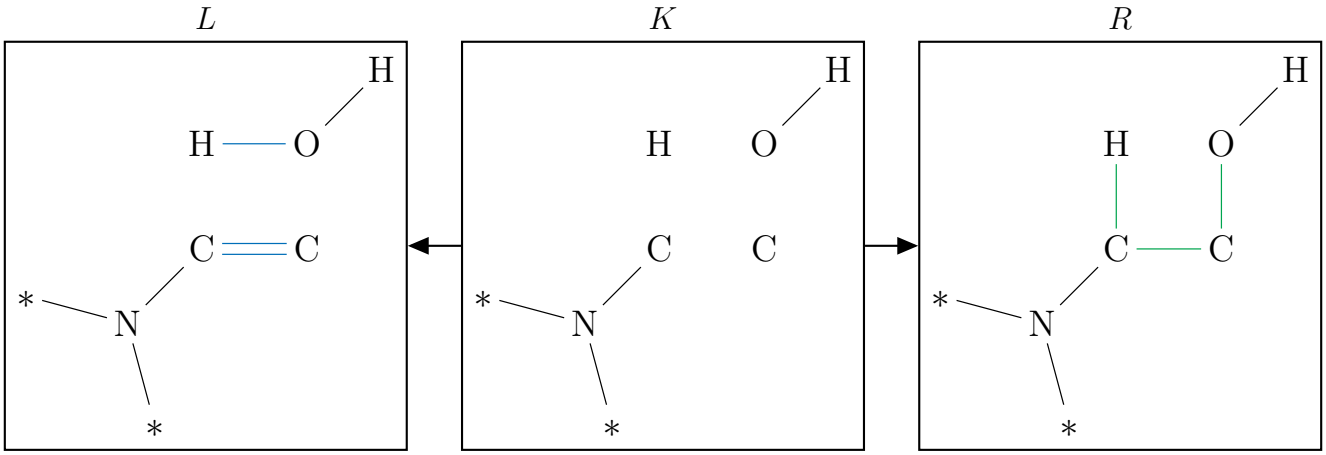


File: out/463_r_95_combined

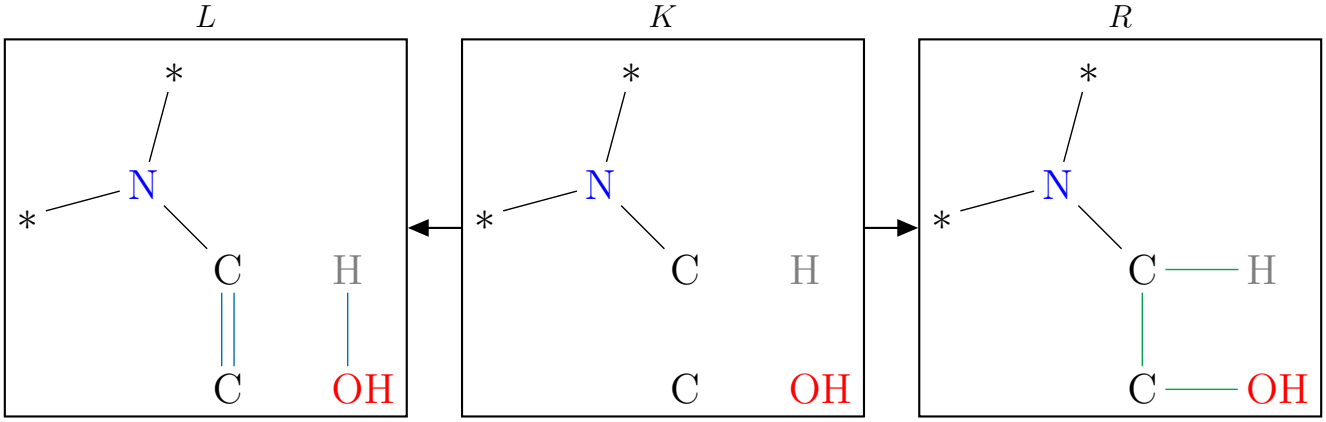
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

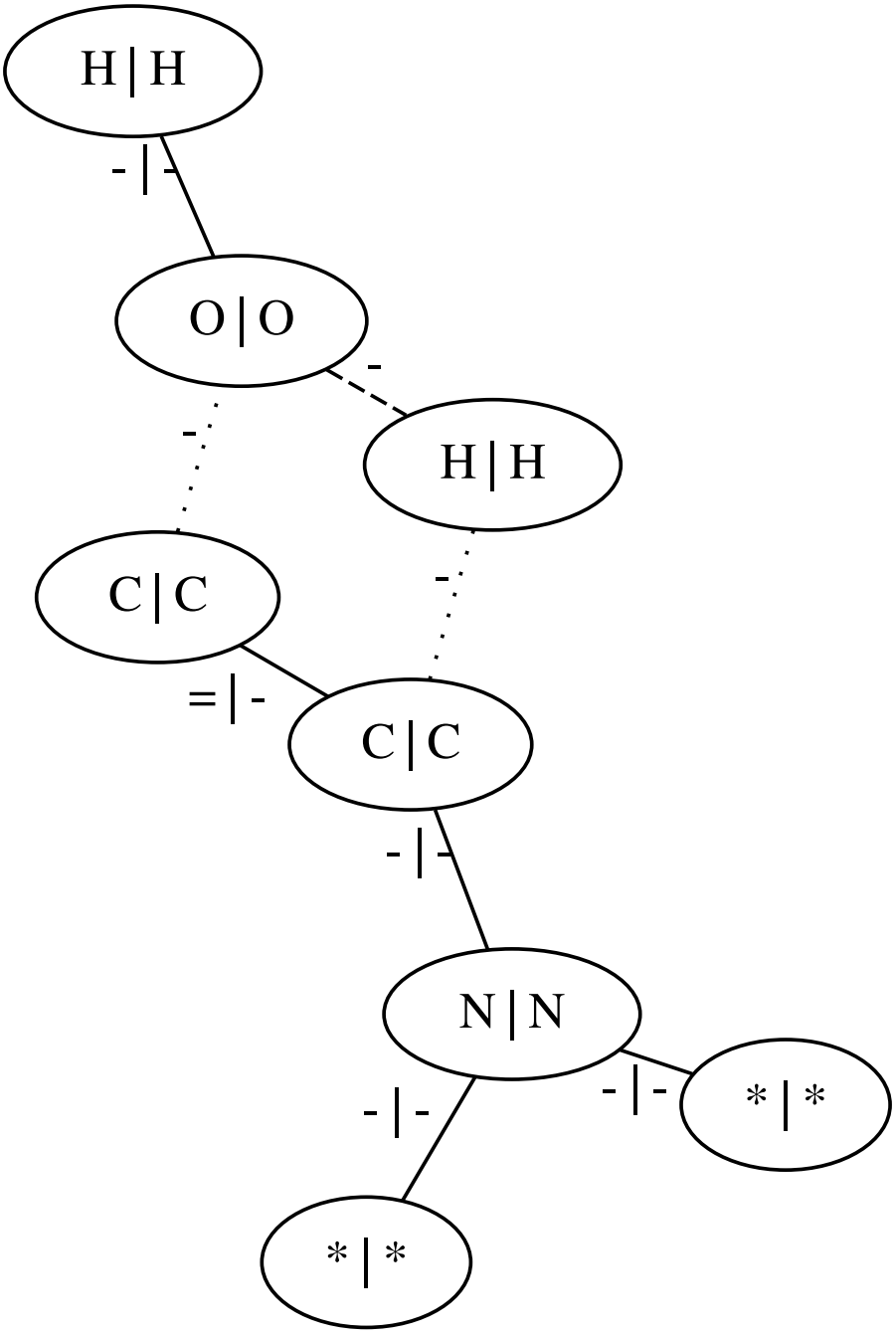
0.0.94 Deydration of Amines (inverse)



Files: out/466_r_96_10300000_{L, K, R}



Files: out/467_r_96_11300100_{L, K, R}



File: out/468_r_96_combined

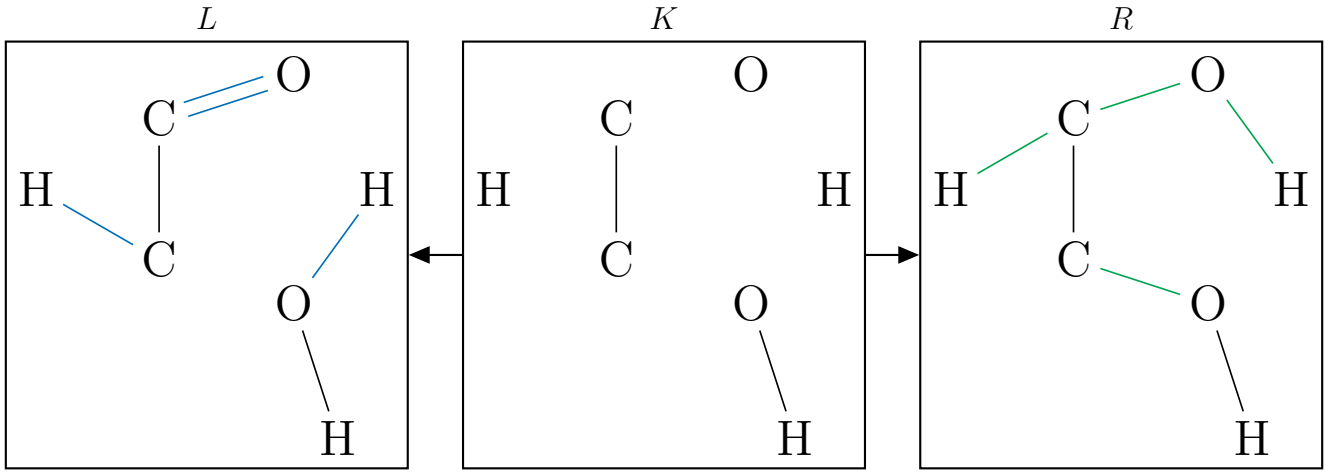
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

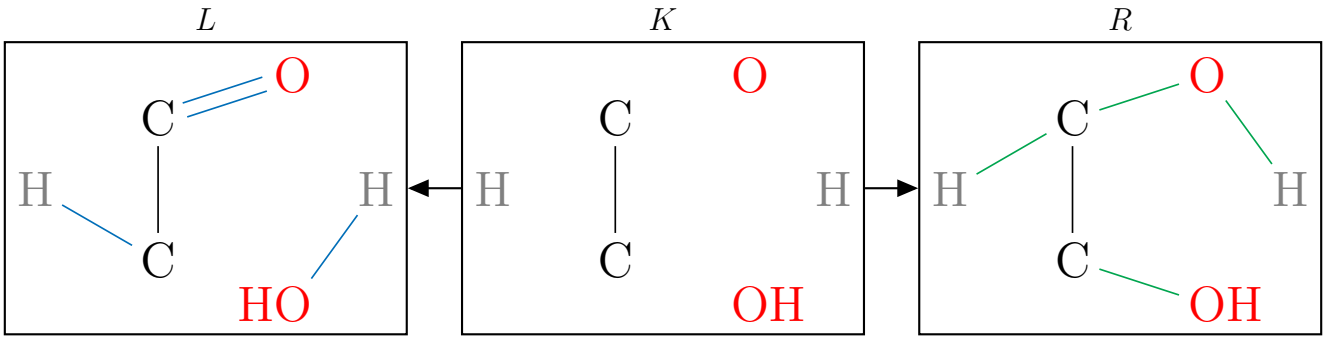
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

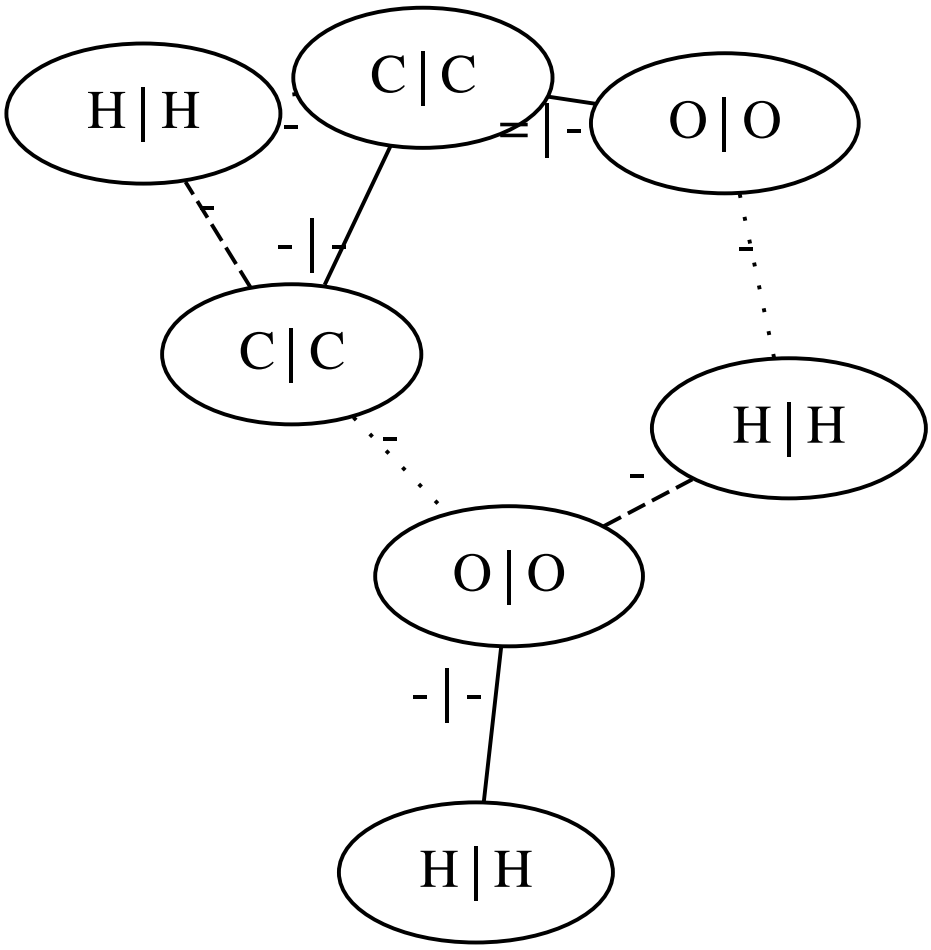
0.0.95 Hydration of C(=O)C



Files: out/471_r_97_10300000_{L, K, R}



Files: out/472_r_97_11300100_{L, K, R}



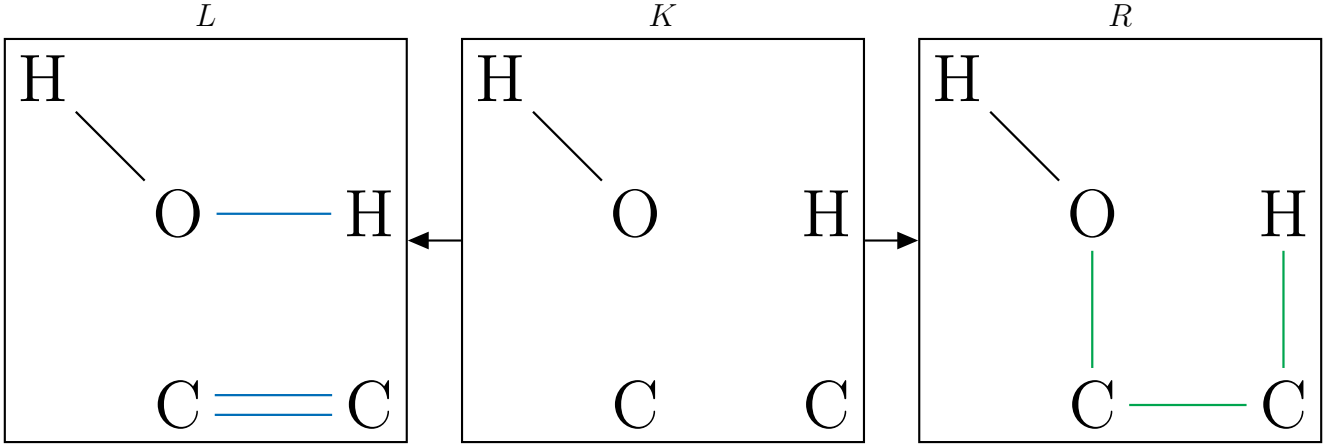
File: out/473_r_97_combined

$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

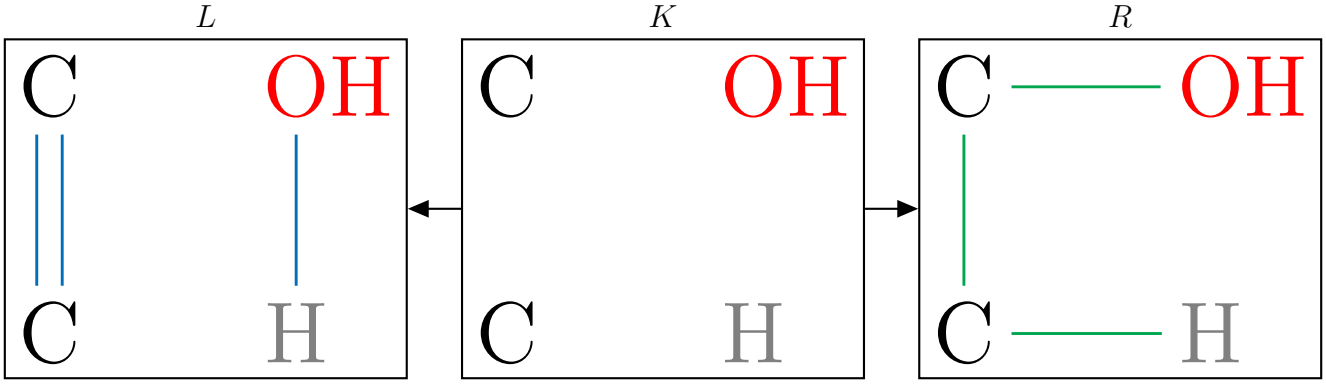
$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}, \text{`='}\}\}| = 0$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

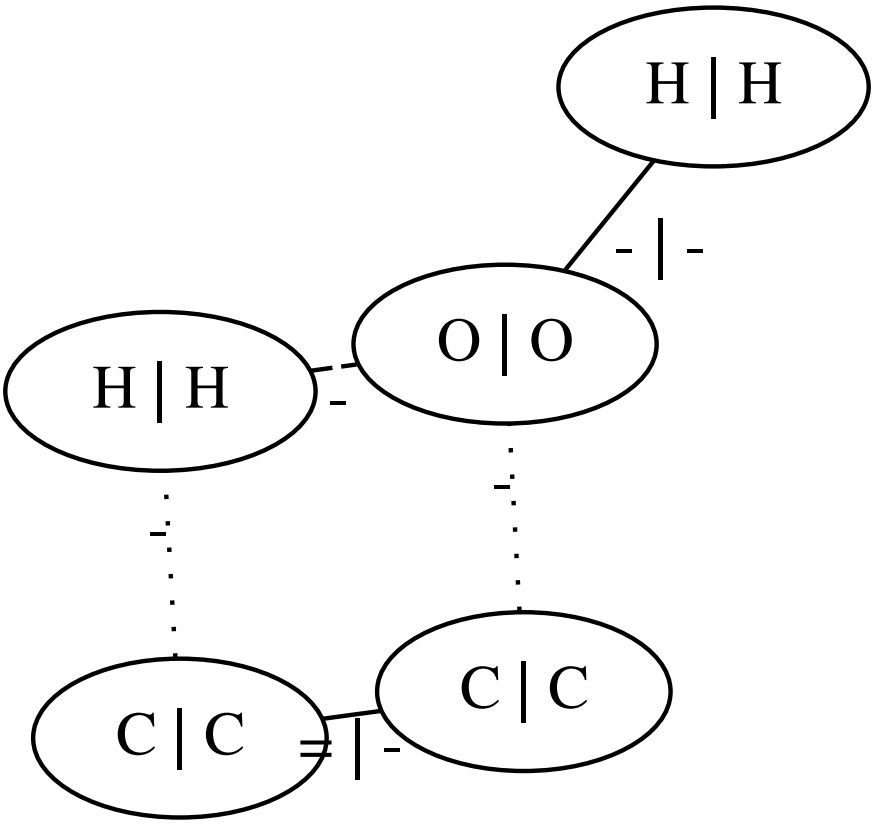
0.0.96 Hydration of C=C(O)



Files: out/476_r_98_10300000_{L, K, R}



Files: out/477_r_98_11300100_{L, K, R}

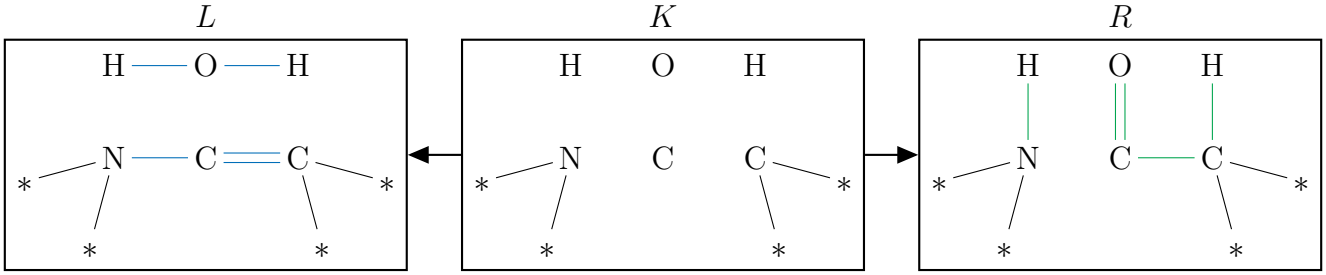


File: out/478_r_98_combined

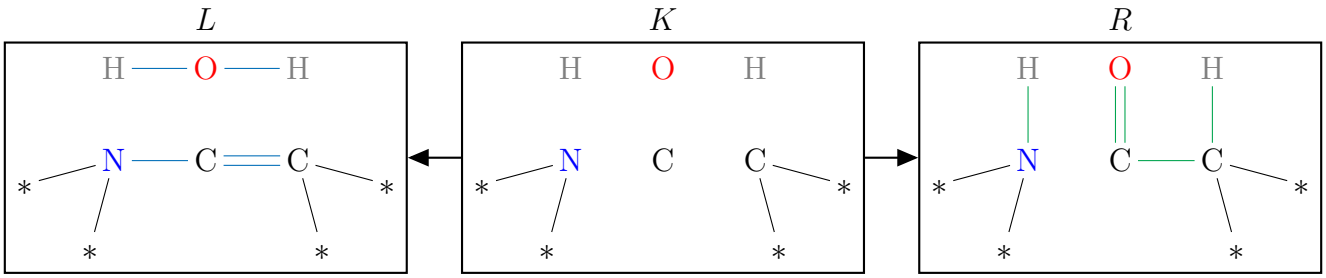
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`='}, \text{`-'}\}\}| = 0$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

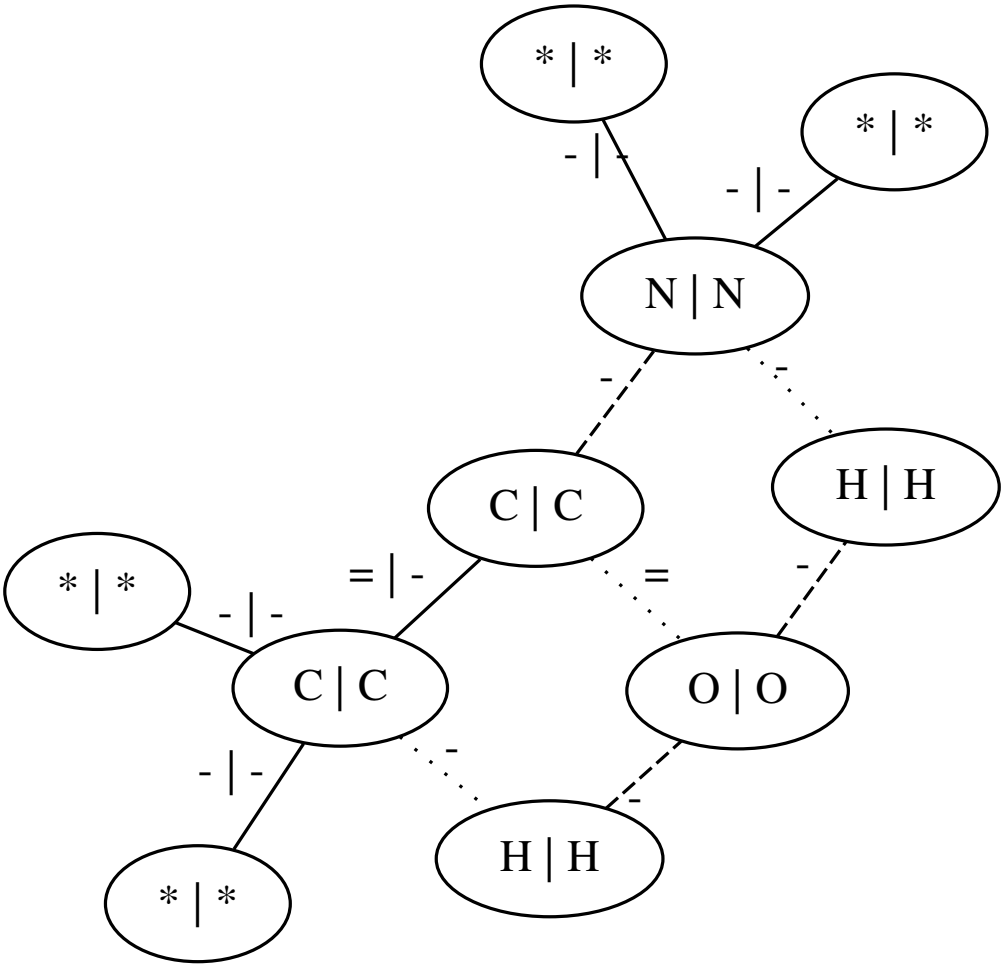
0.0.97 Enamine Hydration and Elimination



Files: out/481_r_99_10300000_{L, K, R}



Files: out/482_r_99_11300100_{L, K, R}



File: out/483_r_99_combined

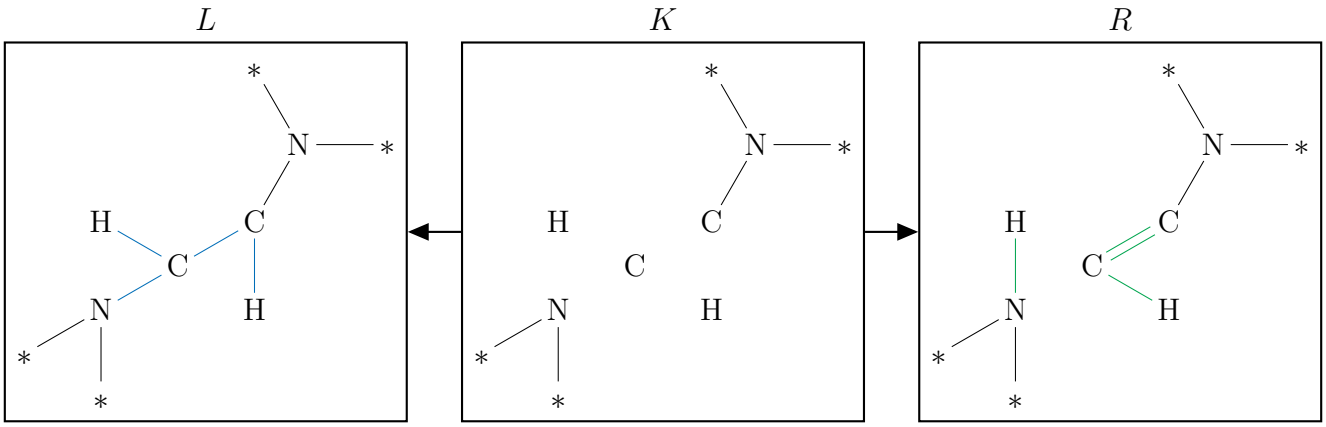
$$|\{e \in \text{outEdges}(3) \mid \\ \quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\ \quad \wedge \\ \quad \text{label}(e) \in \{\text{`='}\} \\ \}| = 0$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

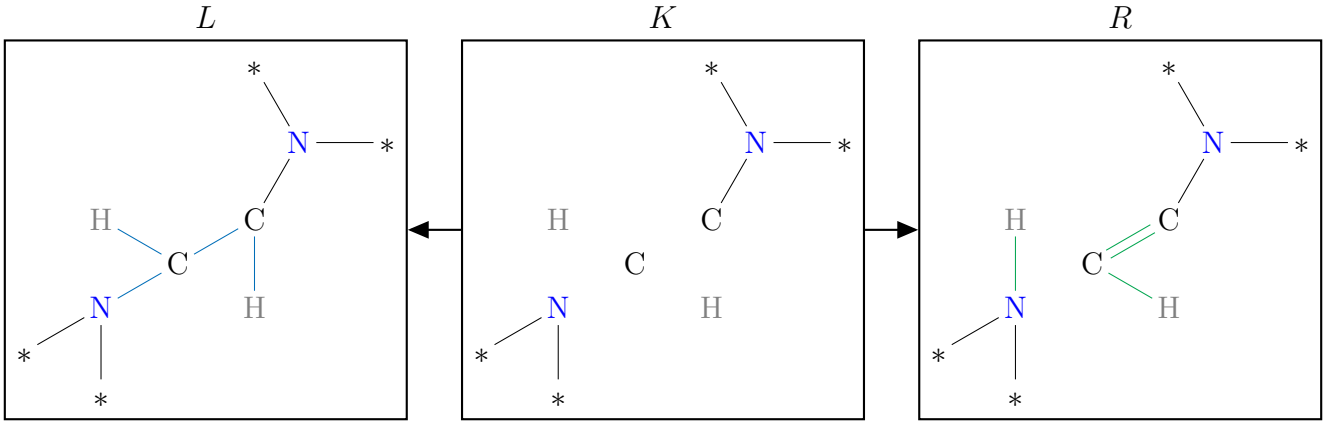
$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

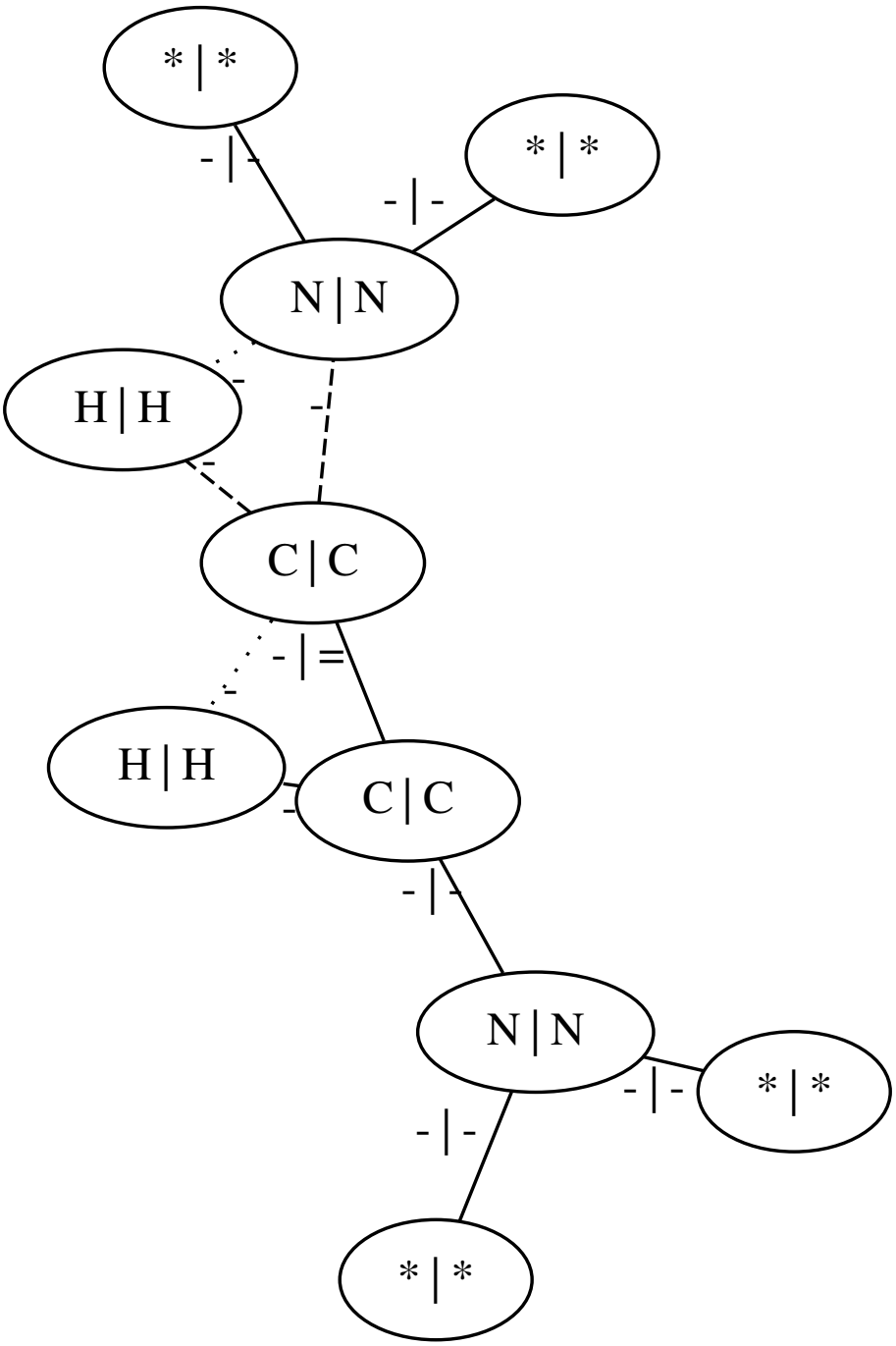
0.0.98 Deamination of Vicinal Diamine



Files: out/486_r_100_10300000_{L, K, R}



Files: out/487_r_100_11300100_{L, K, R}



File: out/488_r_100_combined

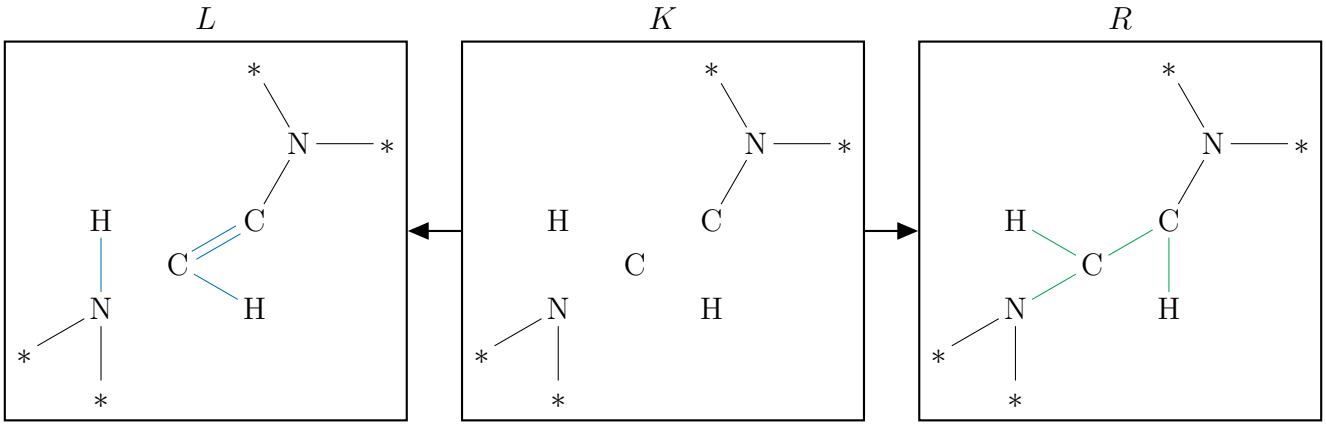
$$
\begin{aligned}
&|\{e \in \text{outEdges}(3) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

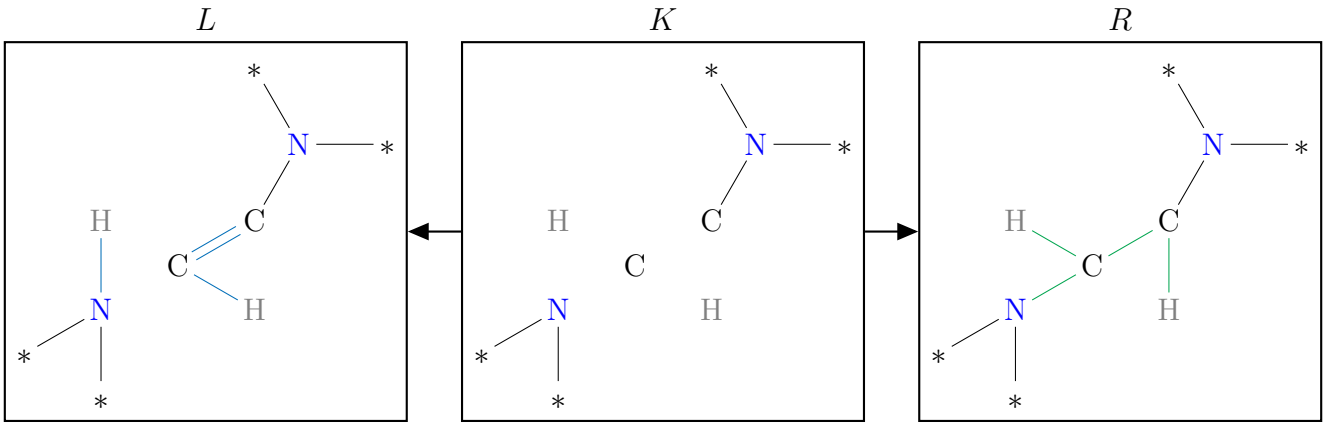
$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

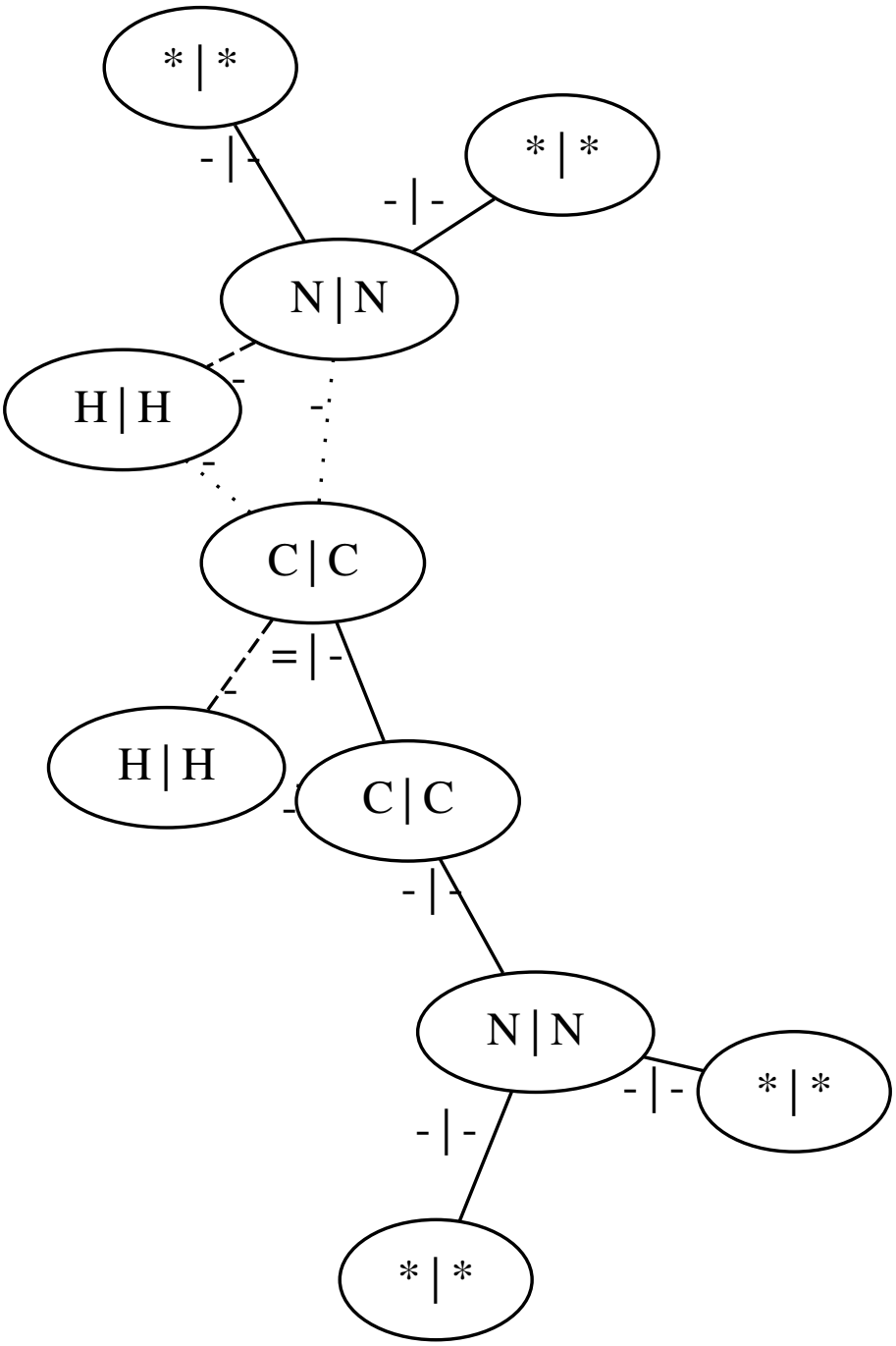
0.0.99 Deamination of Vicinal Diamine, (inverse)



Files: out/491_r_101_10300000_{L, K, R}



Files: out/492_r_101_11300100_{L, K, R}



File: out/493_r_101_combined

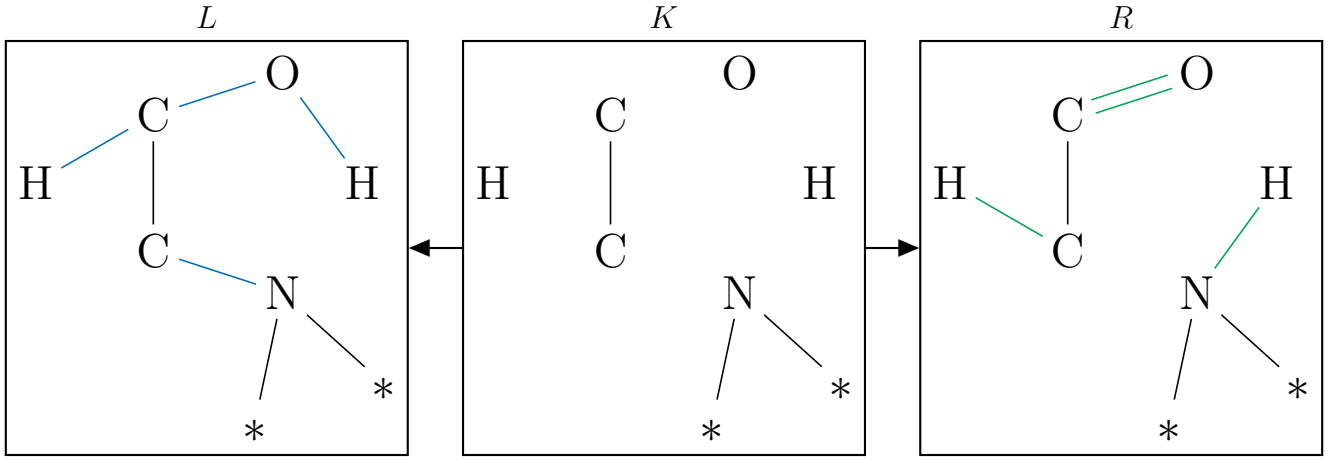
$$
\begin{aligned}
&|\{e \in \text{outEdges}(3) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

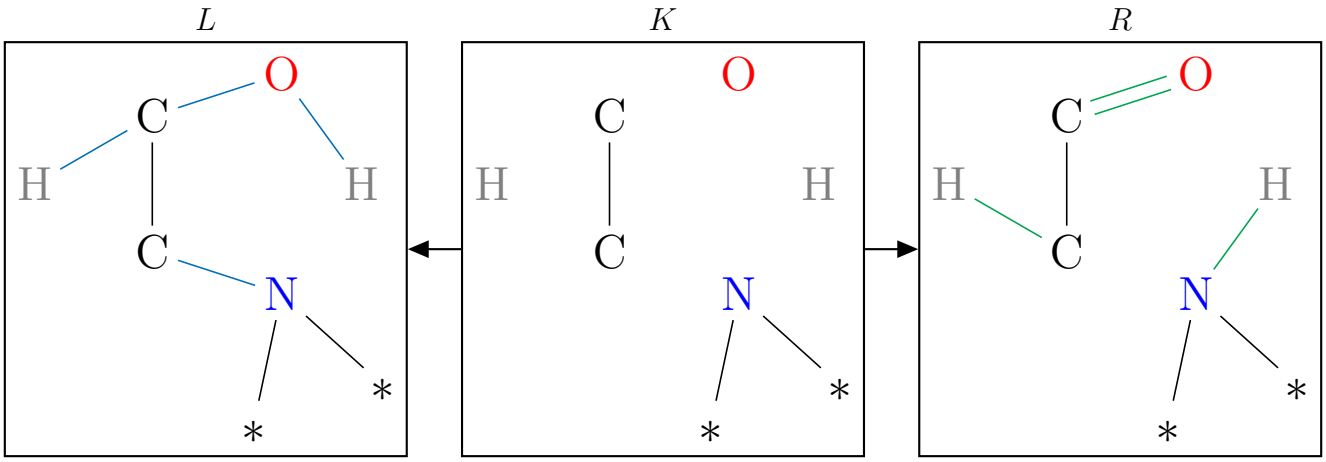
$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

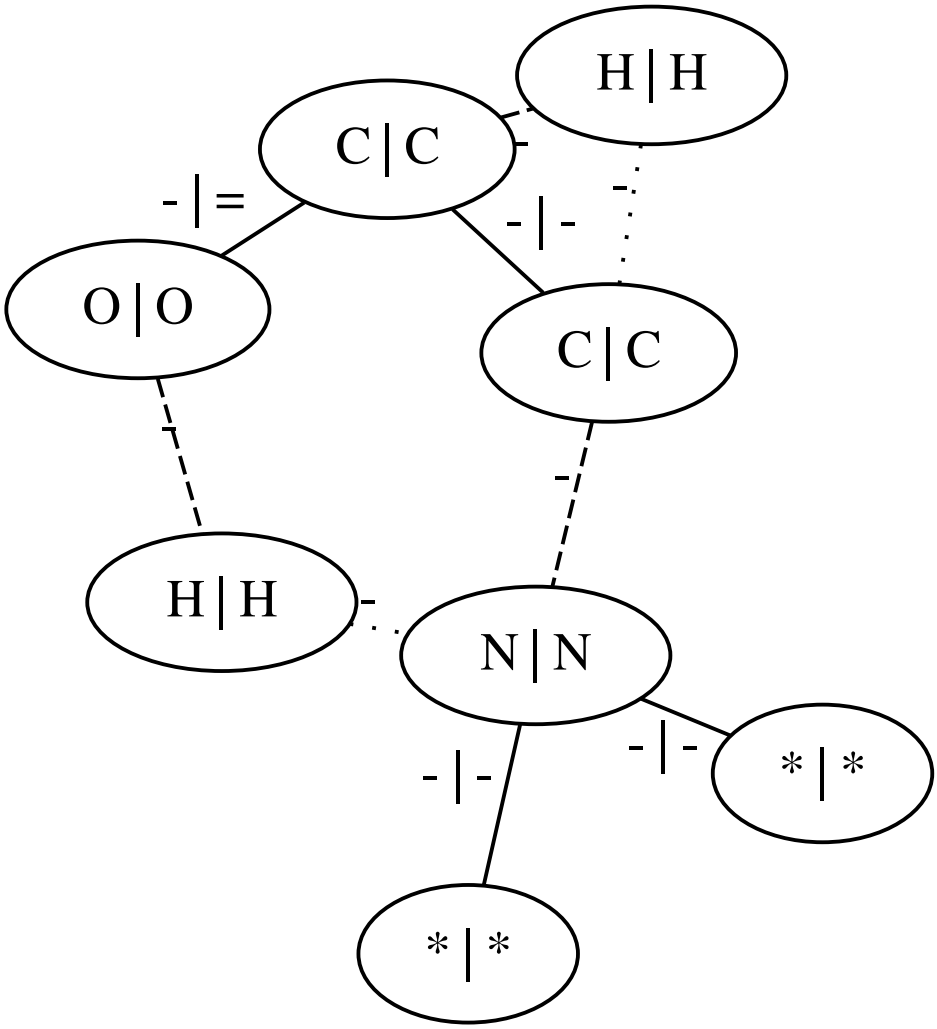
0.0.100 Deamination 2



Files: out/496_r_102_10300000_{L, K, R}



Files: out/497_r_102_11300100_{L, K, R}

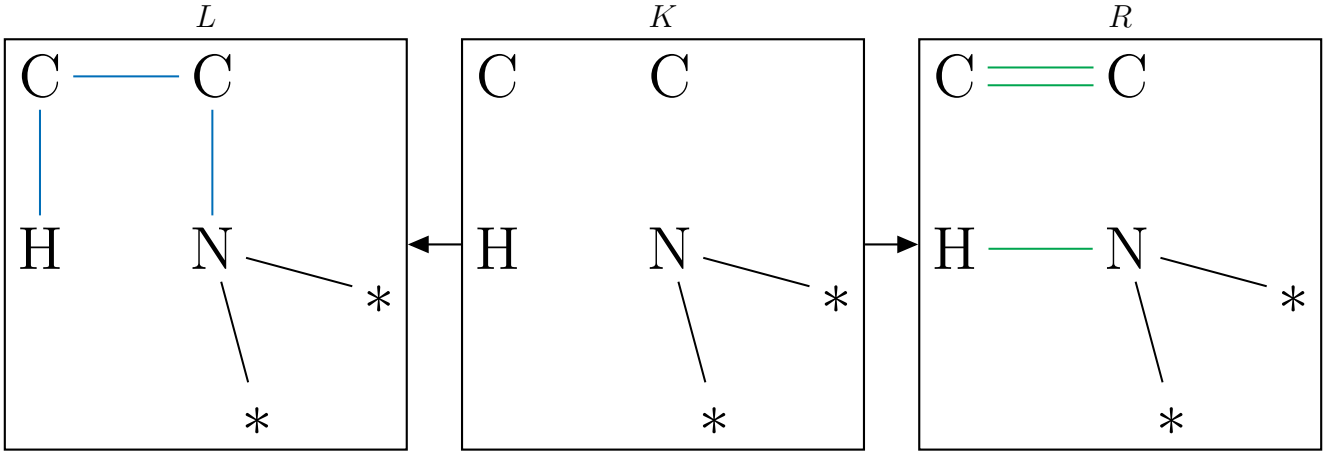


File: out/498_r_102_combined

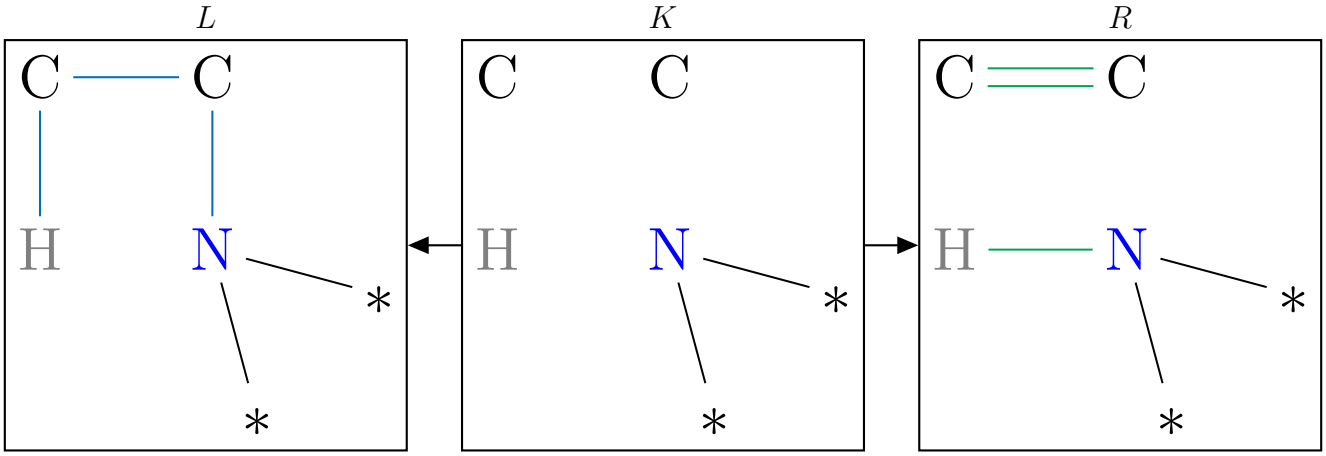
$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

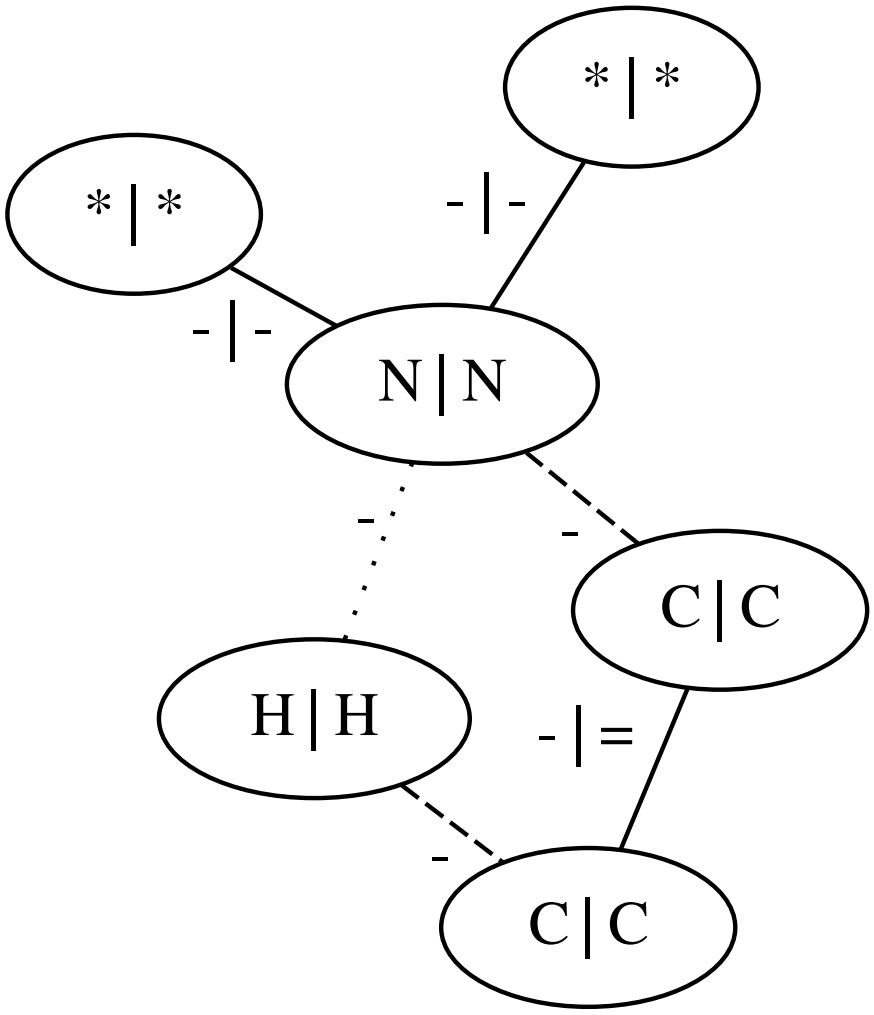
0.0.101 Deamination 3



Files: out/501_r_103_10300000_{L, K, R}



Files: out/502_r_103_11300100_{L, K, R}



File: out/503_r_103_combined

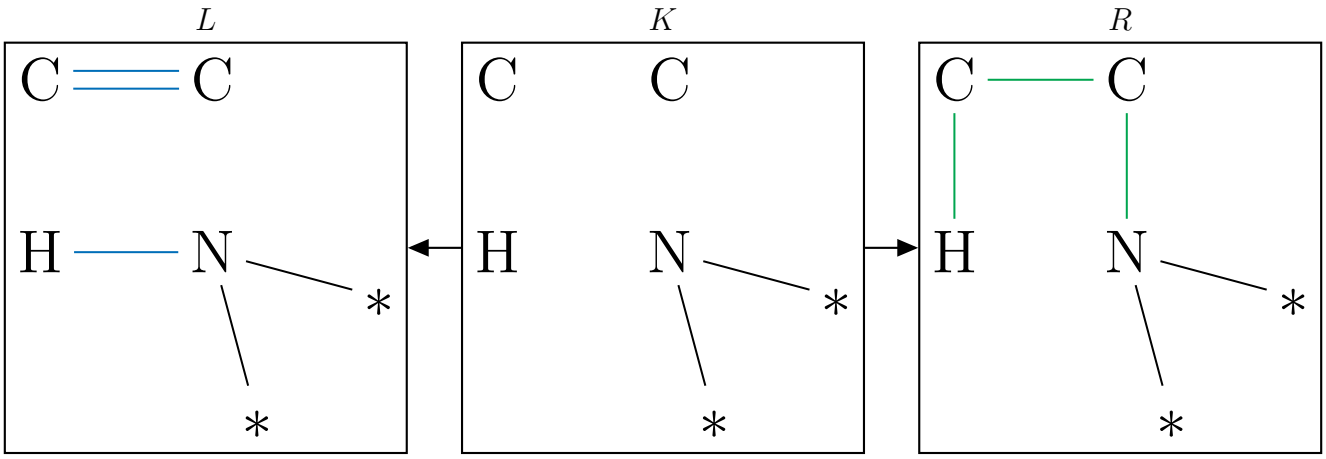
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}, \text{`-'}\}\}| = 0$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

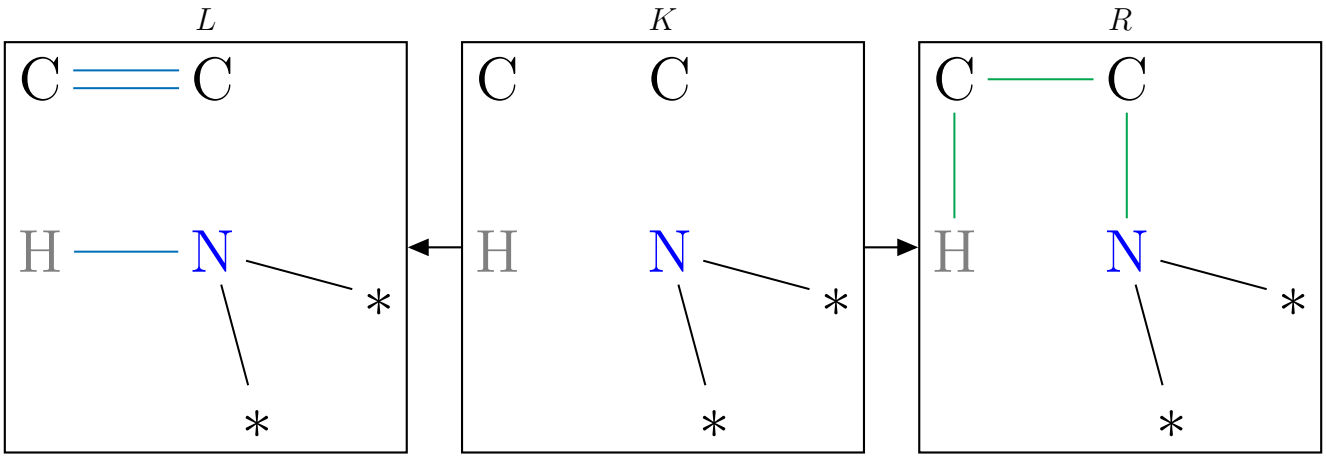
$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

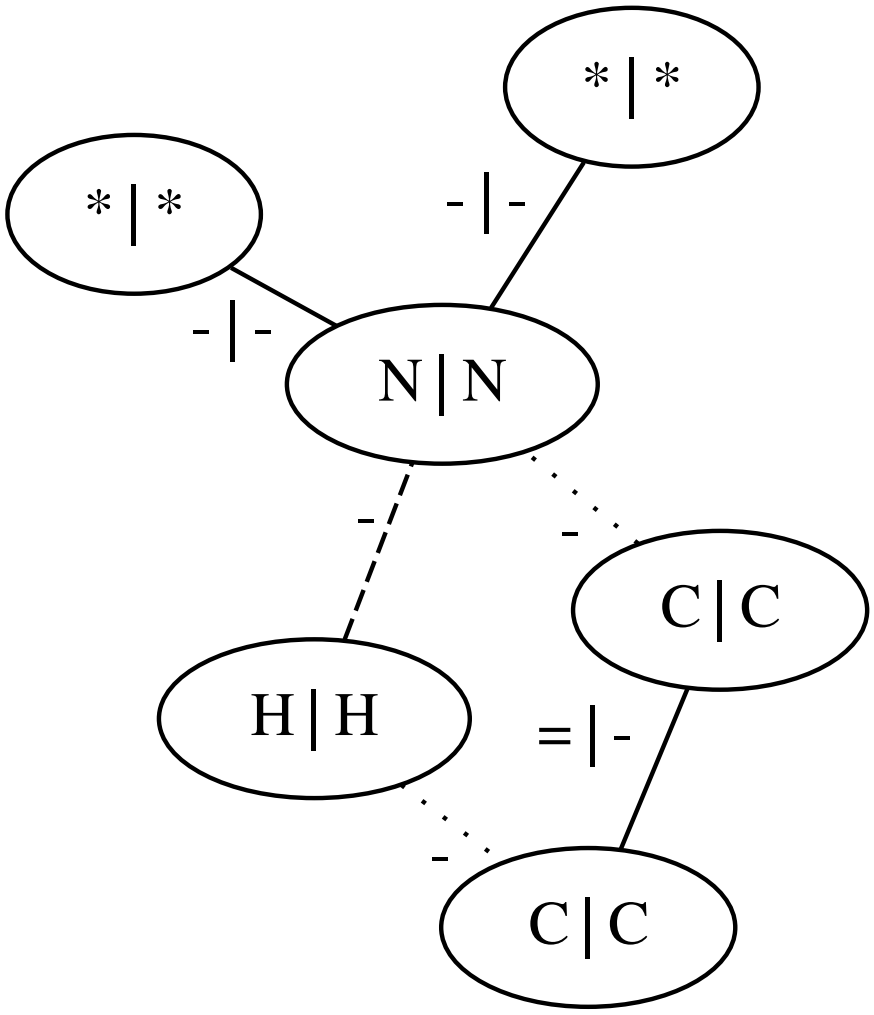
0.0.102 Deamination 3 (inverse)



Files: out/506_r_104_10300000_{L, K, R}



Files: out/507_r_104_11300100_{L, K, R}



File: out/508_r_104_combined

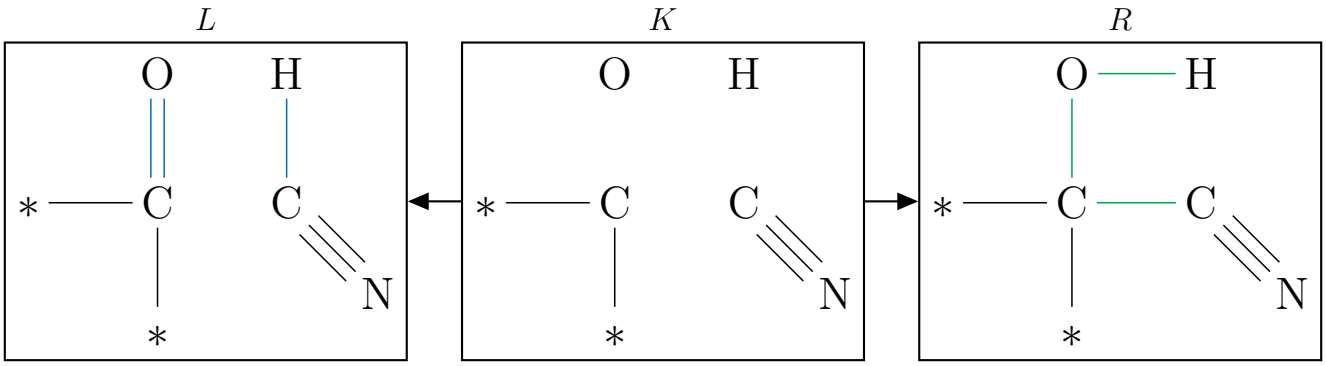
$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`}\texttt{N}\text{'}, \text{`}\texttt{O}\text{'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`}\texttt{=}\text{'}, \text{`}\texttt{-}\text{'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

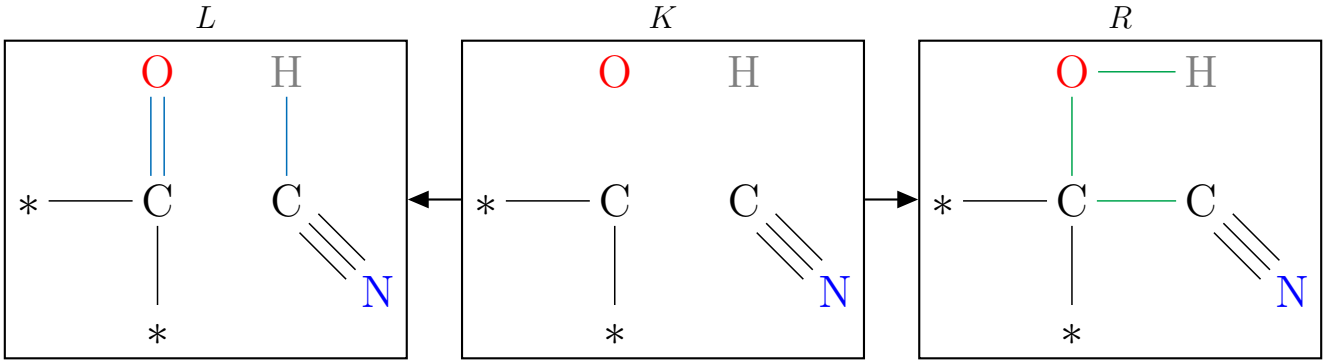
$$
\begin{aligned}
&|\{e \in \text{outEdges}(4) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

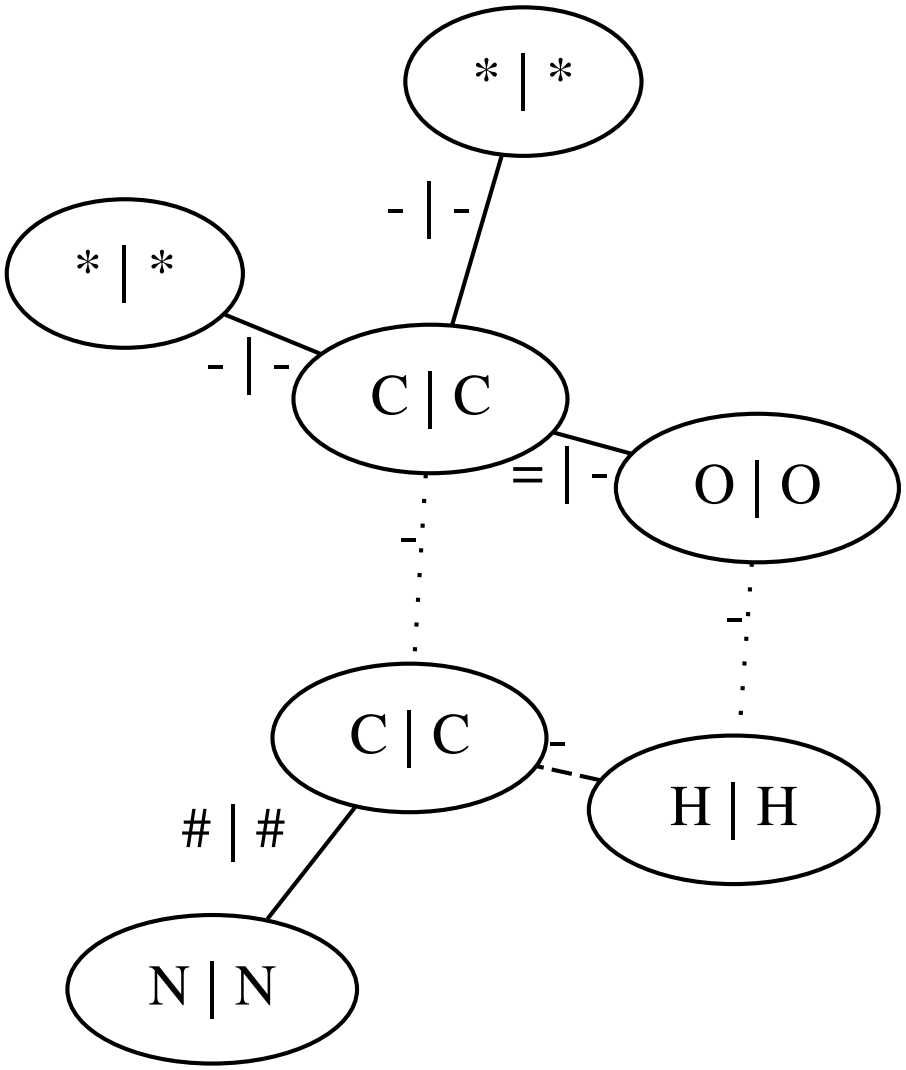
0.0.103 Cyanohydrin Formation



Files: out/511_r_105_10300000_{L, K, R}



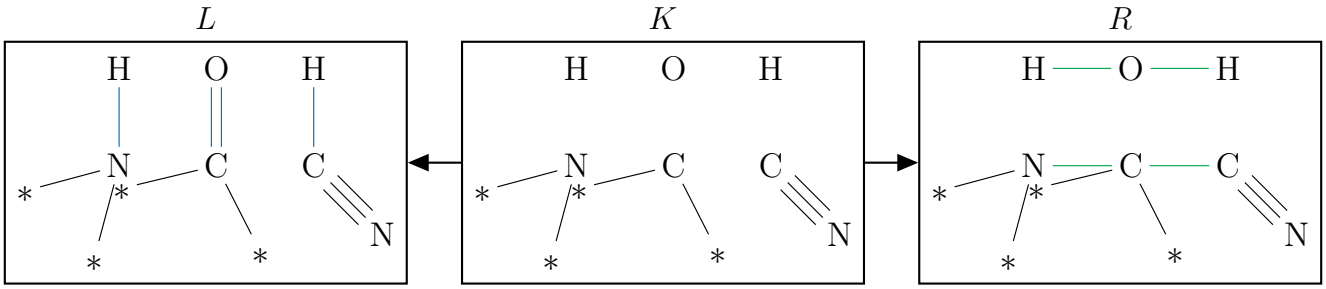
Files: out/512_r_105_11300100_{L, K, R}



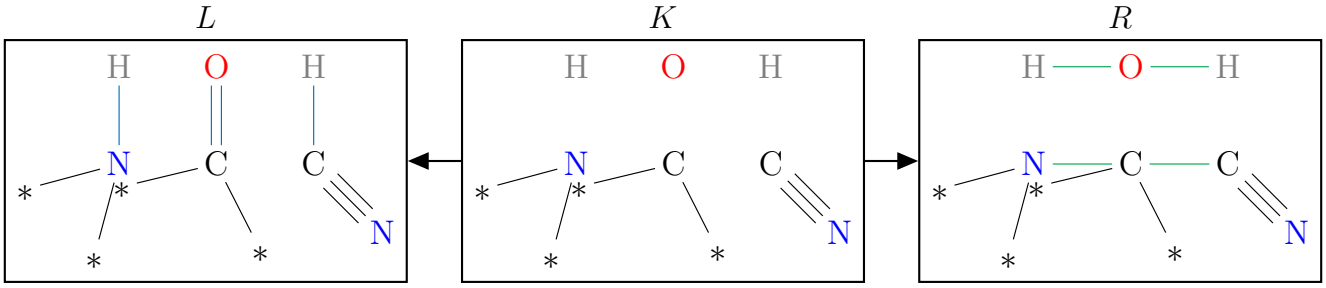
File: out/513_r_105_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

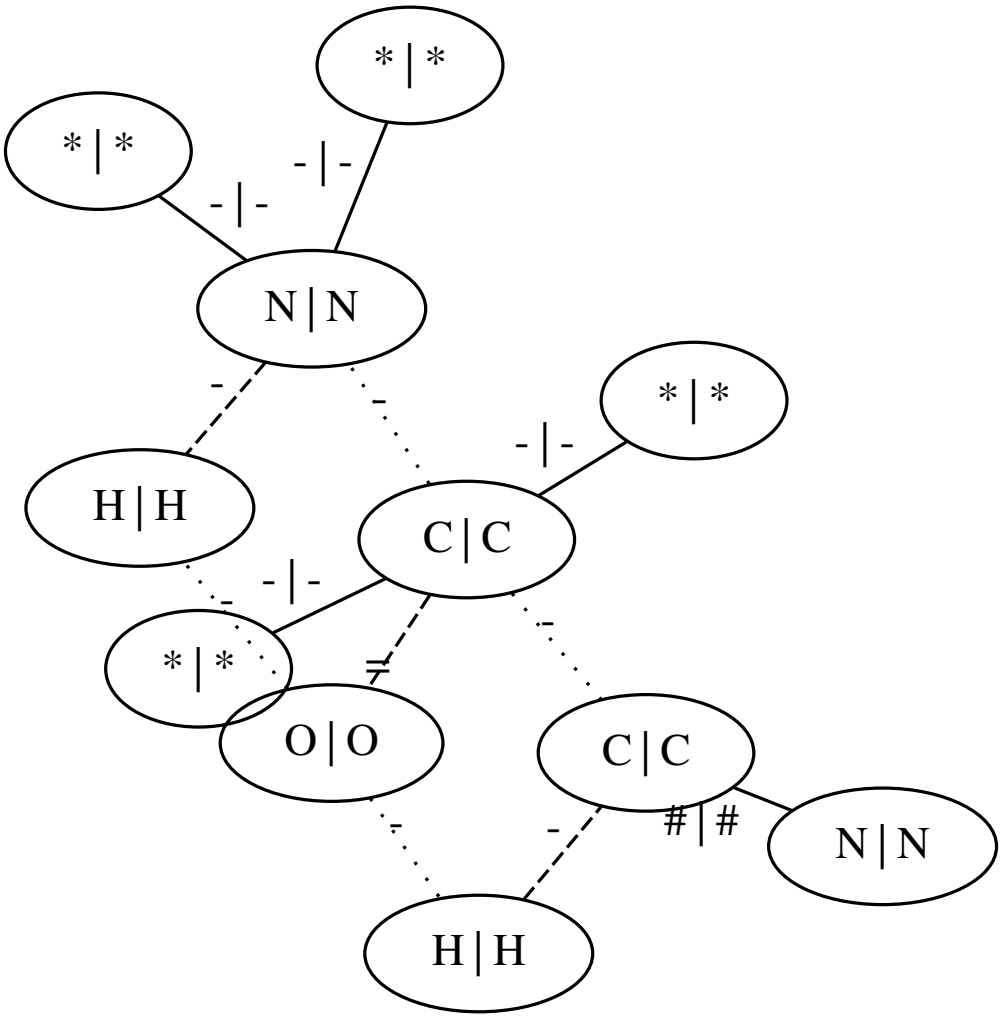
0.0.104 Strecker Synthesis



Files: out/515_r_106_10300000_{L, K, R}



Files: out/516_r_106_11300100_{L, K, R}



File: out/517_r_106_combined

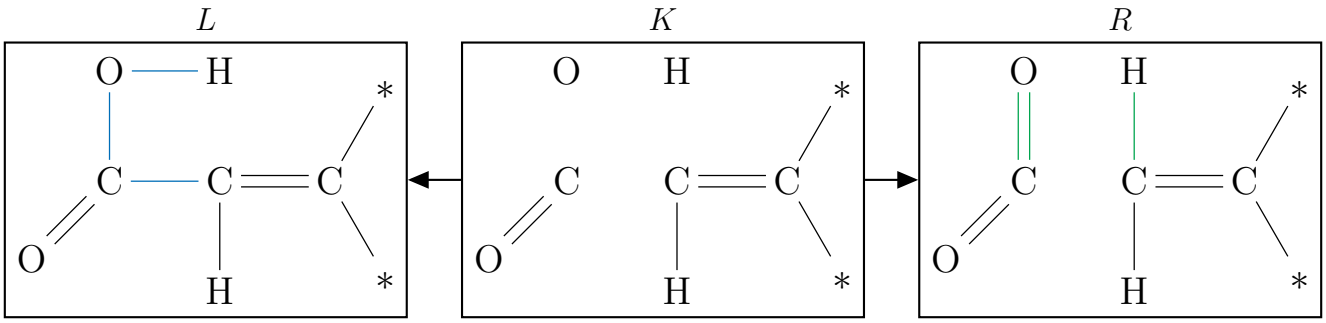
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(4) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

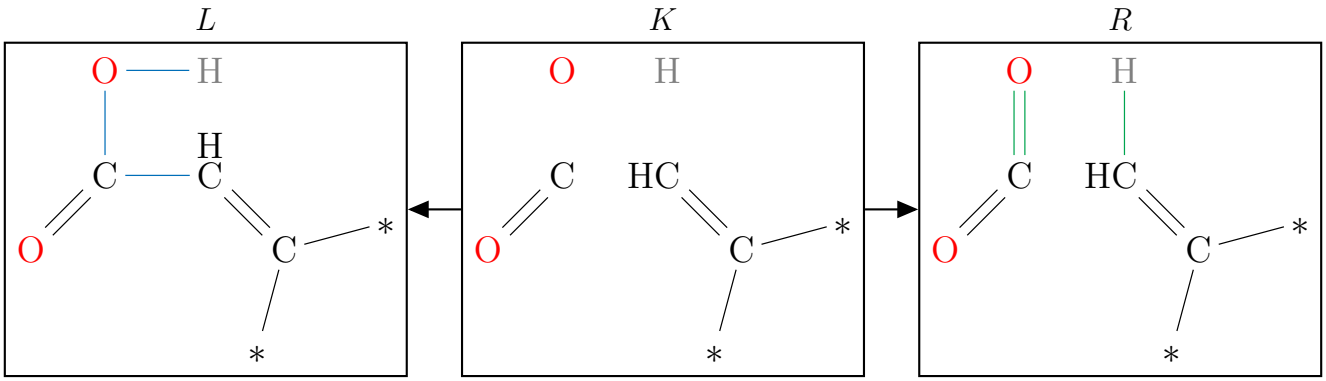
$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

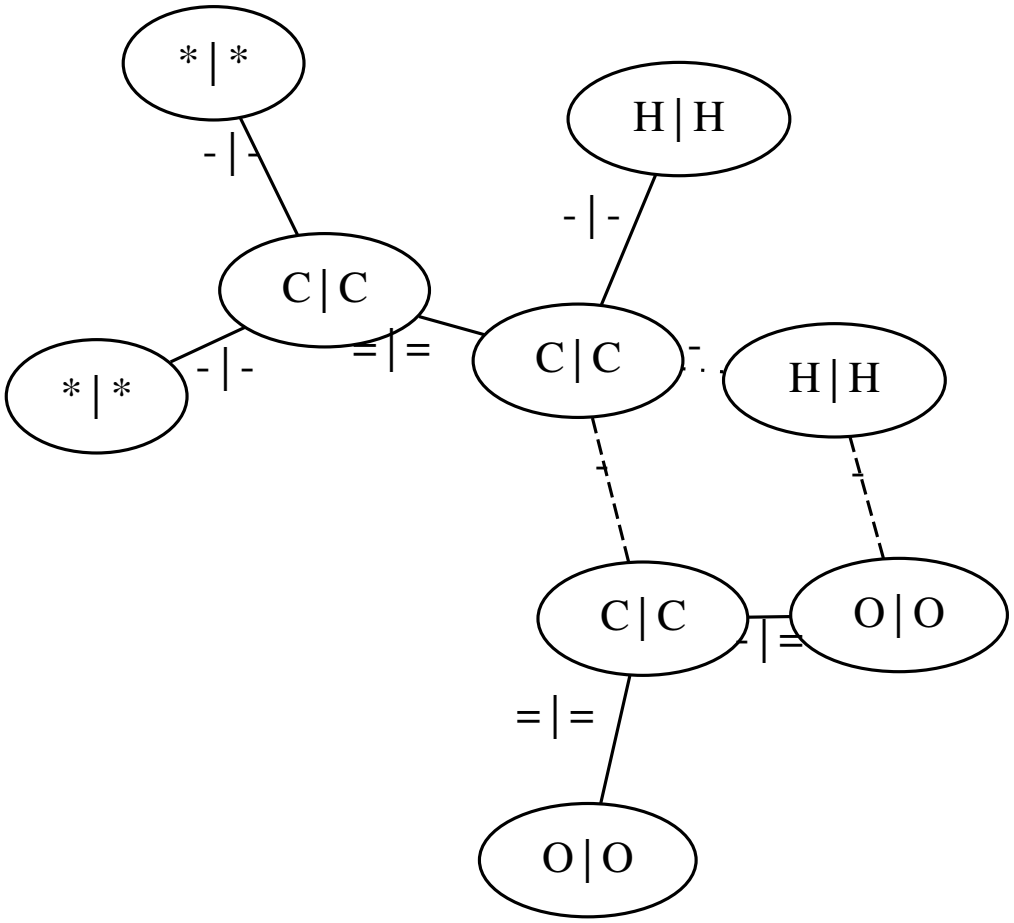
0.0.105 Alpha-Beta Unsaturated Acid Decarboxylation



Files: out/520_r_107_10300000_{L, K, R}

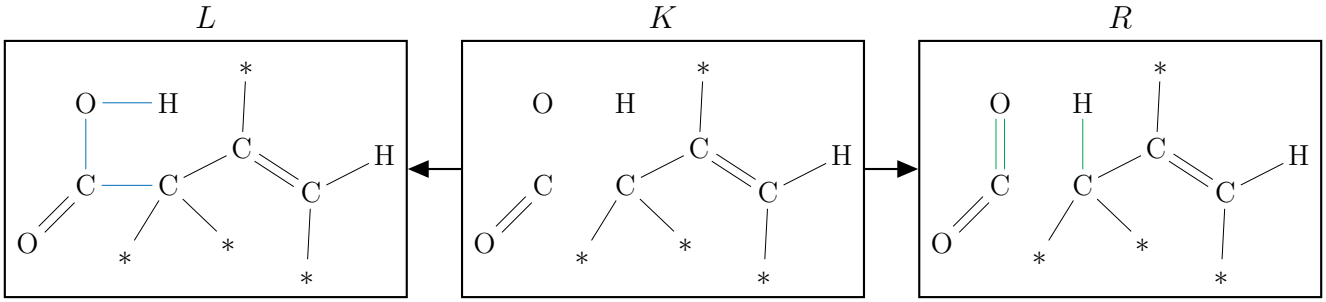


Files: out/521_r_107_11300100_{L, K, R}

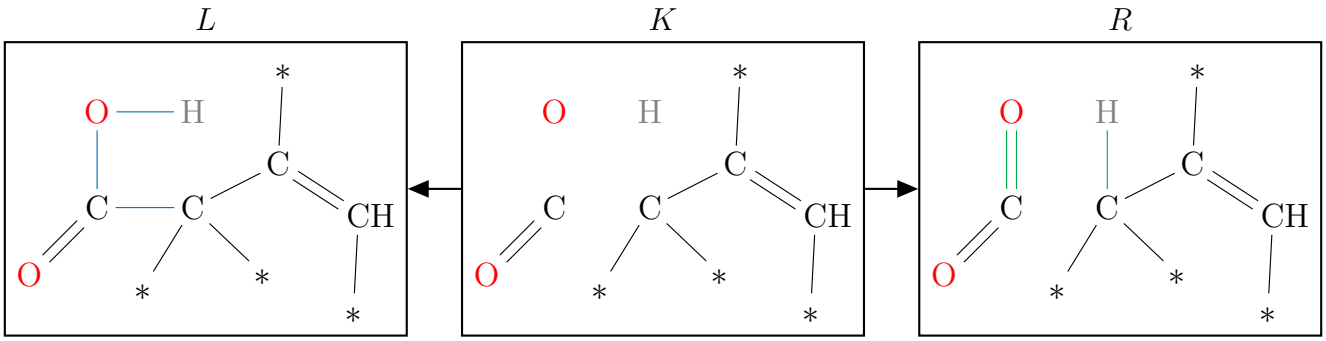


File: out/522_r_107_combined

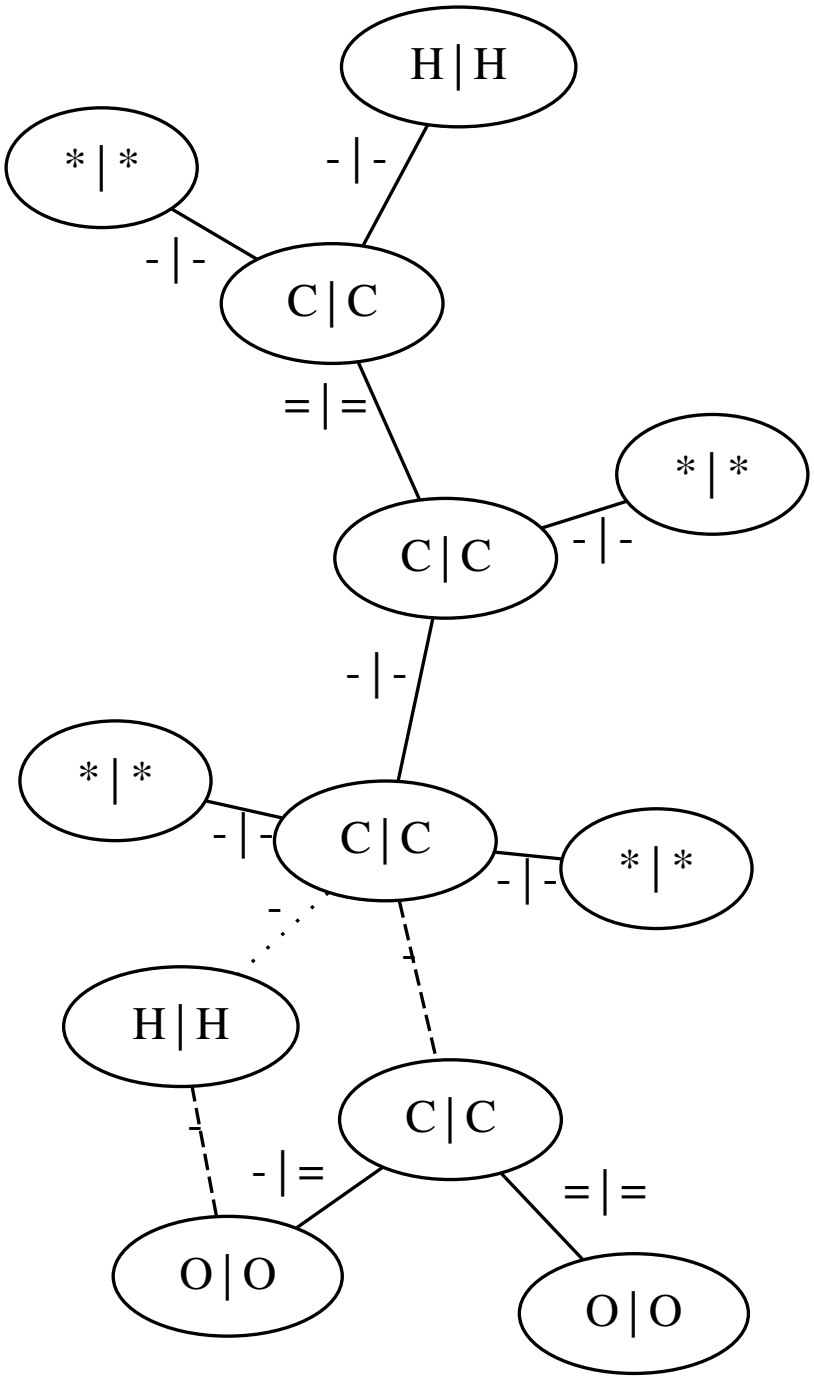
0.0.106 Beta-gamma Unsaturated Acid Decarboxylation



Files: out/525_r_108_10300000_{L, K, R}

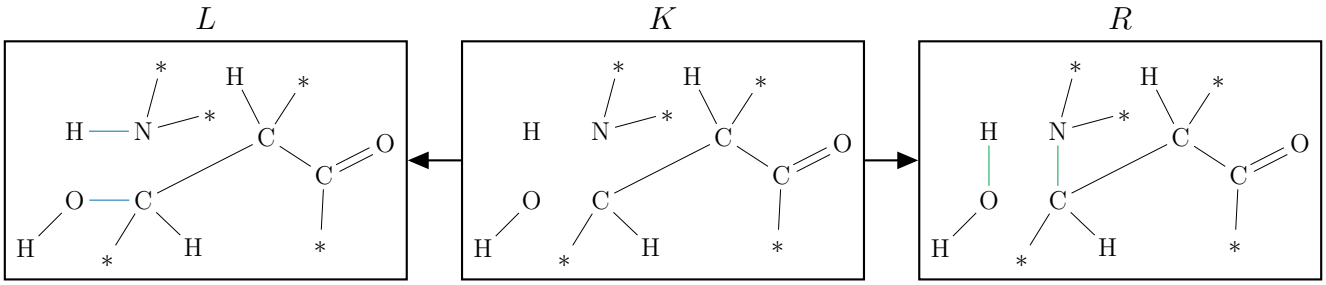


Files: out/526_r_108_11300100_{L, K, R}

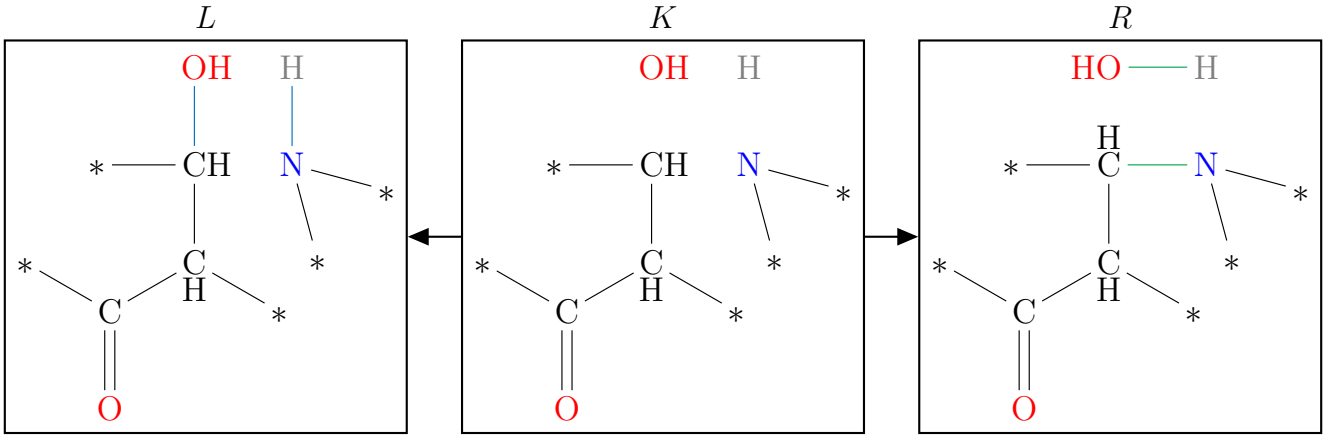


File: out/527_r_108_combined

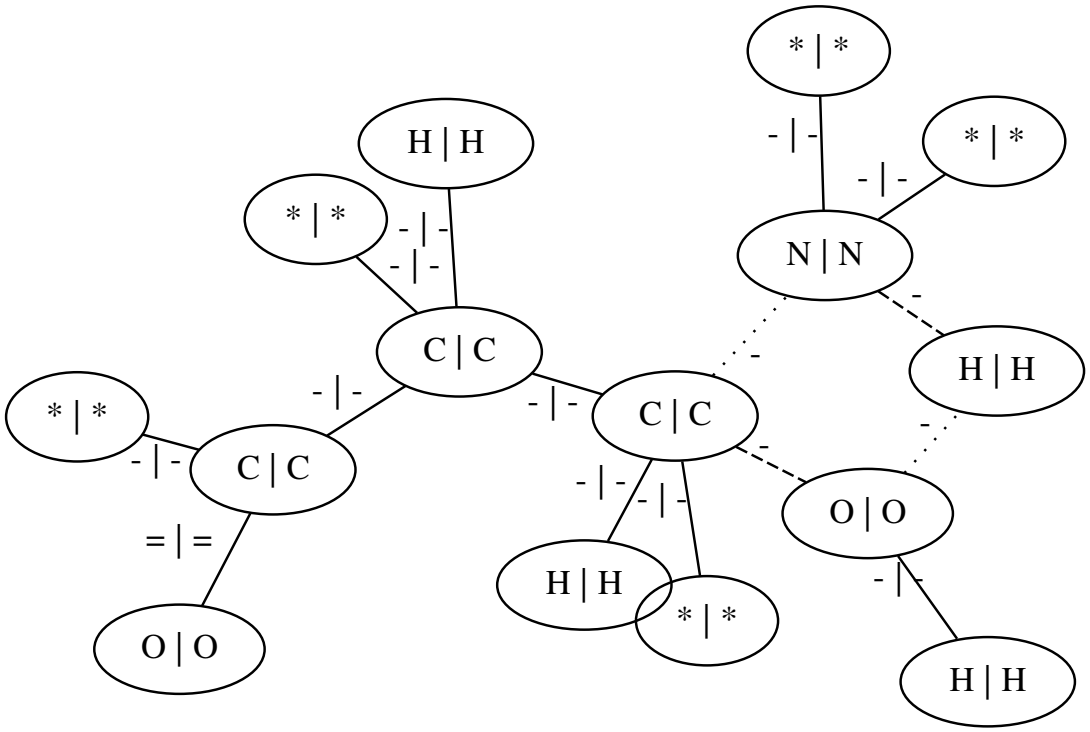
0.0.107 Mannich Addition



Files: out/530_r_109_10300000_{L, K, R}



Files: out/531_r_109_11300100_{L, K, R}



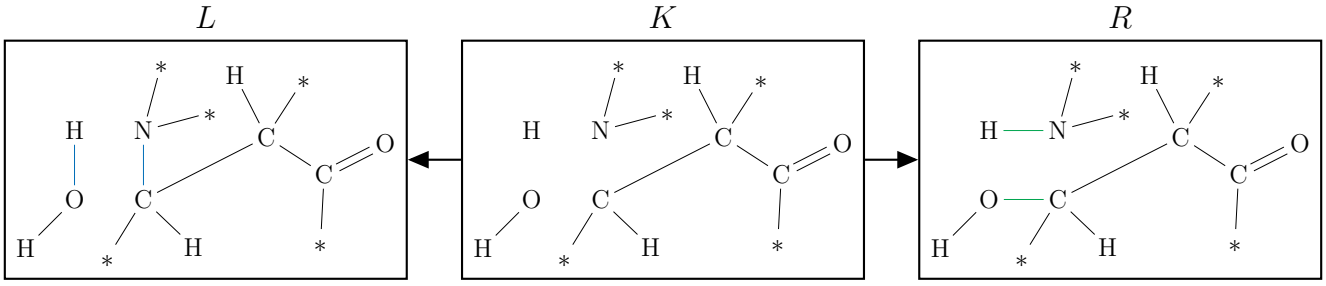
$$|\{e \in \text{outEdges}(12) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(12) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

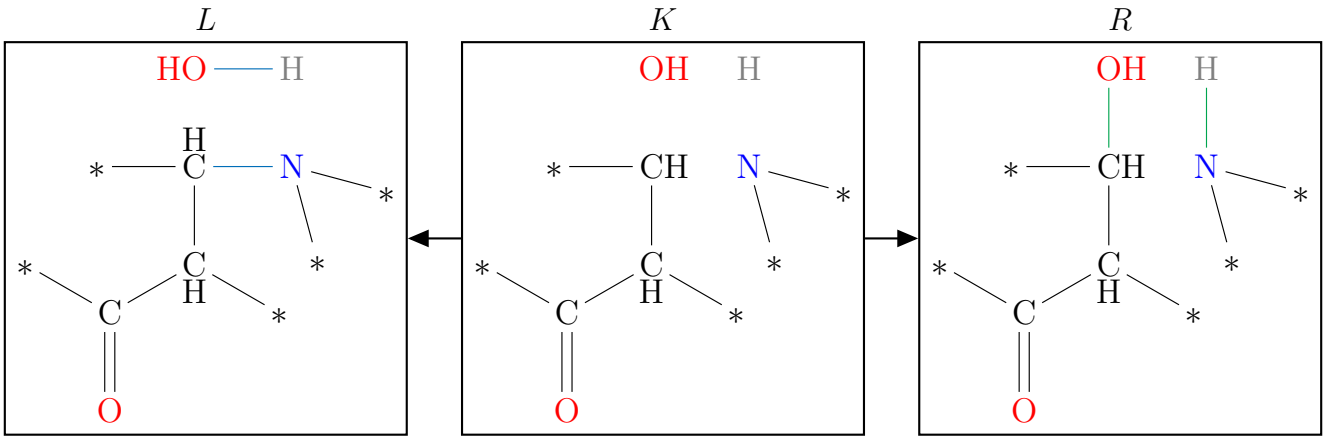
$$|\{e \in \text{outEdges}(13) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(13) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

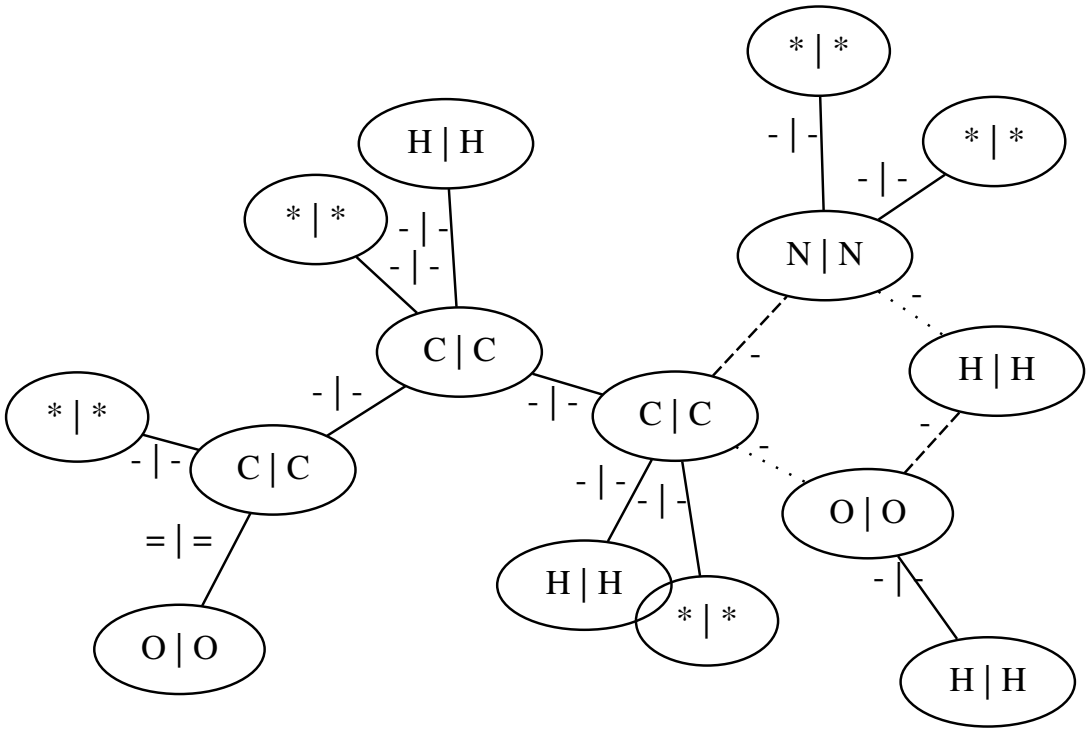
0.0.108 Mannich Addition (reverse)



Files: out/535_r_110_10300000_{L, K, R}



Files: out/536_r_110_11300100_{L, K, R}



File: out/537_r_110_combined

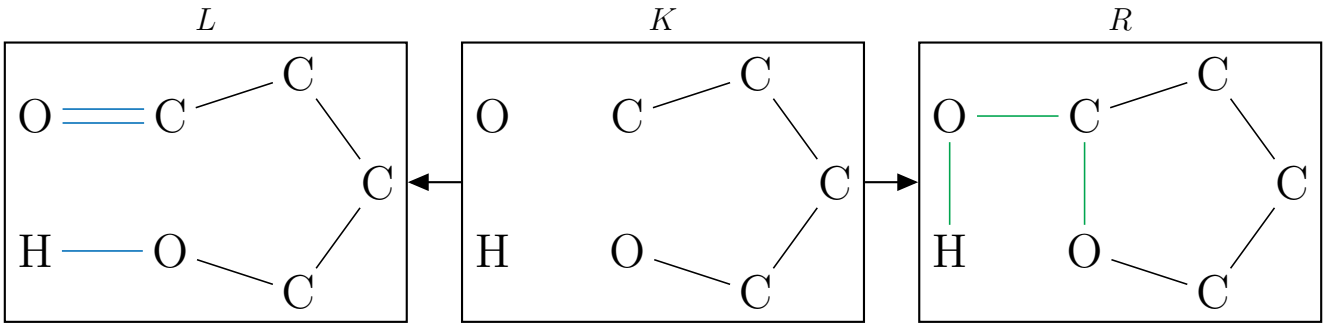
$$
\begin{aligned}
&|\{e \in \text{outEdges}(12) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(12) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

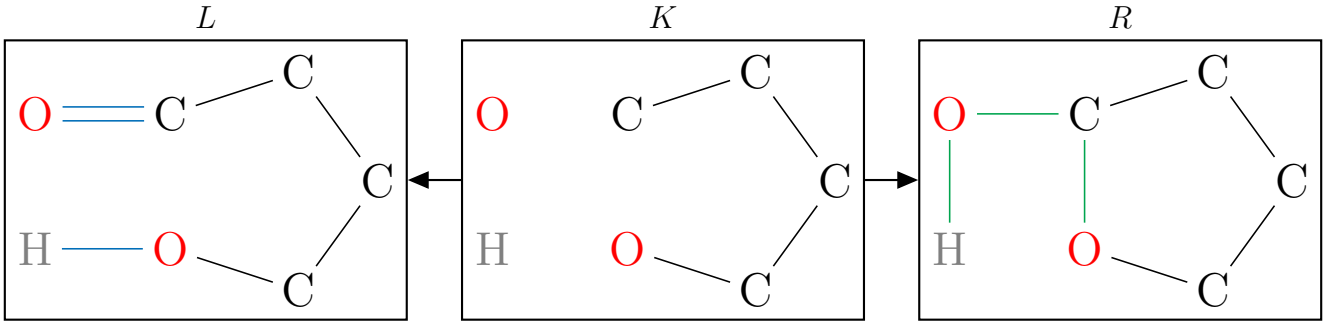
$$
\begin{aligned}
&|\{e \in \text{outEdges}(13) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(13) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

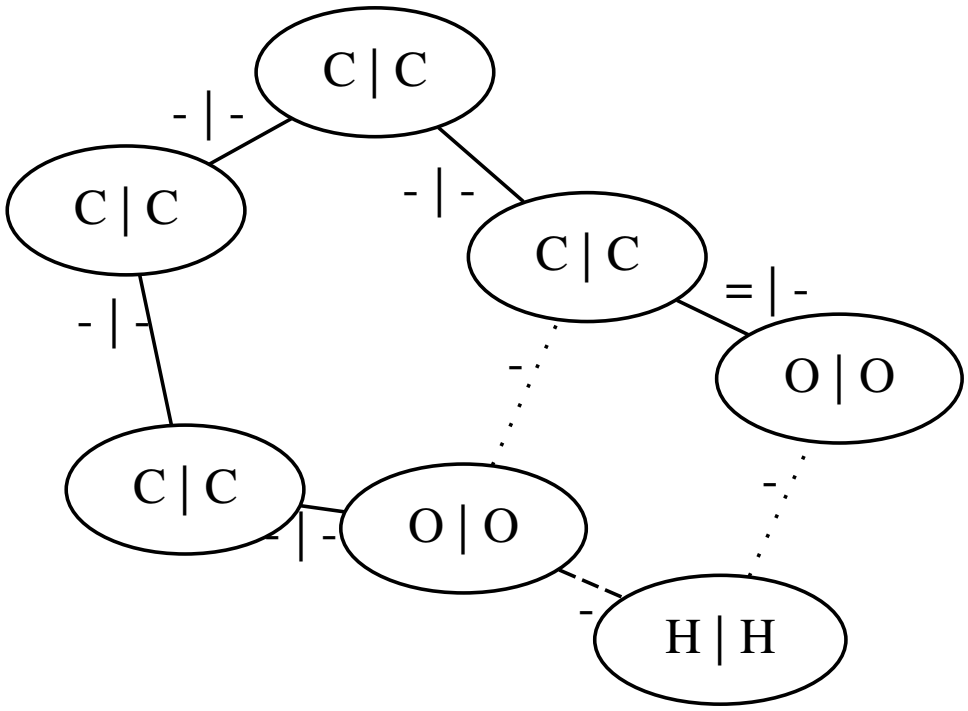
0.0.109 Hemiacetal Formation for 5 membered rings



Files: out/540_r_111_10300000_{L, K, R}



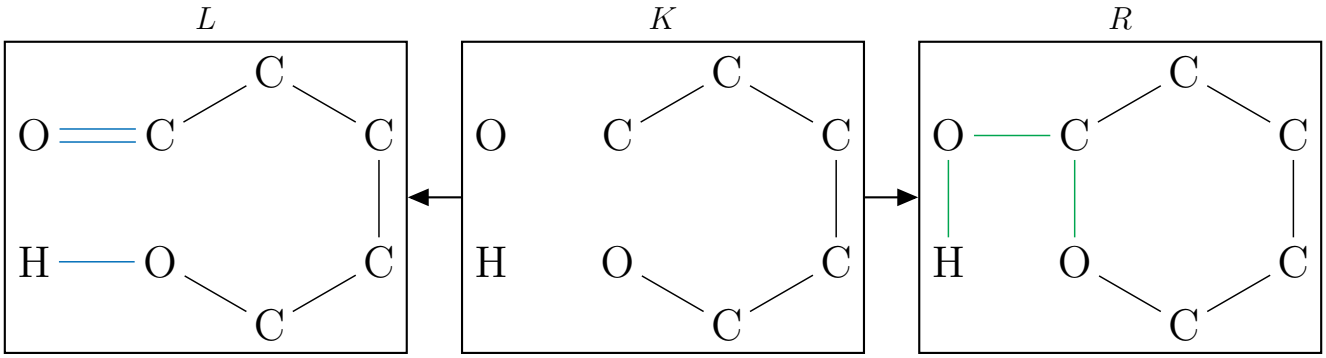
Files: out/541_r_111_11300100_{L, K, R}



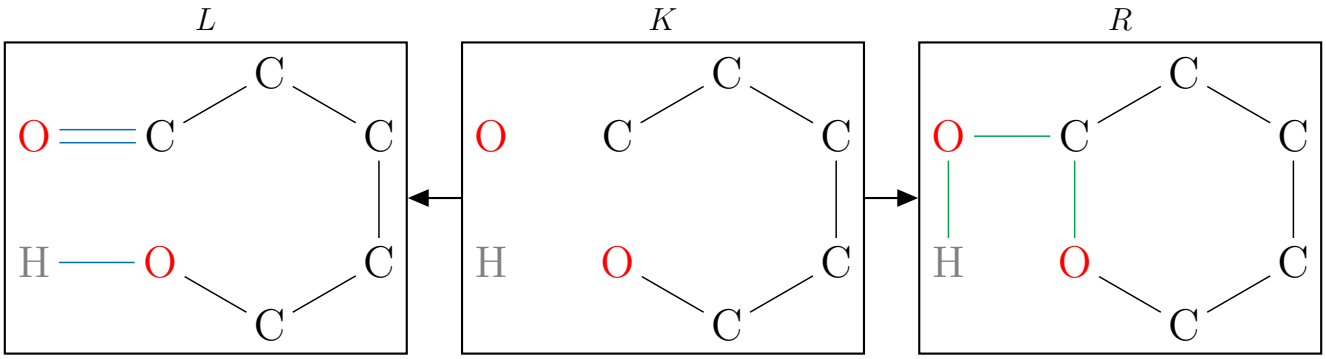
File: out/542_r_111_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(3) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

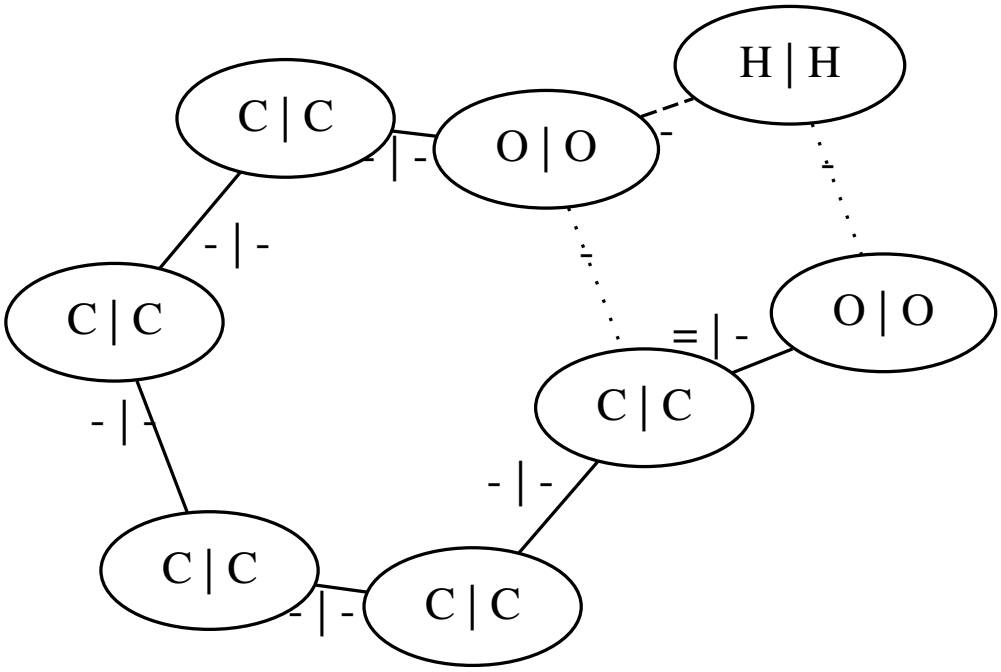
0.0.110 Hemiacetal Formation for 6 membered rings



Files: out/545_r_112_10300000_{L, K, R}



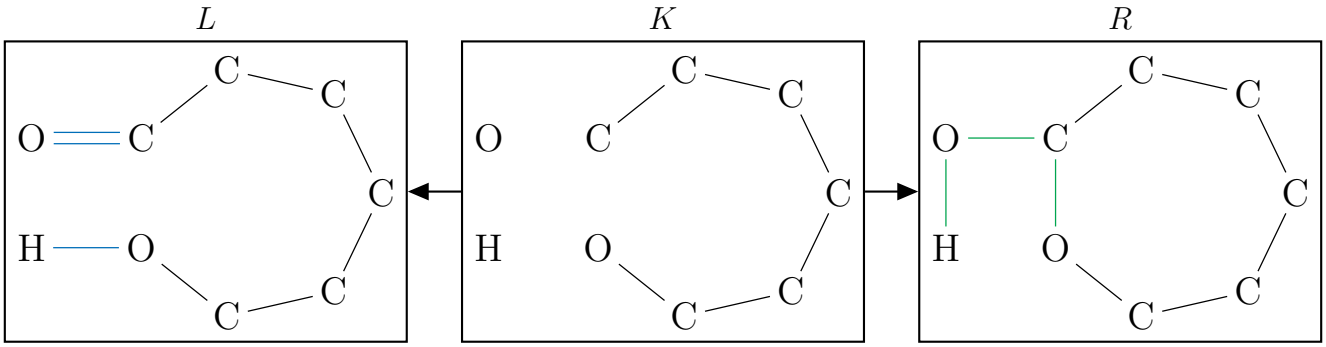
Files: out/546_r_112_11300100_{L, K, R}



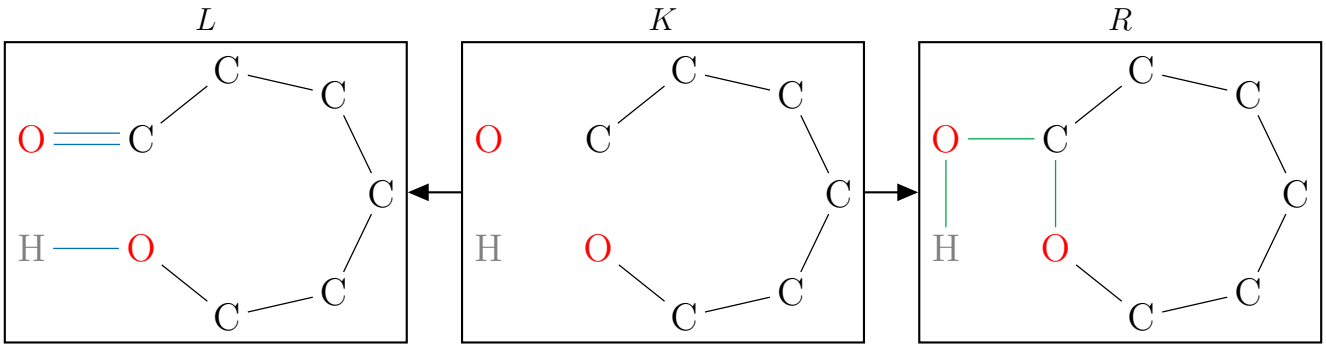
File: out/547_r_112_combined

$$|\{e \in \text{outEdges}(3) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

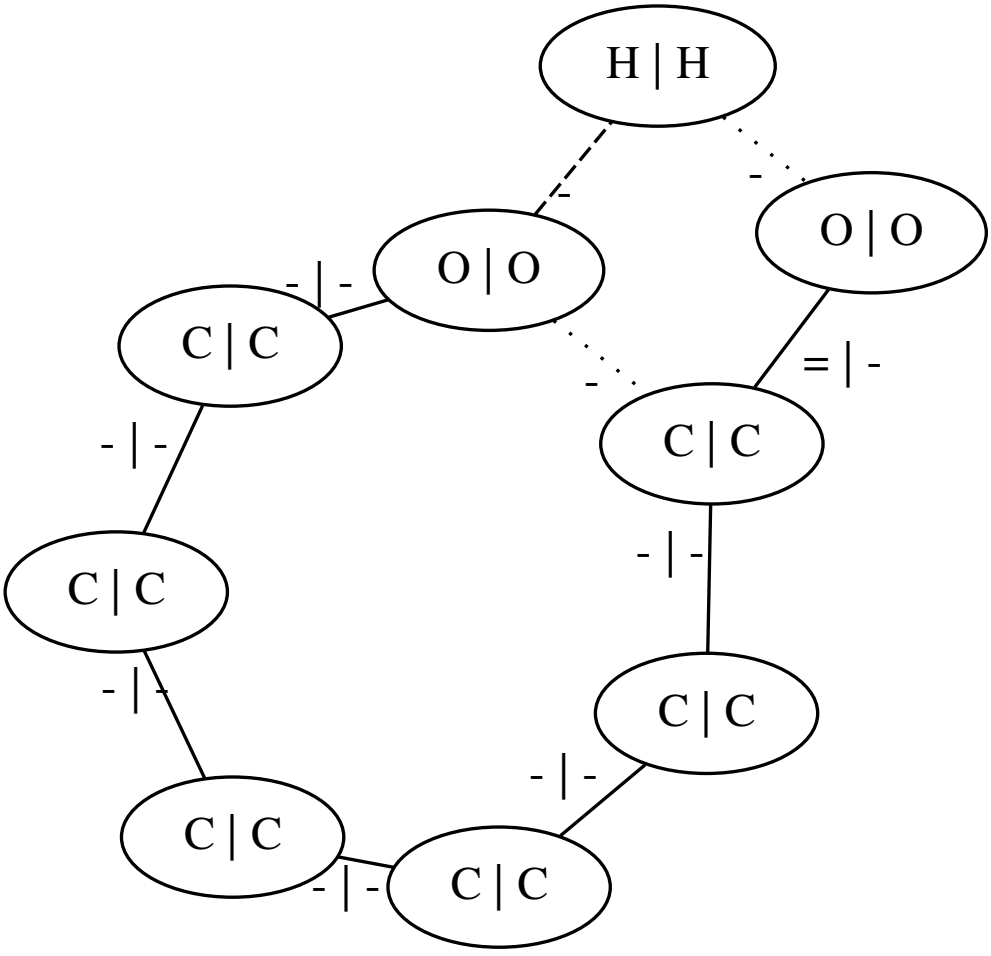
0.0.111 Hemiacetal Formation for 7 membered rings



Files: out/550_r_113_10300000_{L, K, R}



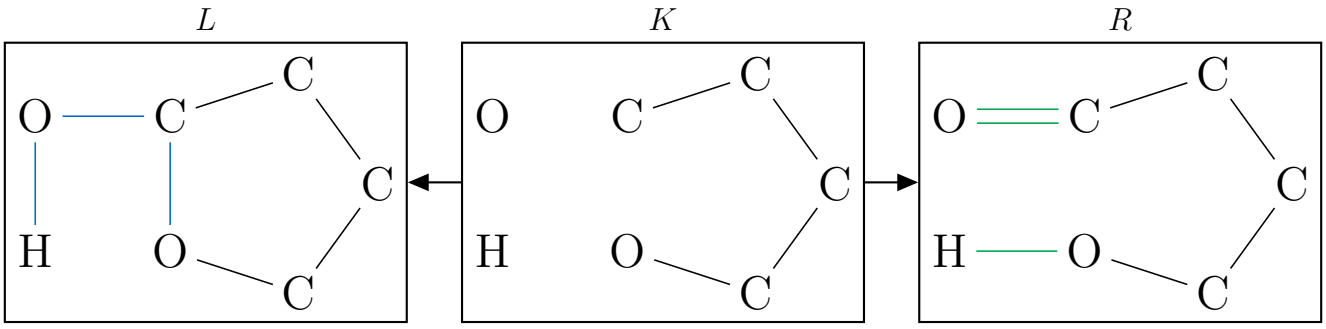
Files: out/551_r_113_11300100_{L, K, R}



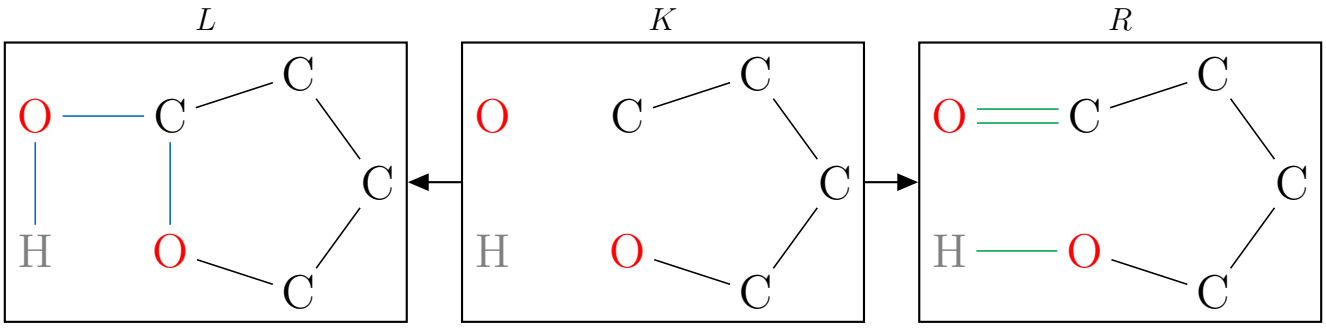
File: out/552_r_113_combined

$$|\{e \in \text{outEdges}(3) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

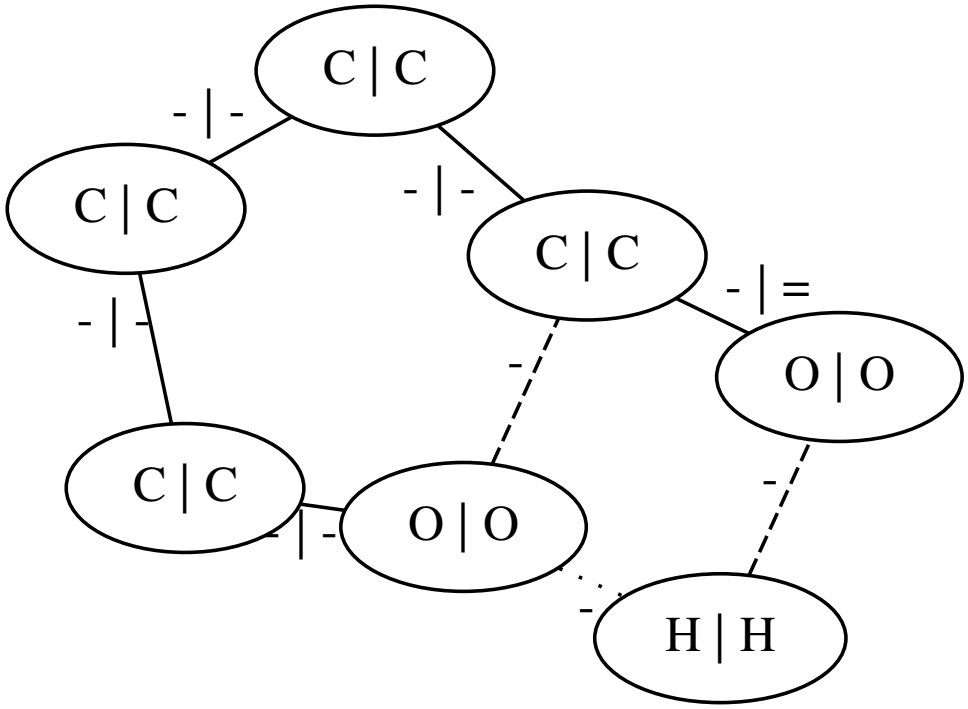
0.0.112 Hemiacetal Formation for 5 membered rings, inverse



Files: out/555_r_114_10300000_{L, K, R}

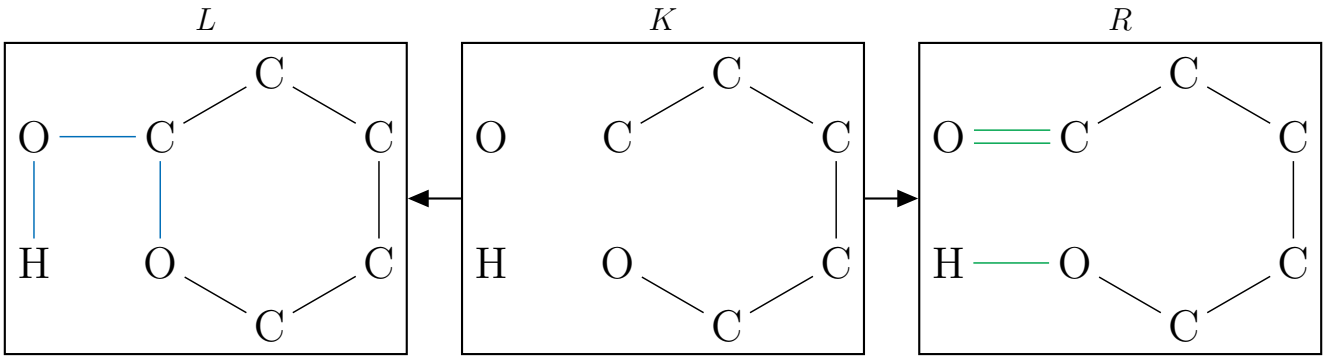


Files: out/556_r_114_11300100_{L, K, R}

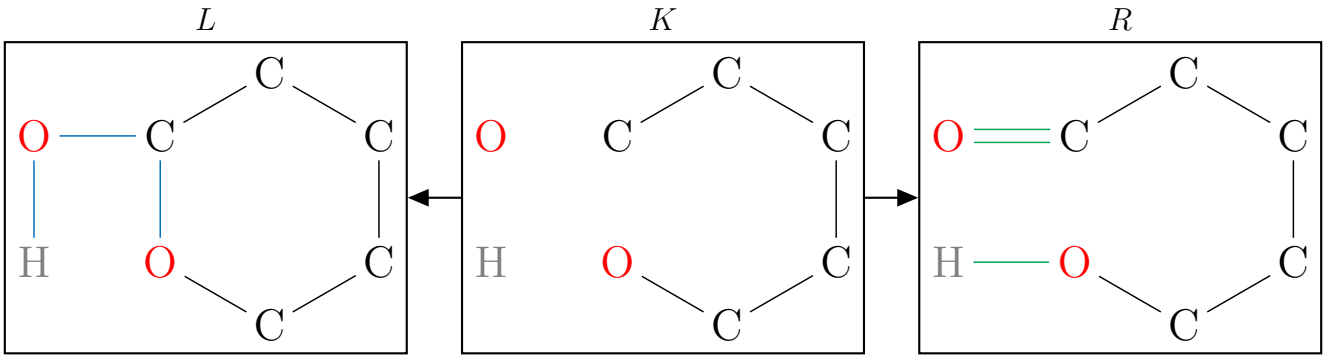


File: out/557_r_114_combined

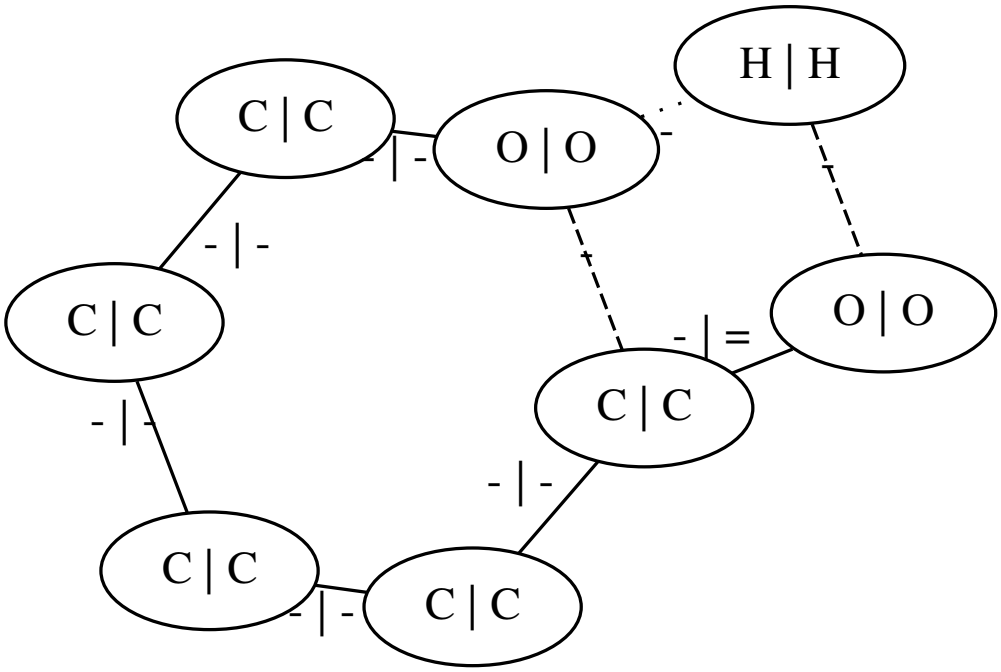
0.0.113 Hemiacetal Formation for 6 membered rings, inverse



Files: out/560_r_115_10300000_{L, K, R}

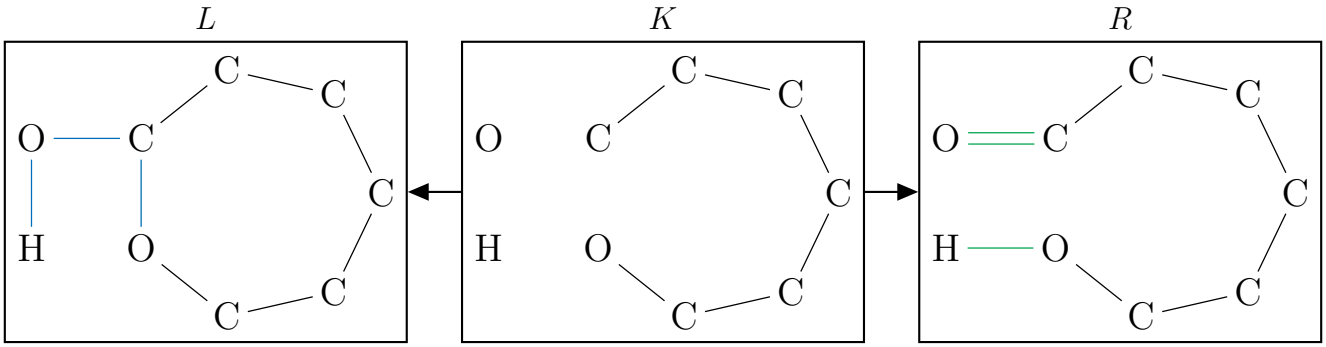


Files: out/561_r_115_11300100_{L, K, R}

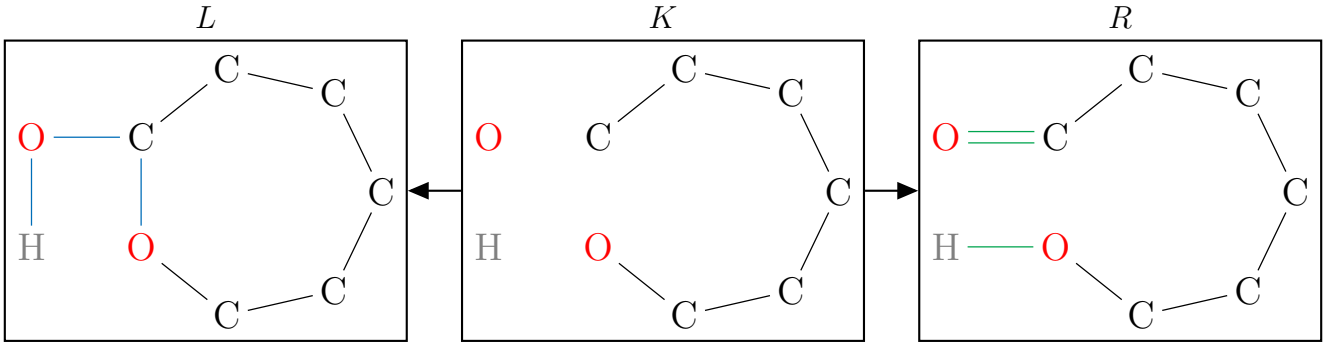


File: out/562_r_115_combined

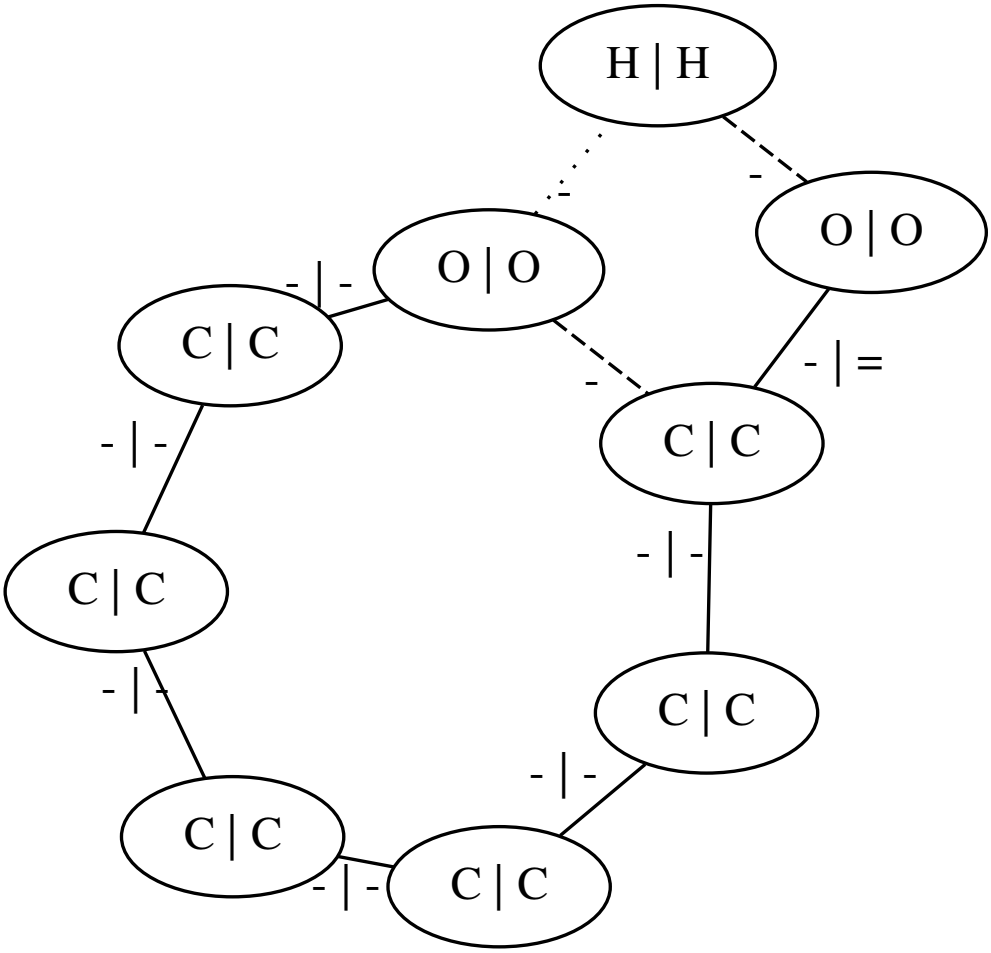
0.0.114 Hemiacetal Formation for 7 membered rings, inverse



Files: out/565_r_116_10300000_{L, K, R}

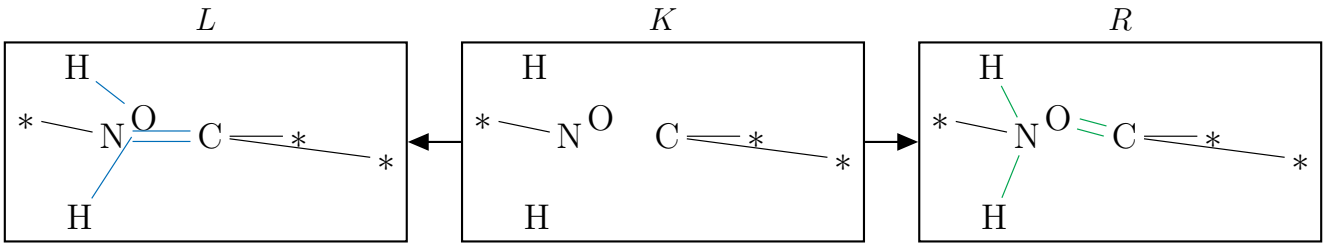


Files: out/566_r_116_11300100_{L, K, R}

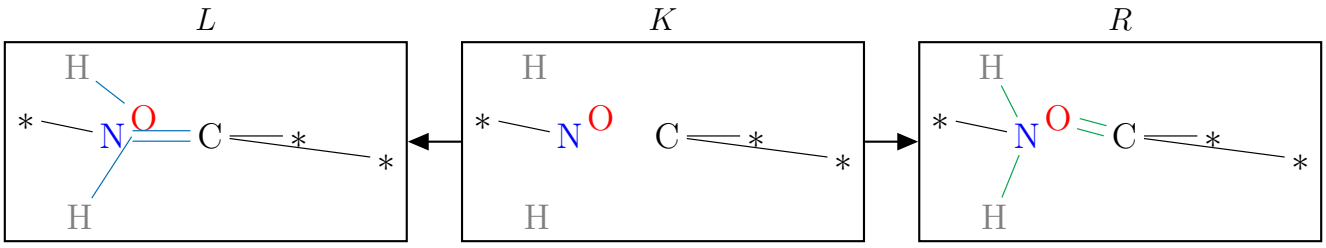


File: out/567_r_116_combined

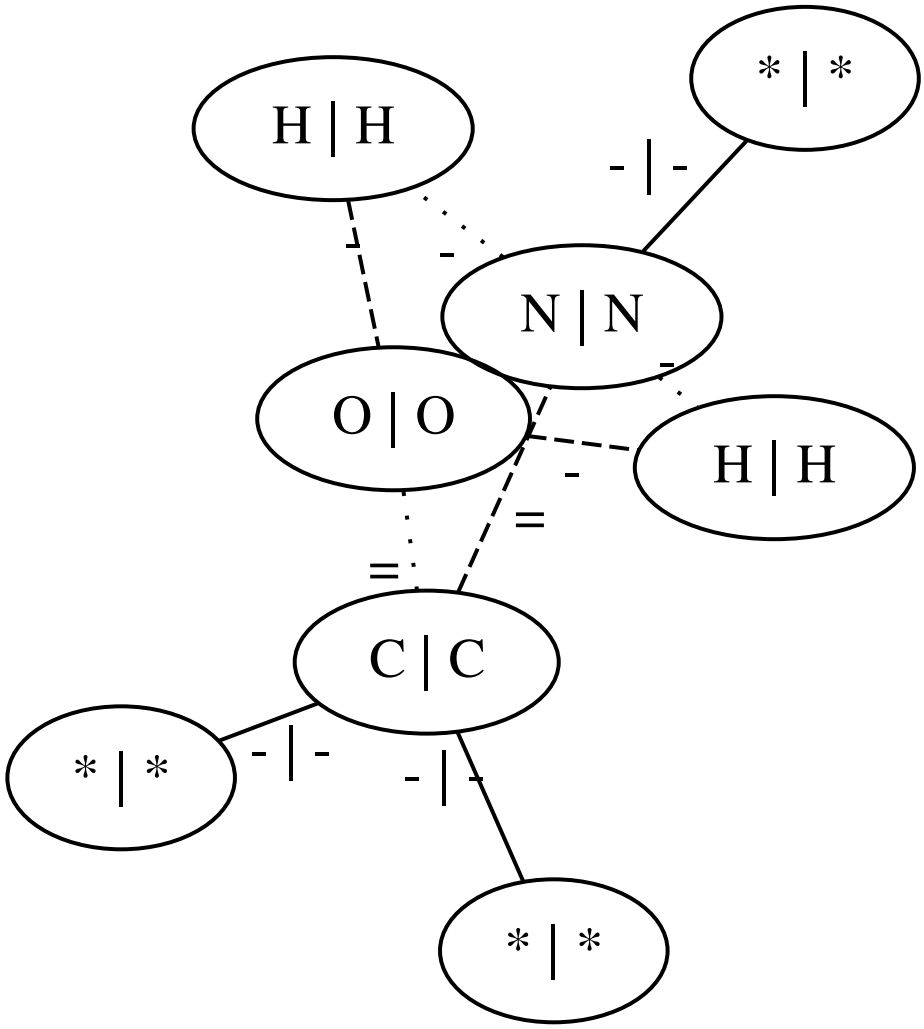
0.0.115 Imine to Carbonyl



Files: out/570_r_117_10300000_{L, K, R}

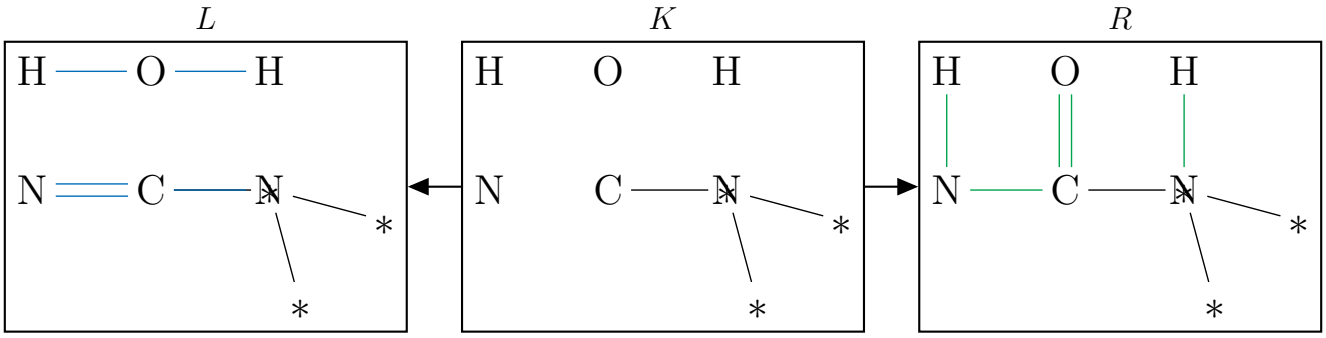


Files: out/571_r_117_11300100_{L, K, R}

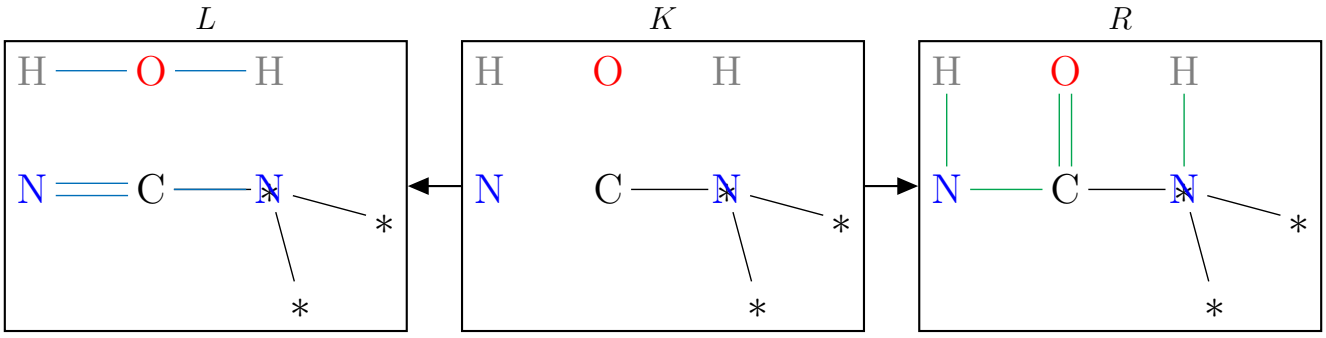


File: out/572_r_117_combined

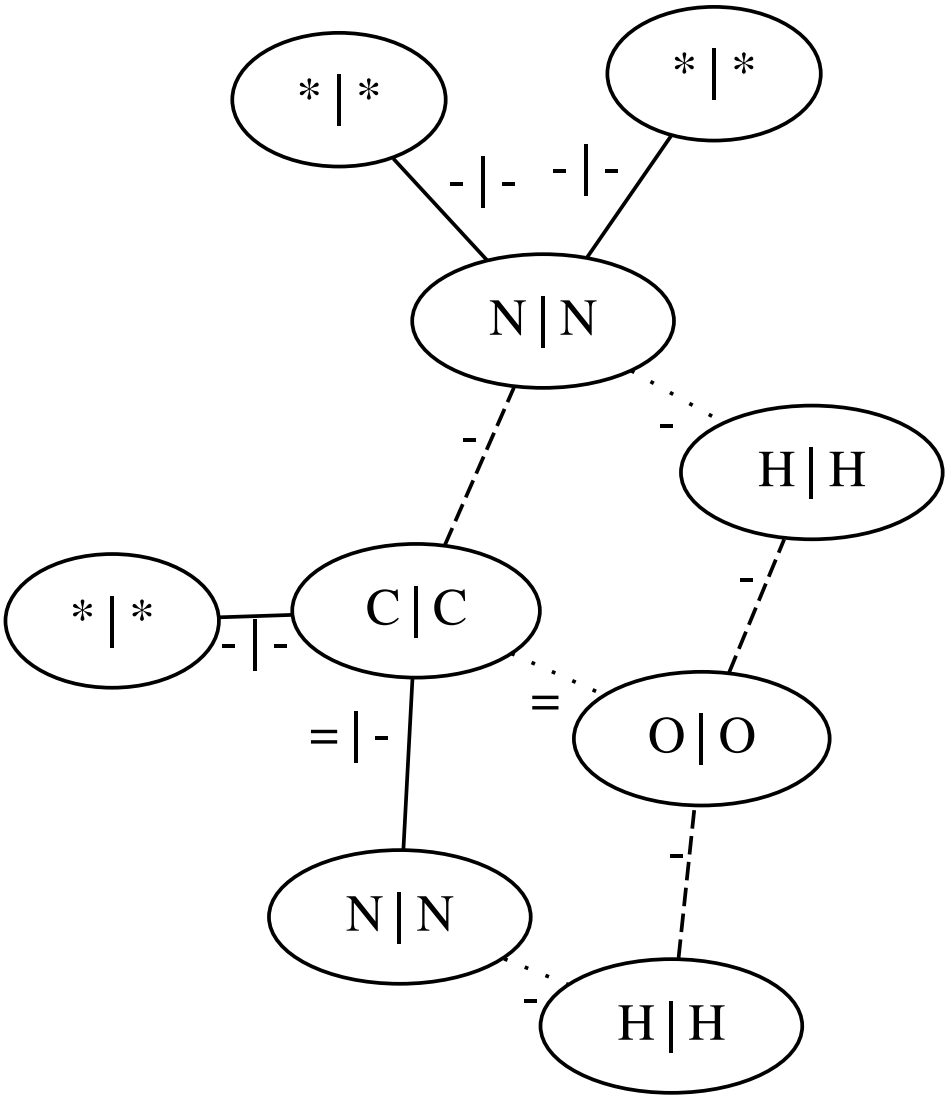
0.0.116 Amidine to Amide Hydrolysis



Files: out/575_r_118_10300000_{L, K, R}

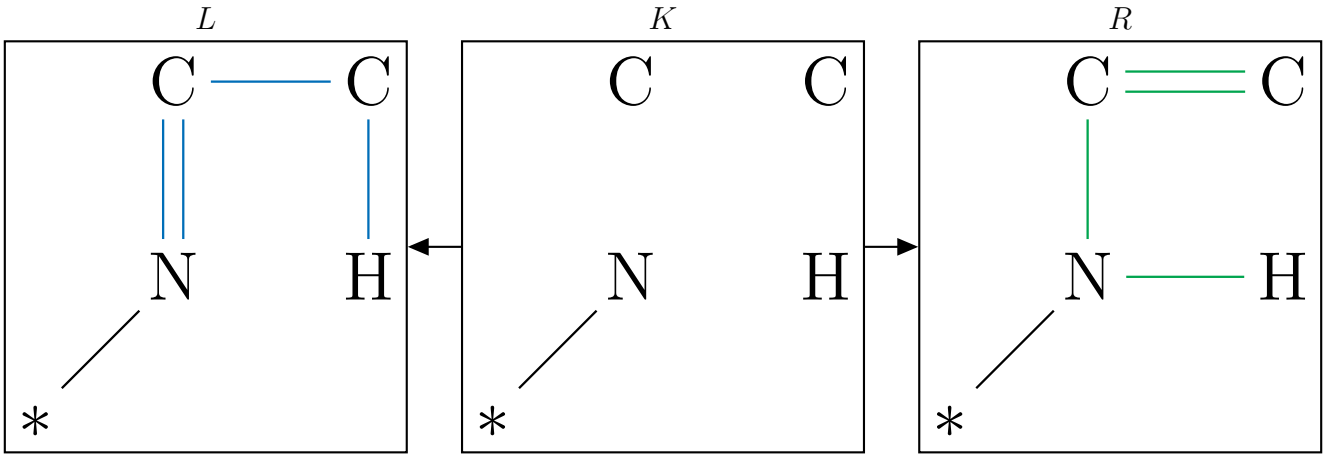


Files: out/576_r_118_11300100_{L, K, R}

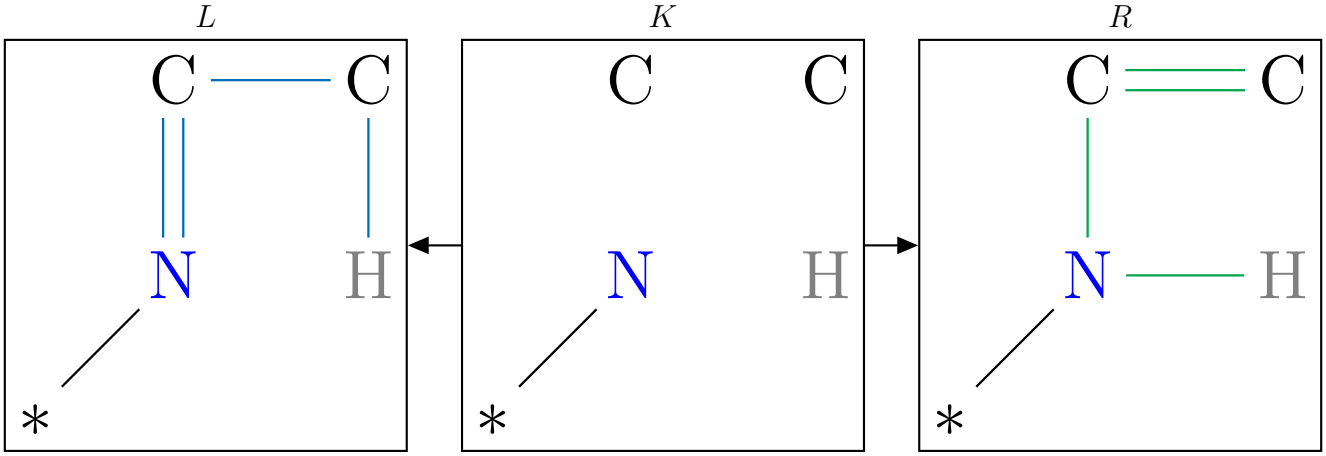


File: out/577_r_118_combined

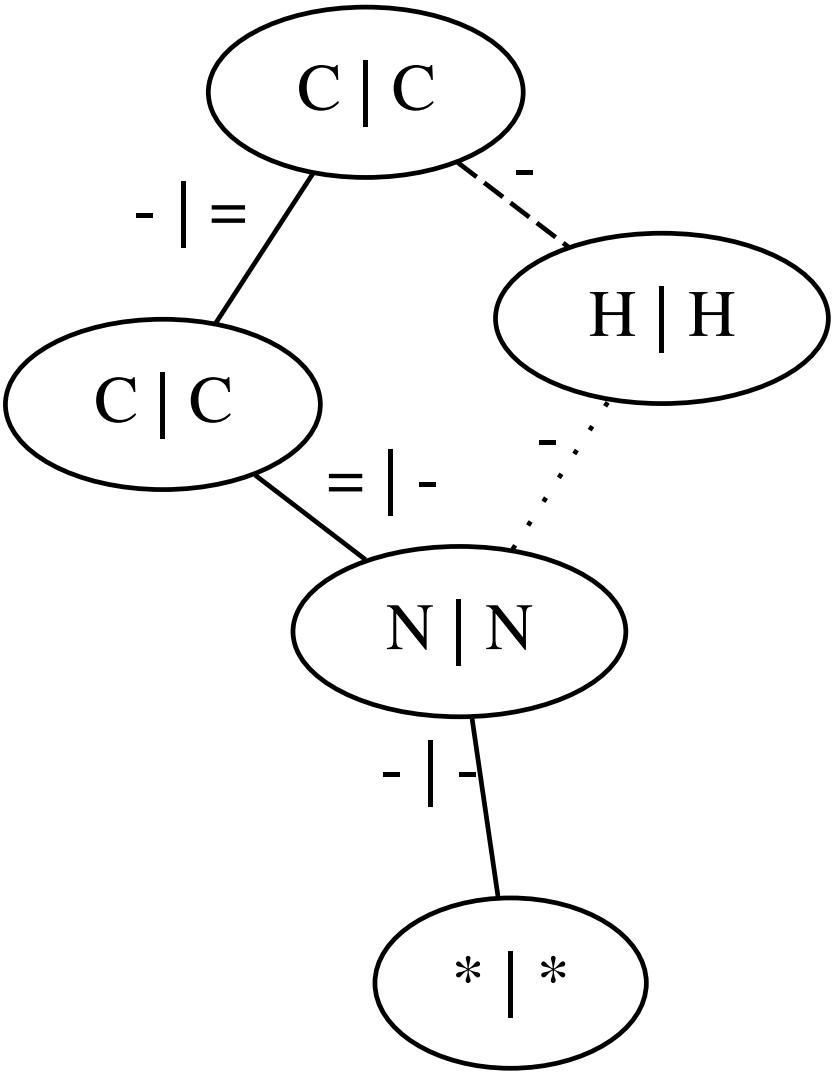
0.0.117 Imine to Enamine



Files: out/580_r_119_10300000_{L, K, R}



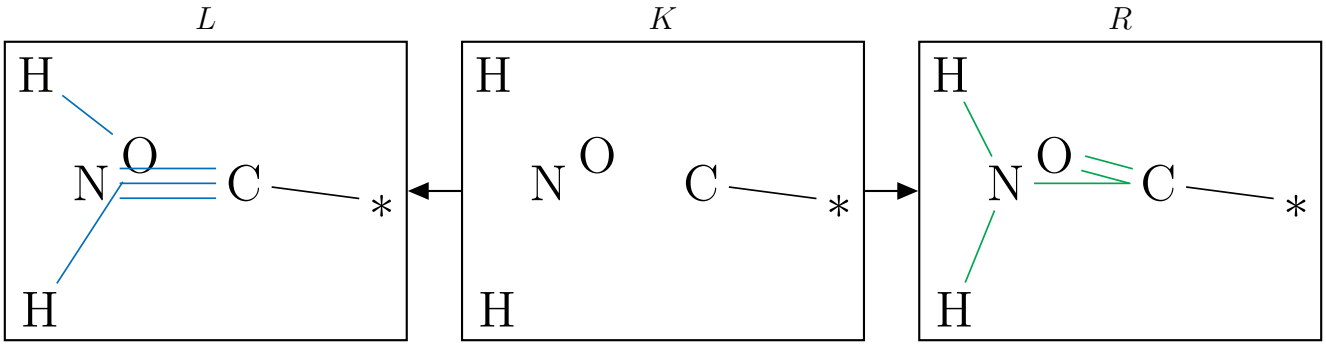
Files: out/581_r_119_11300100_{L, K, R}



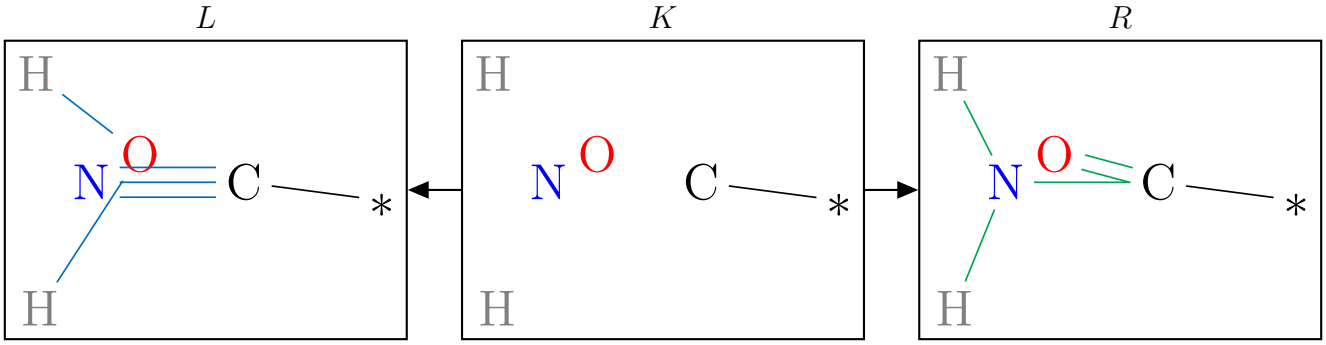
File: out/582_r_119_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

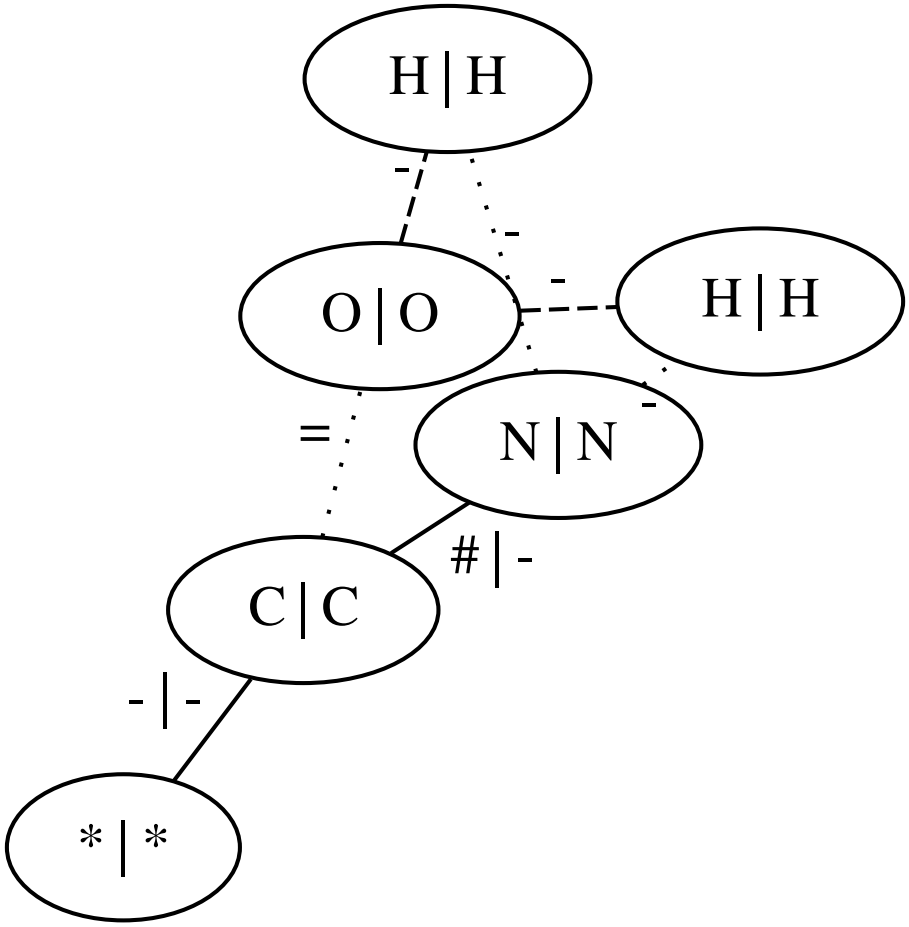
0.0.118 Nitrile Hydrolysis



Files: out/585_r_120_10300000_{L, K, R}

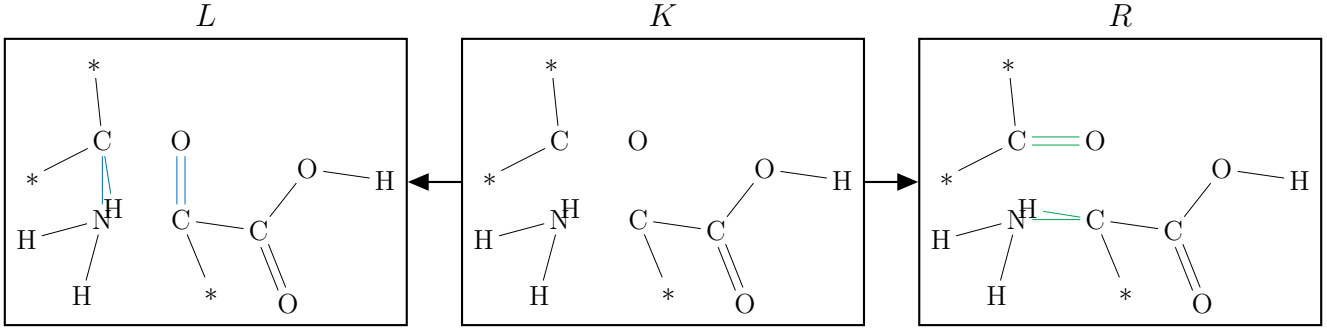


Files: out/586_r_120_11300100_{L, K, R}

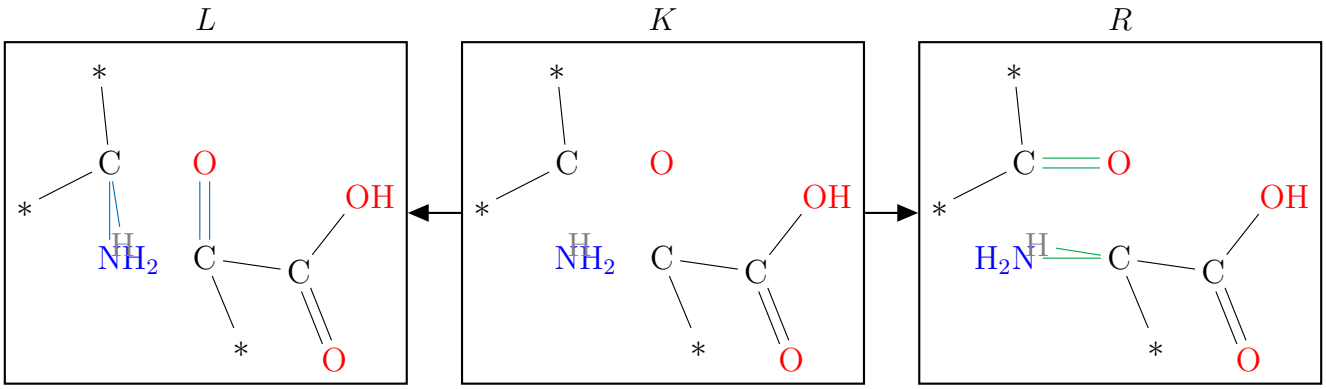


File: out/587_r_120_combined

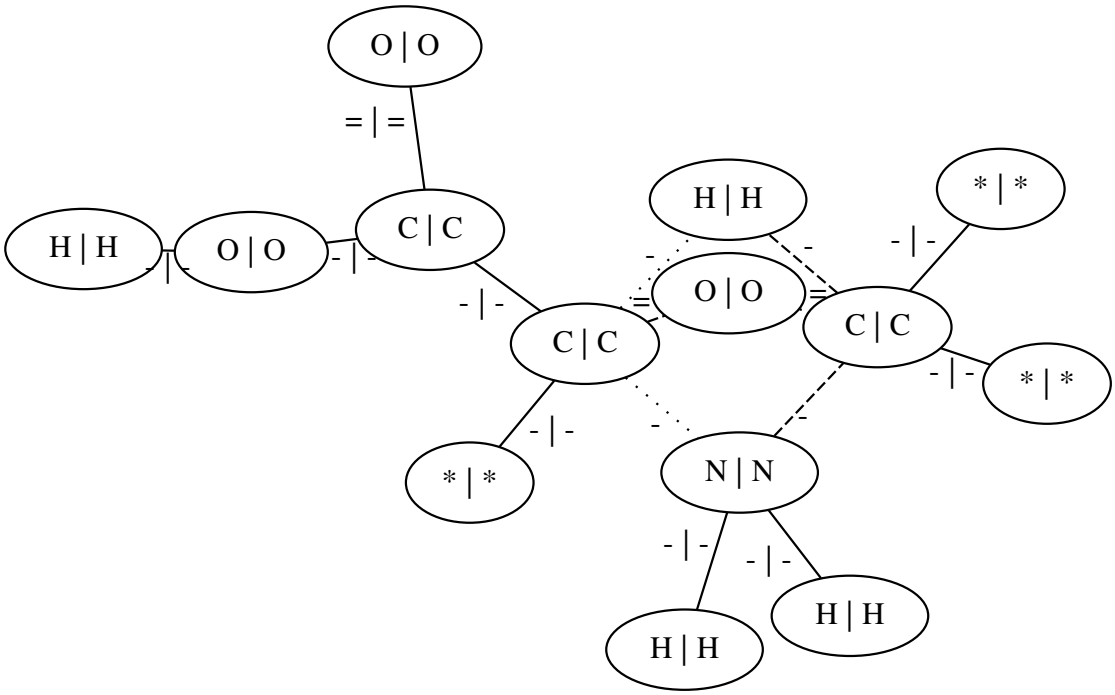
0.0.119 Transamination



Files: out/590_r_121_10300000_{L, K, R}



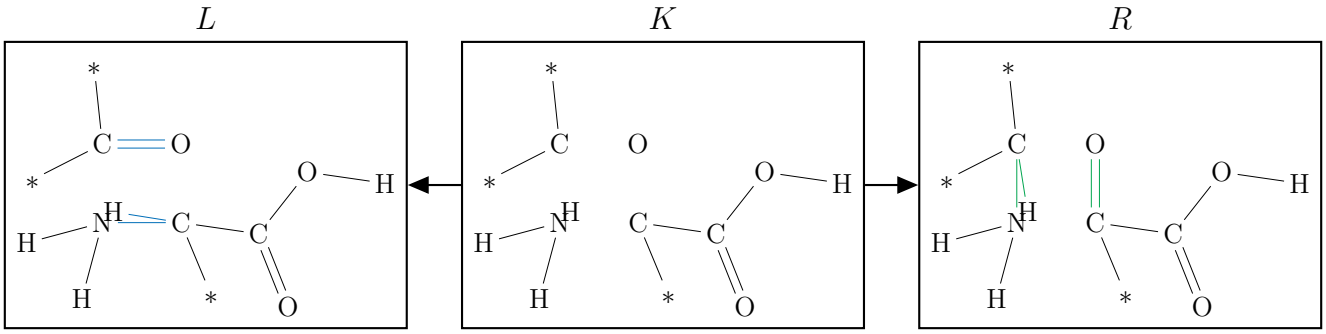
Files: out/591_r_121_11300100_{L, K, R}



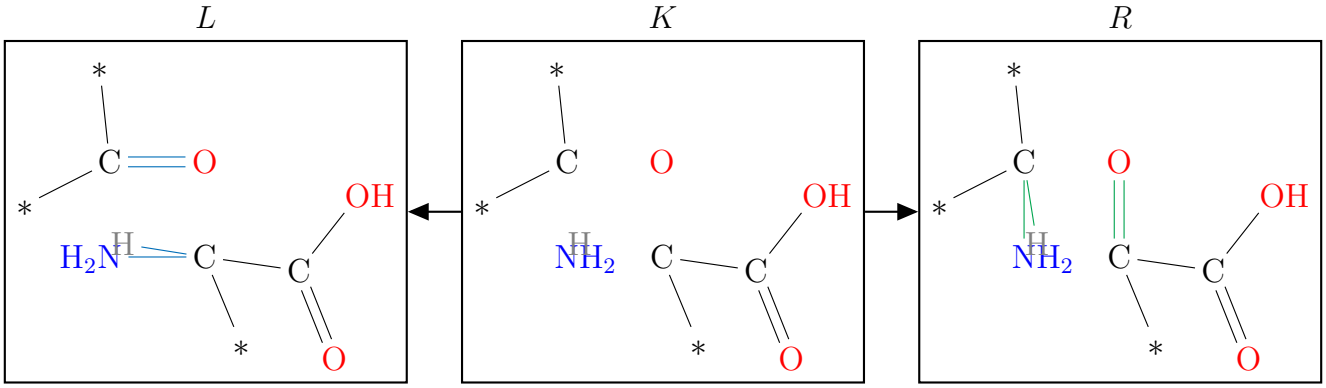
File: out/592_r_121_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

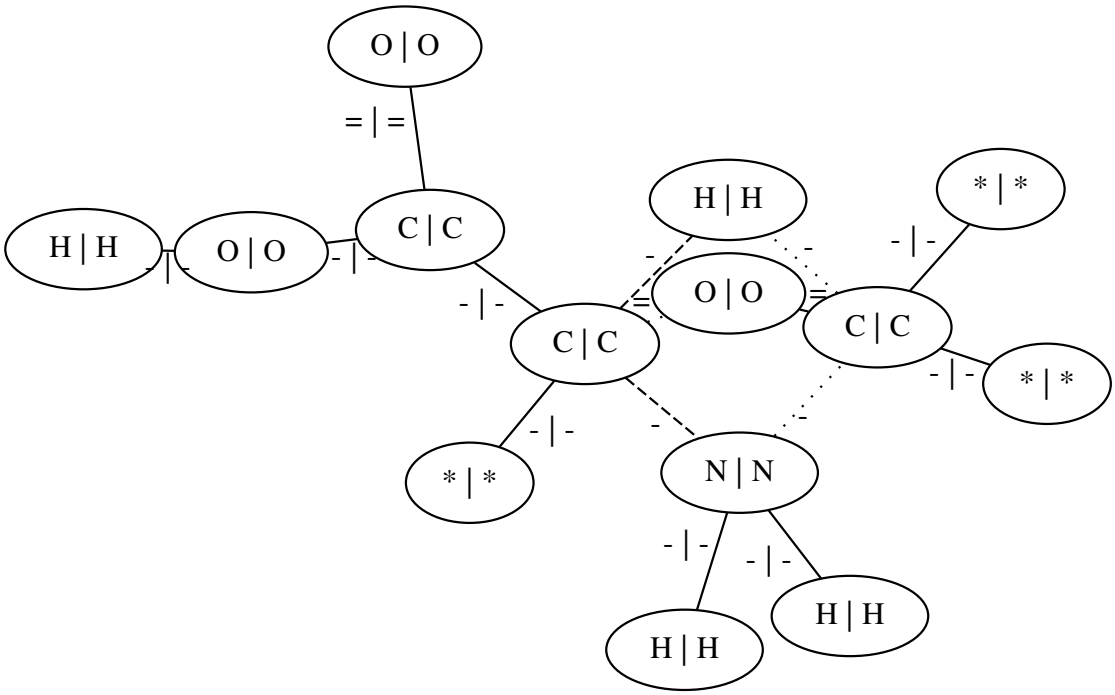
0.0.120 Transamination (inverse)



Files: out/595_r_122_10300000_{L, K, R}



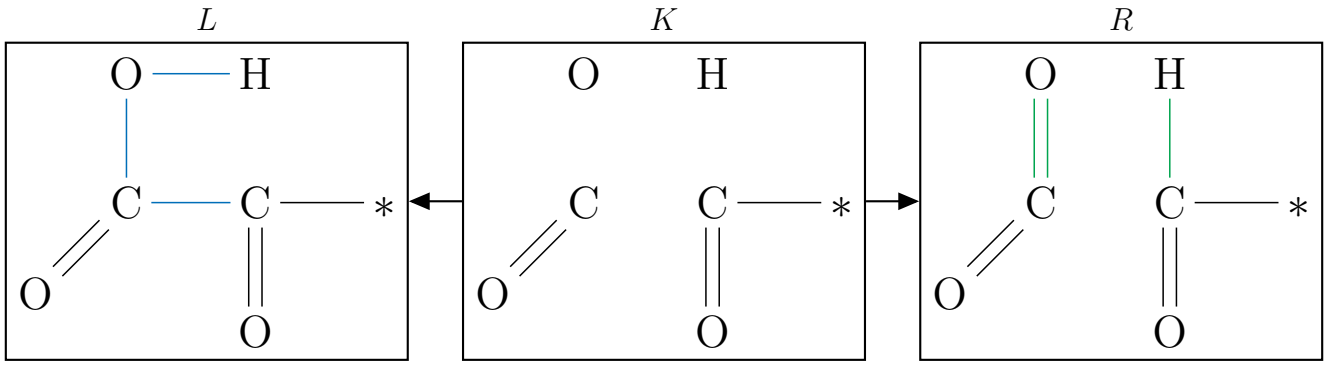
Files: out/596_r_122_11300100_{L, K, R}



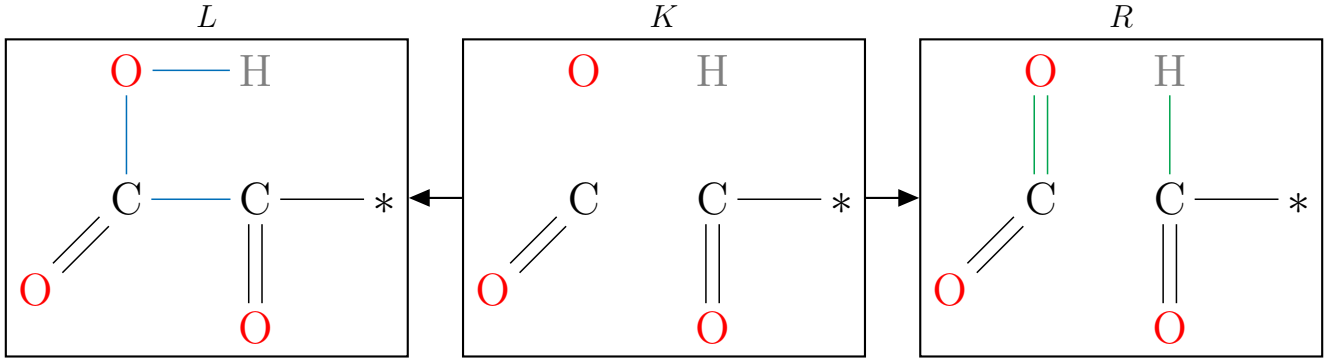
File: out/597_r_122_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

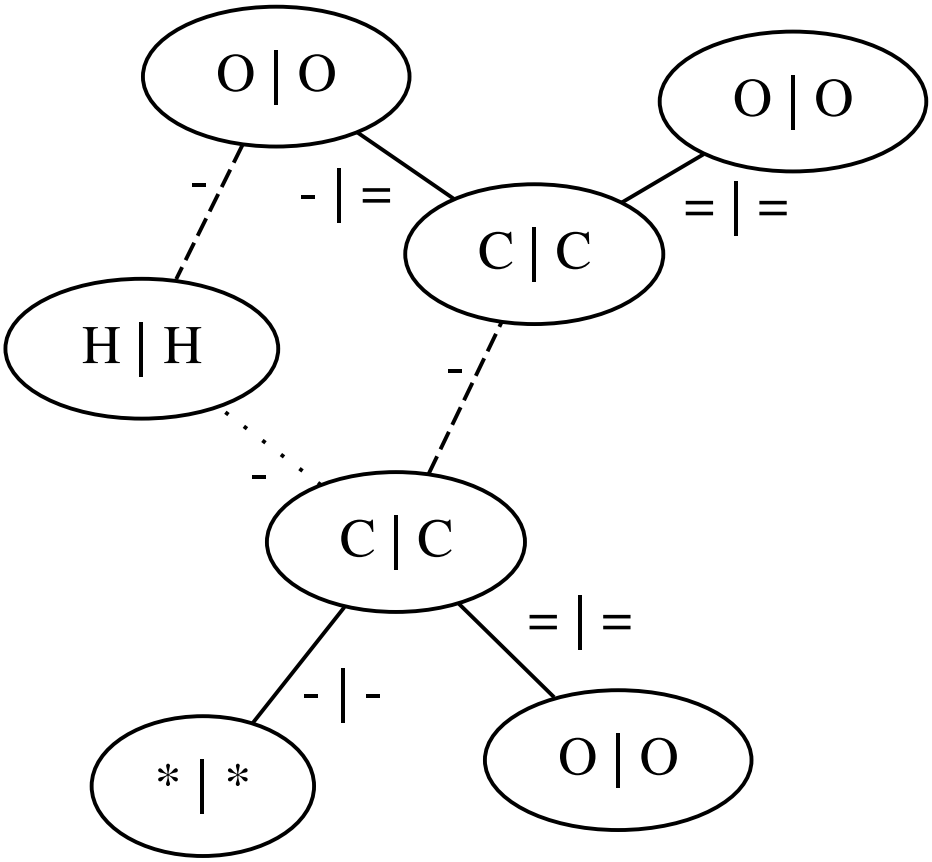
0.0.121 Alpha-Keto Acid Decarboxylation



Files: out/600_r_123_10300000_{L, K, R}

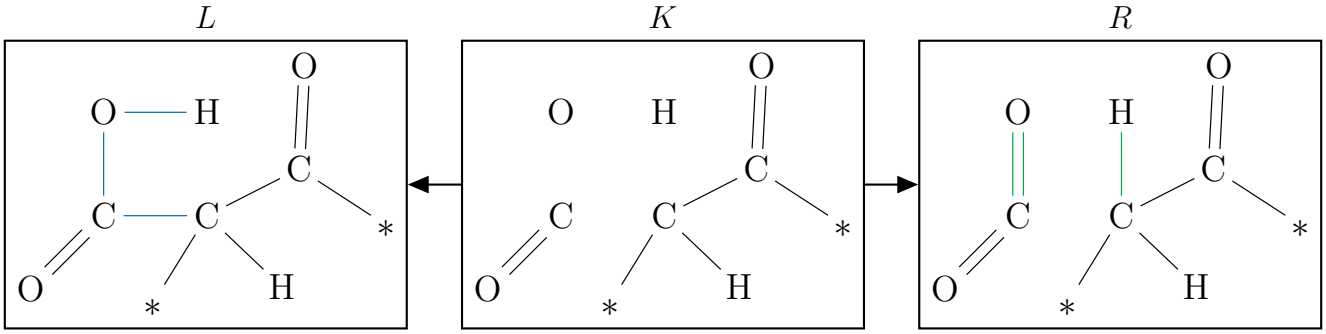


Files: out/601_r_123_11300100_{L, K, R}

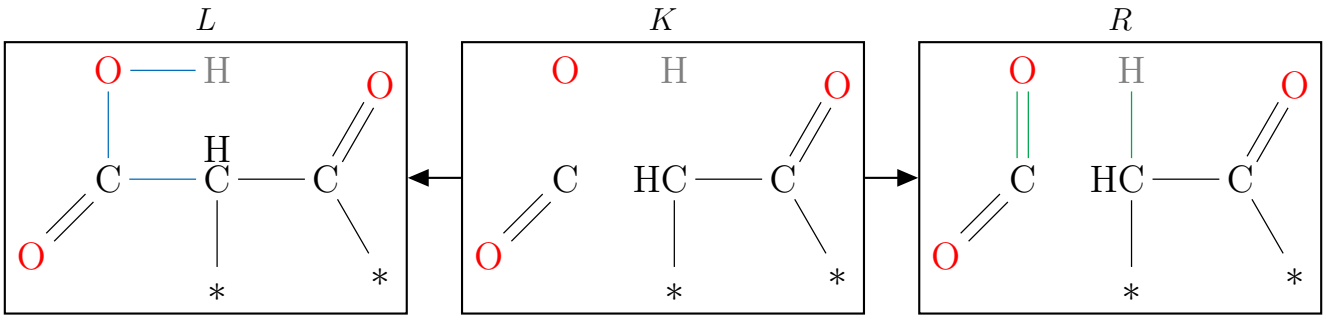


File: out/602_r_123_combined

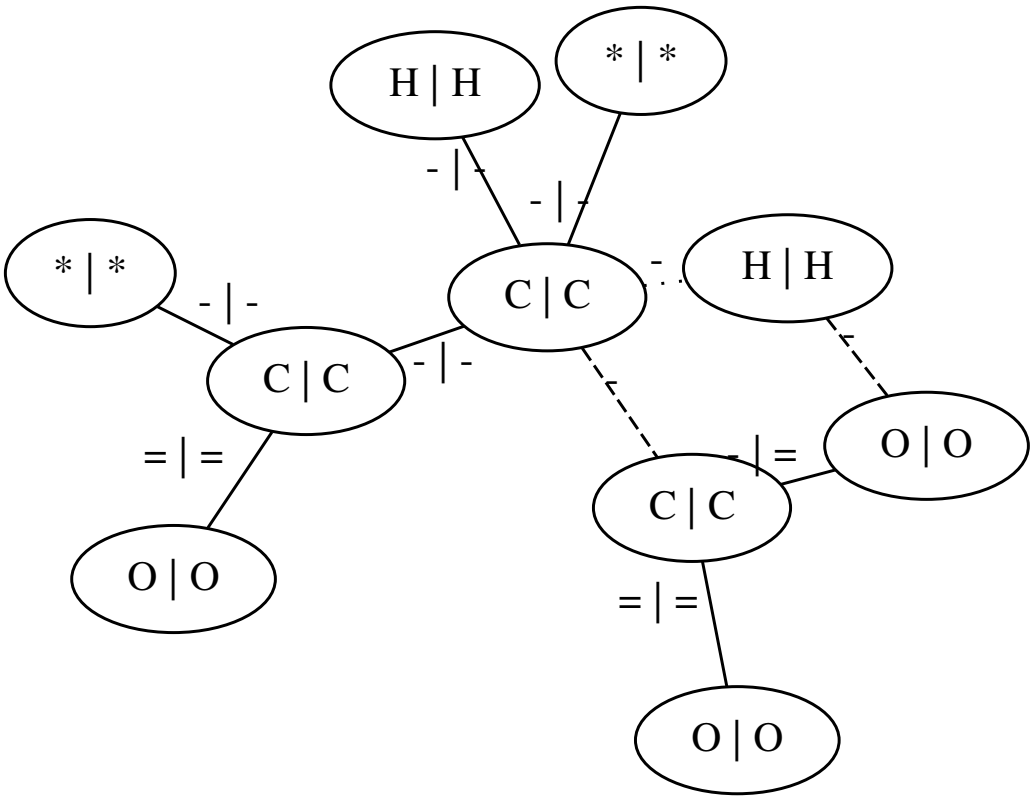
0.0.122 Beta Decarboxylation



Files: out/605_r_124_10300000_{L, K, R}

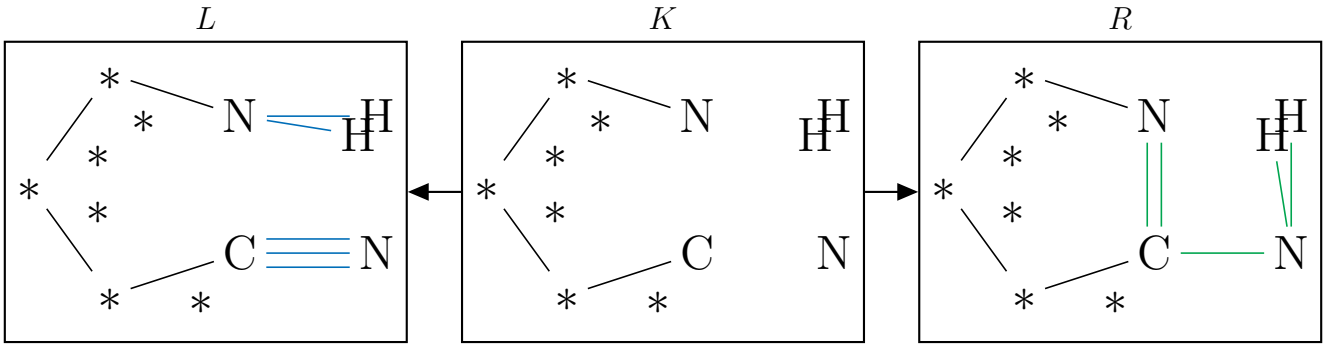


Files: out/606_r_124_11300100_{L, K, R}

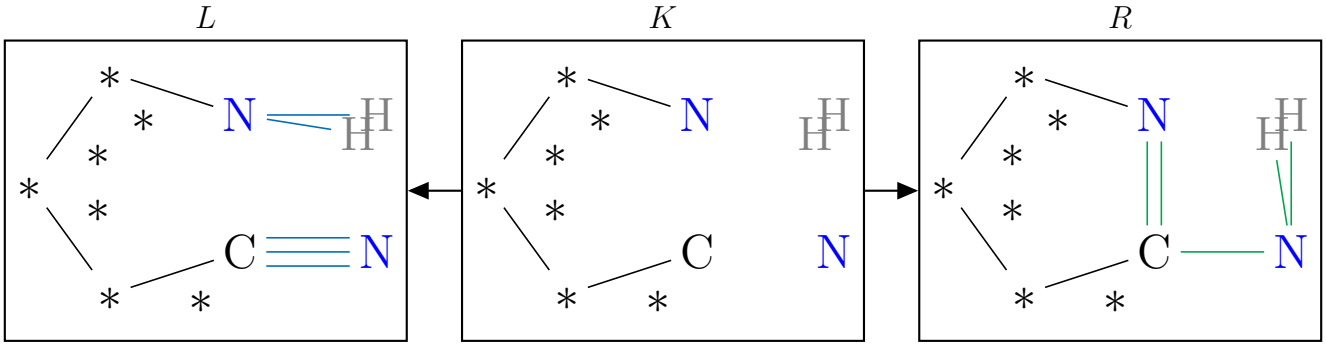


File: out/607_r_124_combined

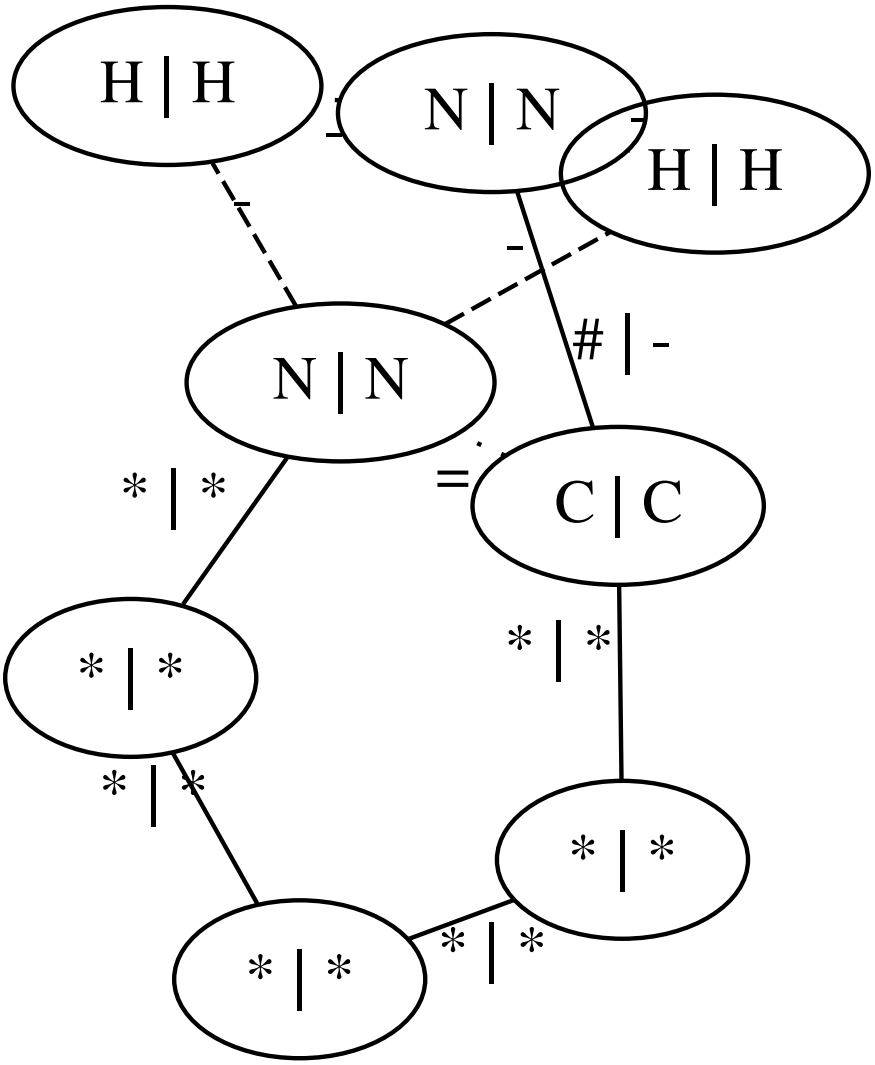
0.0.123 Nitrile Ring Closure 5



Files: out/610_r_125_10300000_{L, K, R}



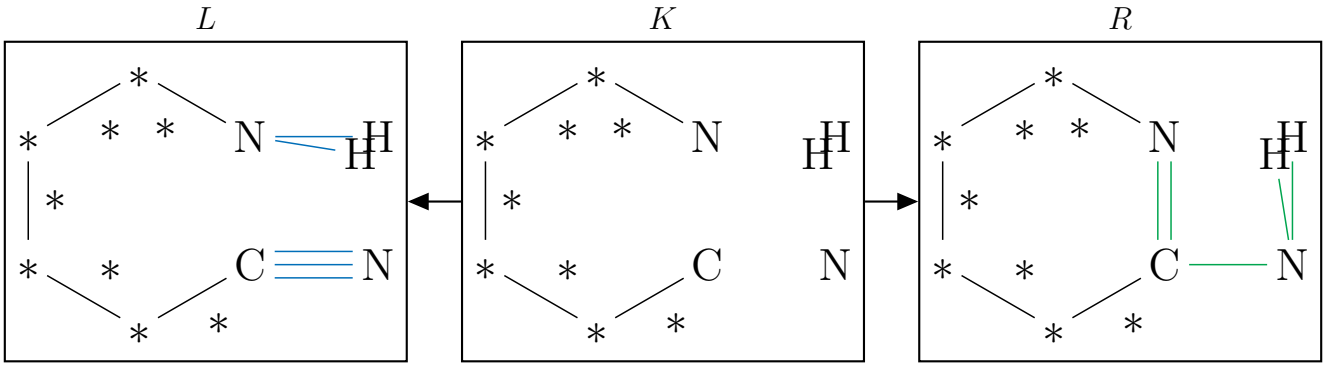
Files: out/611_r_125_11300100_{L, K, R}



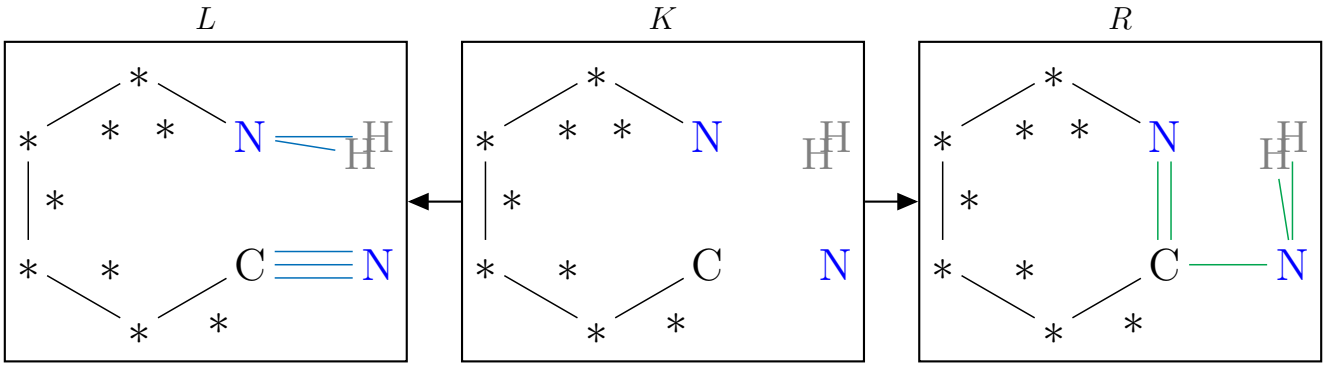
File: out/612_r_125_combined

$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

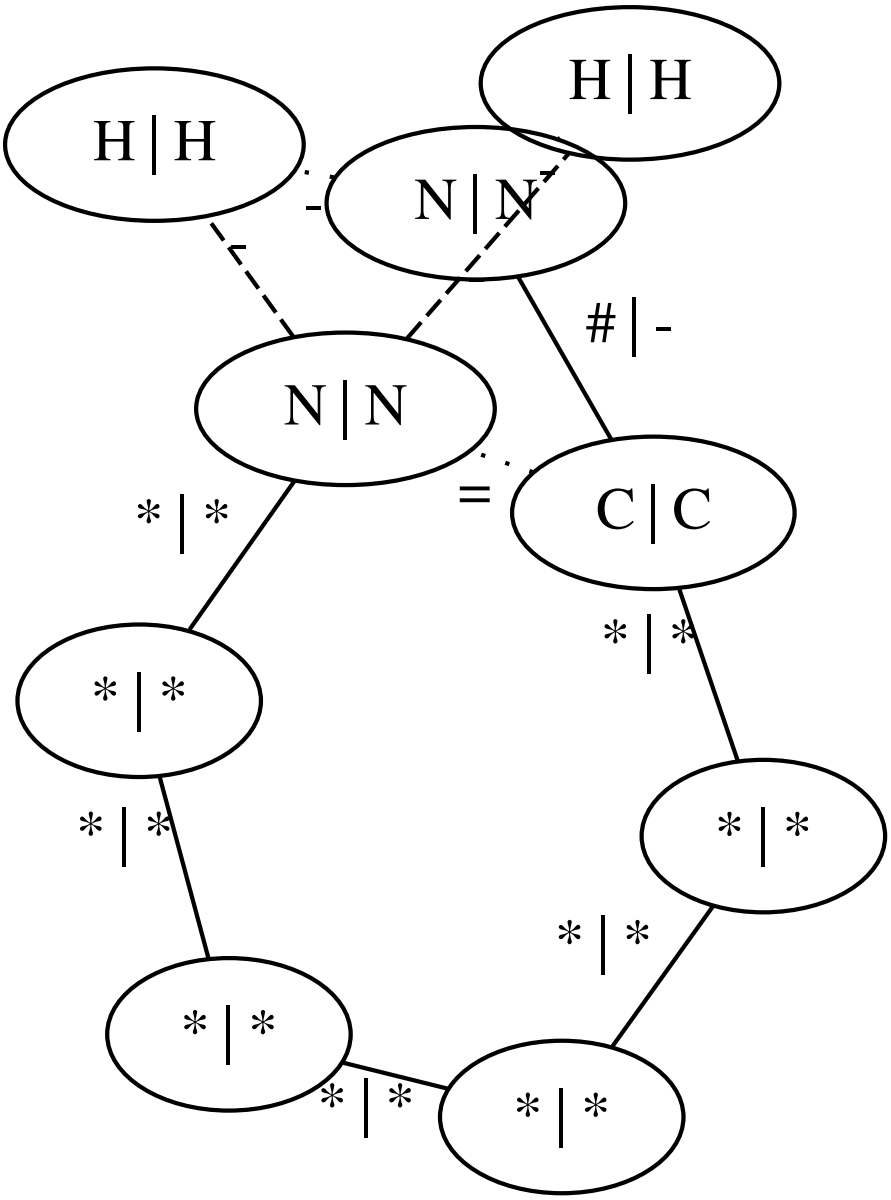
0.0.124 Nitrile Ring Closure 6



Files: out/615_r_126_10300000_{L, K, R}



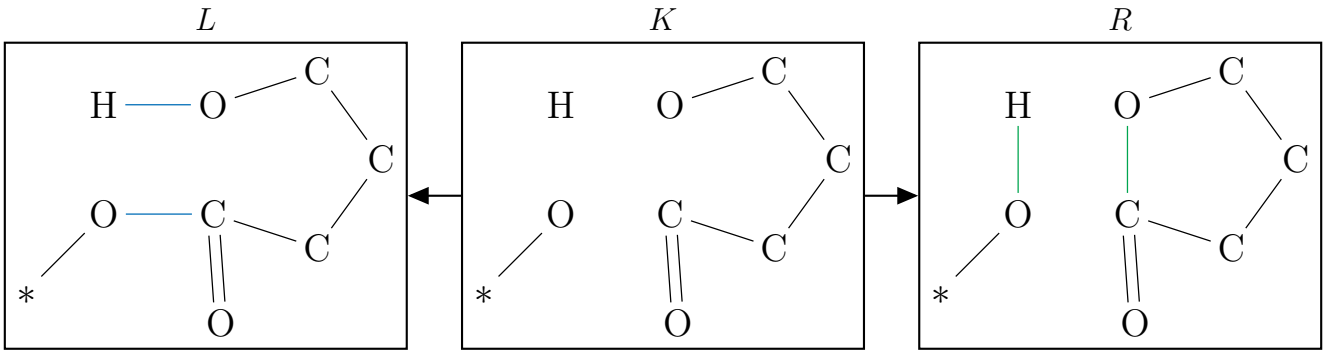
Files: out/616_r_126_11300100_{L, K, R}



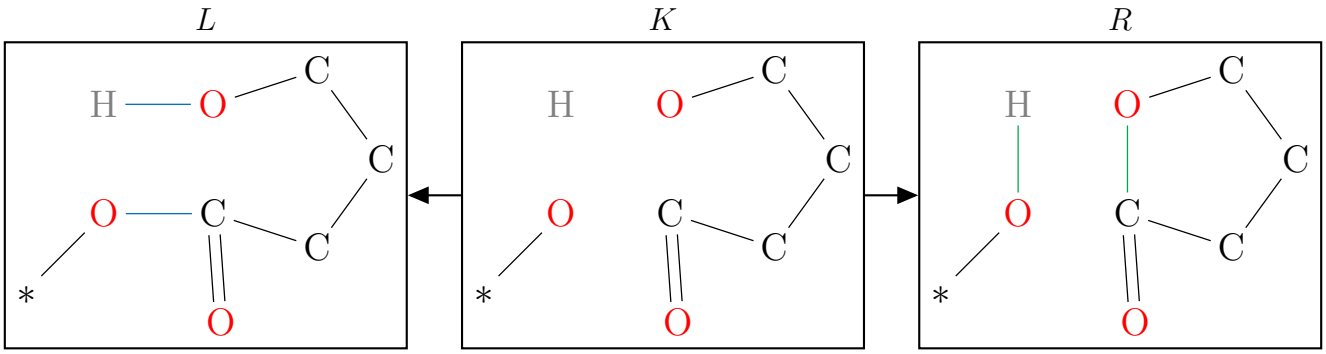
File: out/617_r_126_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

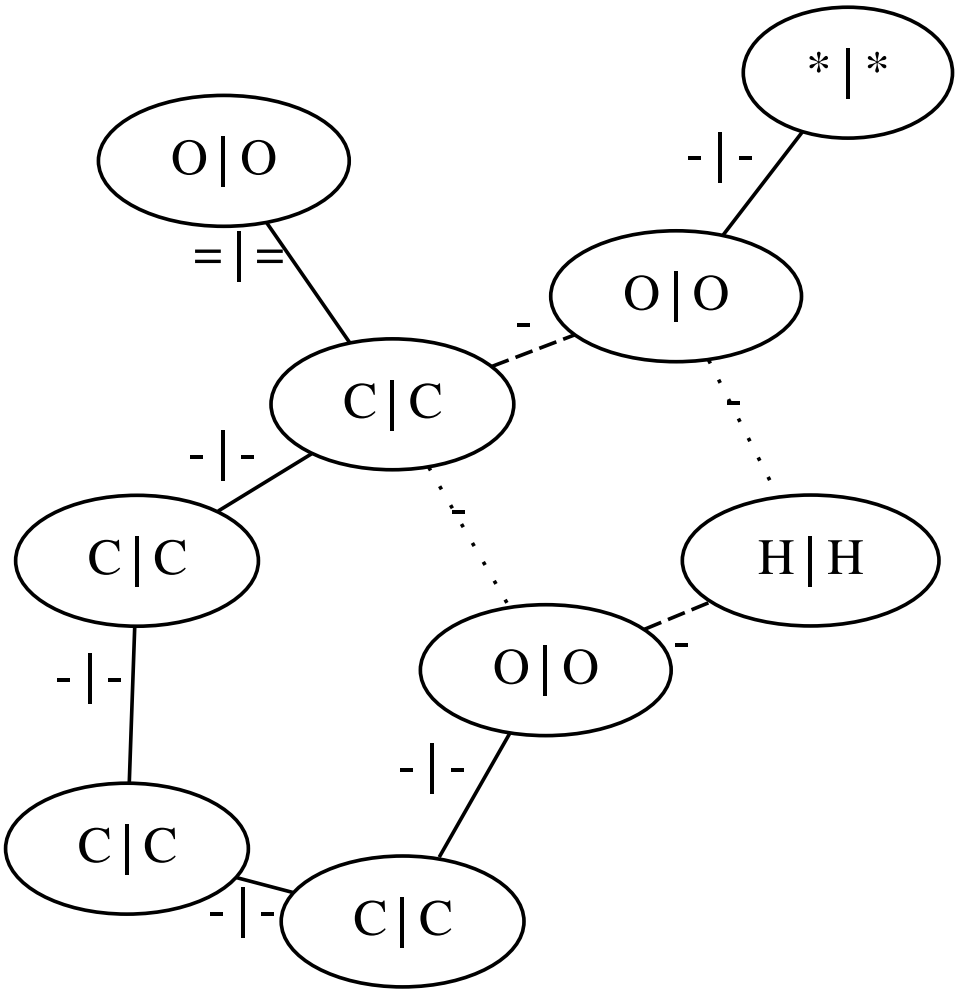
0.0.125 Ring Closure 5 membered O, O



Files: out/620_r_127_10300000_{L, K, R}



Files: out/621_r_127_11300100_{L, K, R}

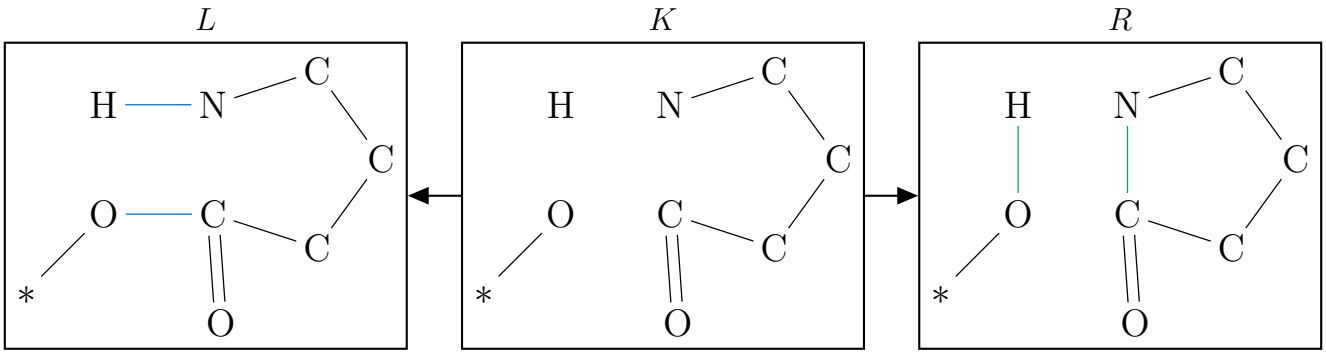


File: out/622_r_127_combined

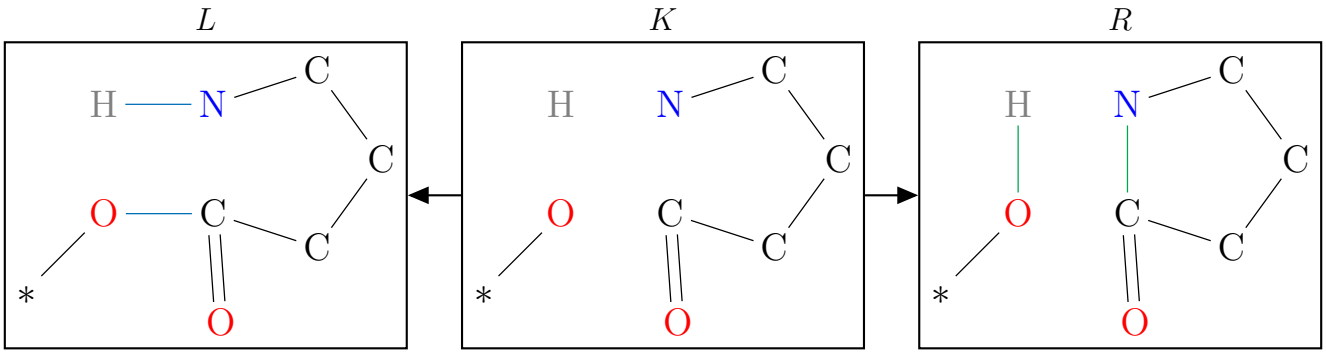
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

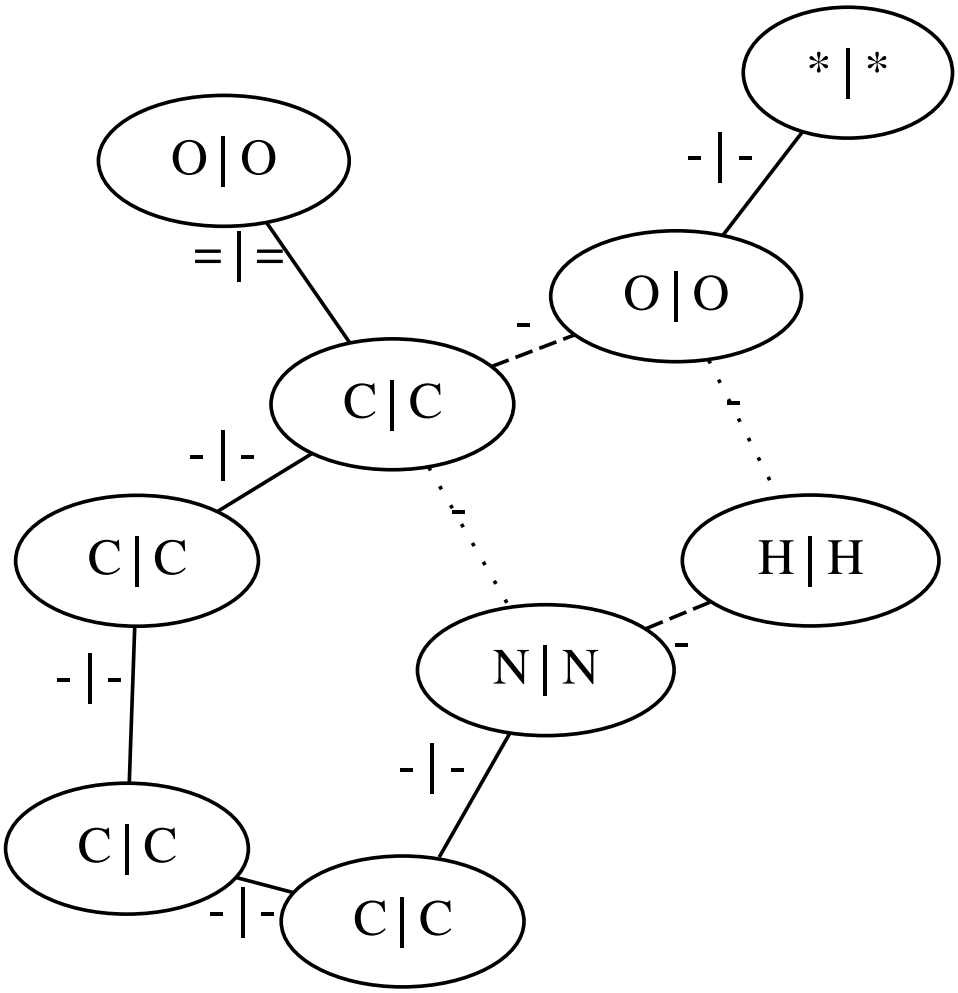
0.0.126 Ring Closure 5 membered O, N



Files: out/625_r_128_10300000_{L, K, R}



Files: out/626_r_128_11300100_{L, K, R}

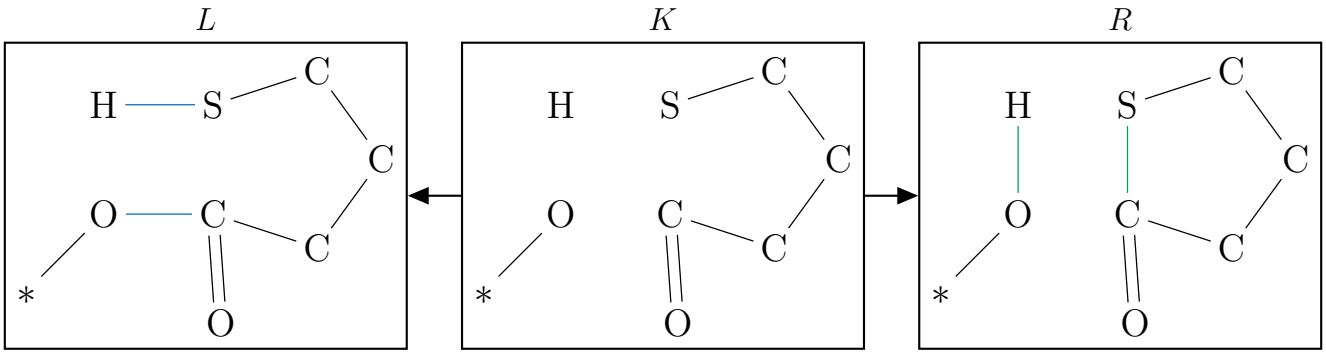


File: out/627_r_128_combined

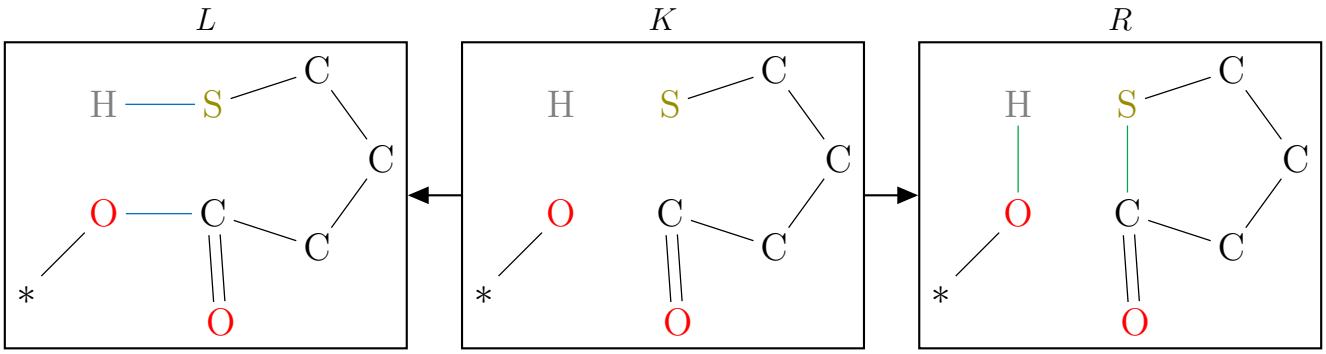
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

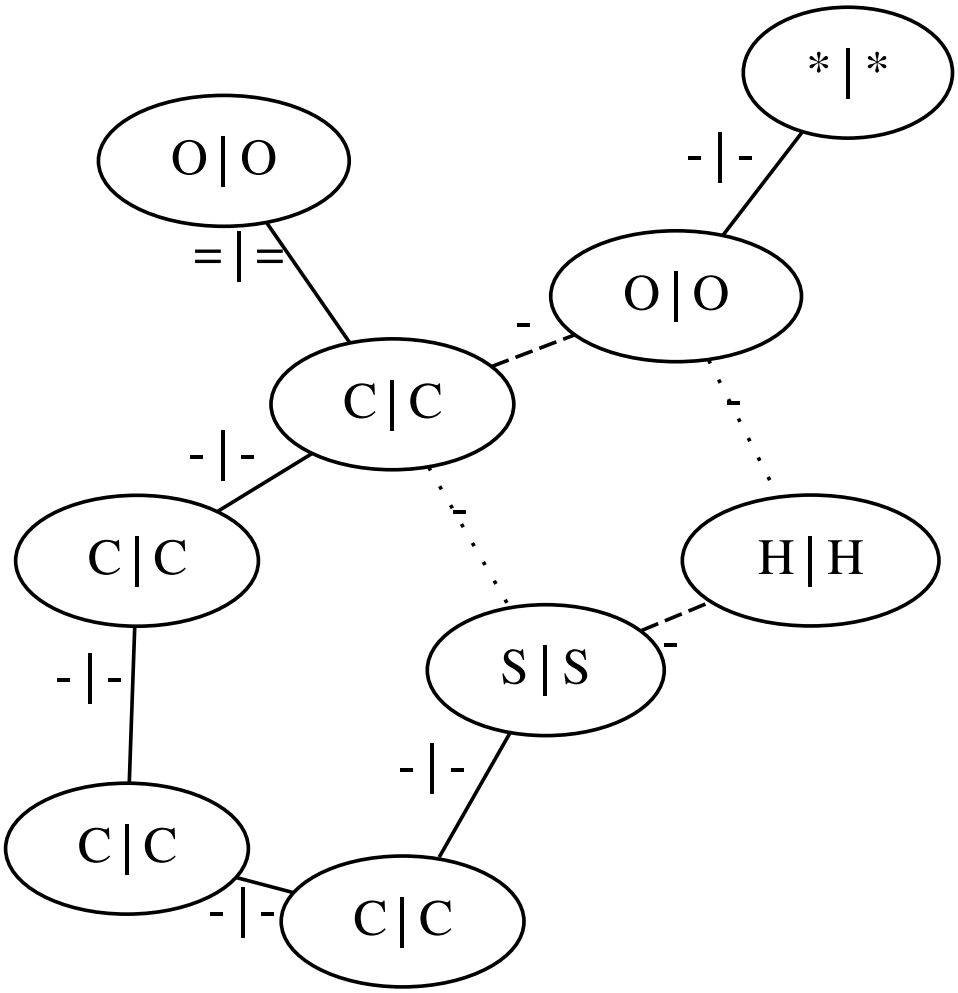
0.0.127 Ring Closure 5 membered O, S



Files: out/630_r_129_10300000_{L, K, R}



Files: out/631_r_129_11300100_{L, K, R}

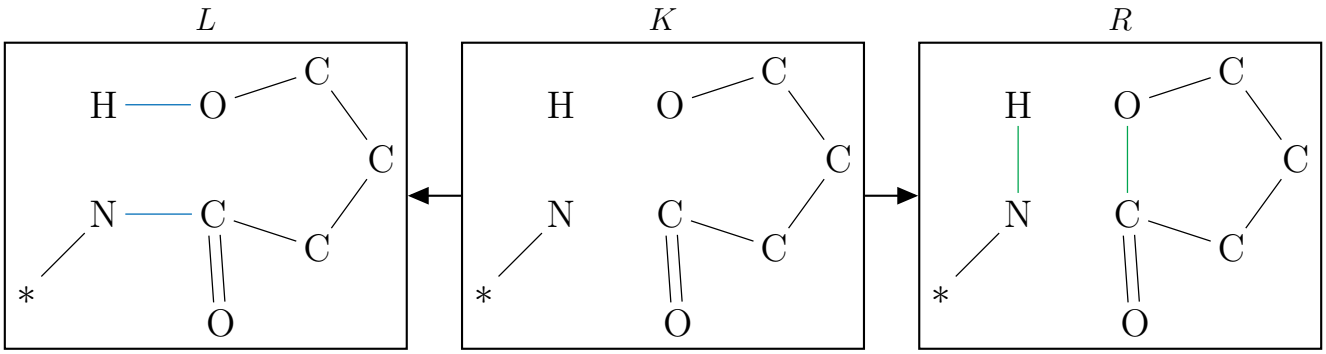


File: out/632_r_129_combined

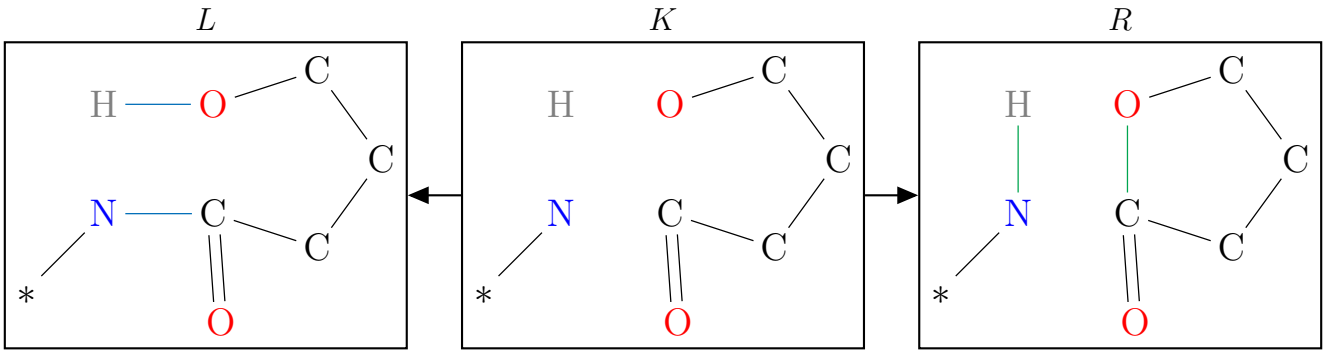
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

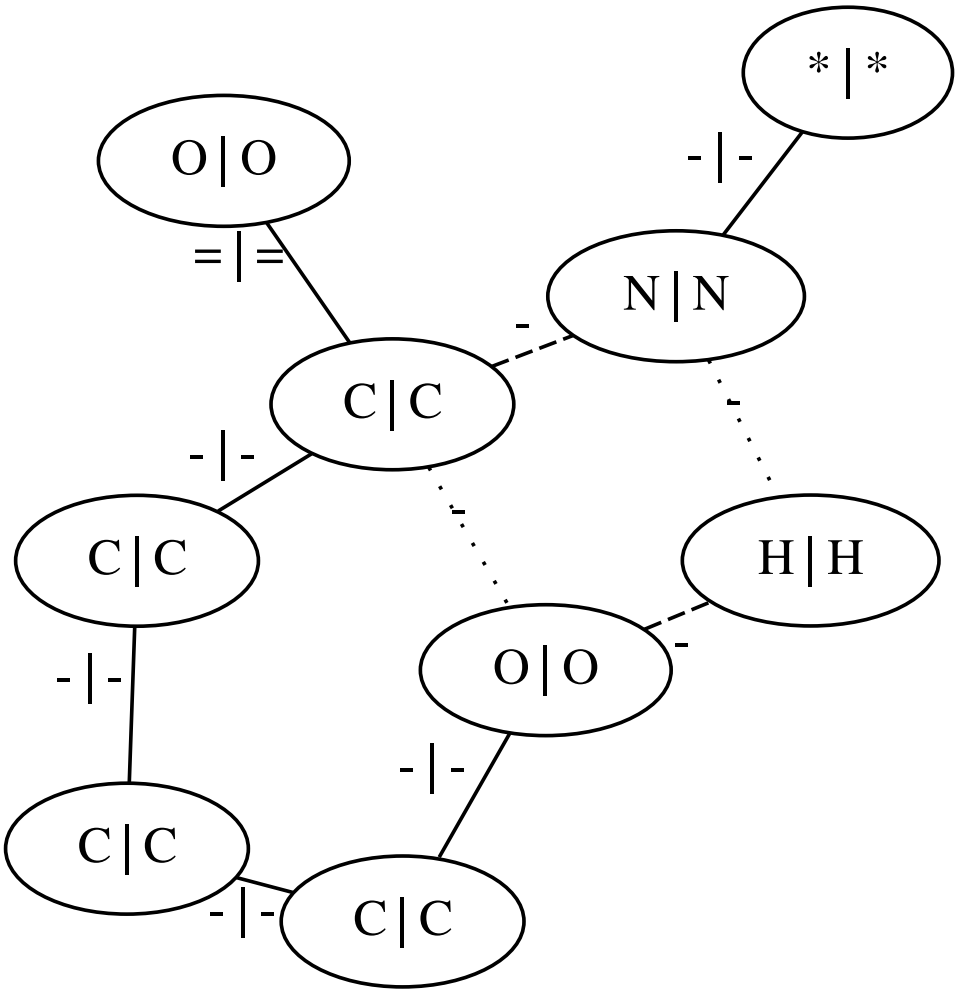
0.0.128 Ring Closure 5 membered N, O



Files: out/635_r_130_10300000_{L, K, R}



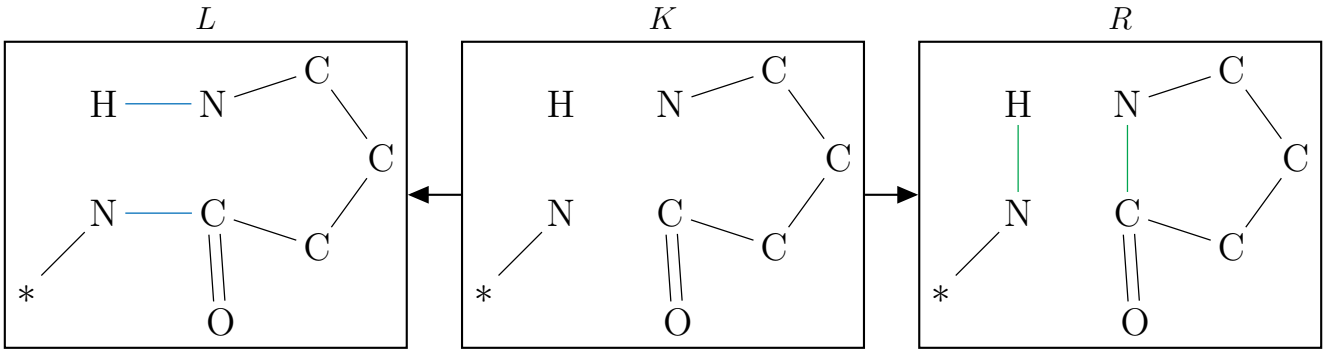
Files: out/636_r_130_11300100_{L, K, R}



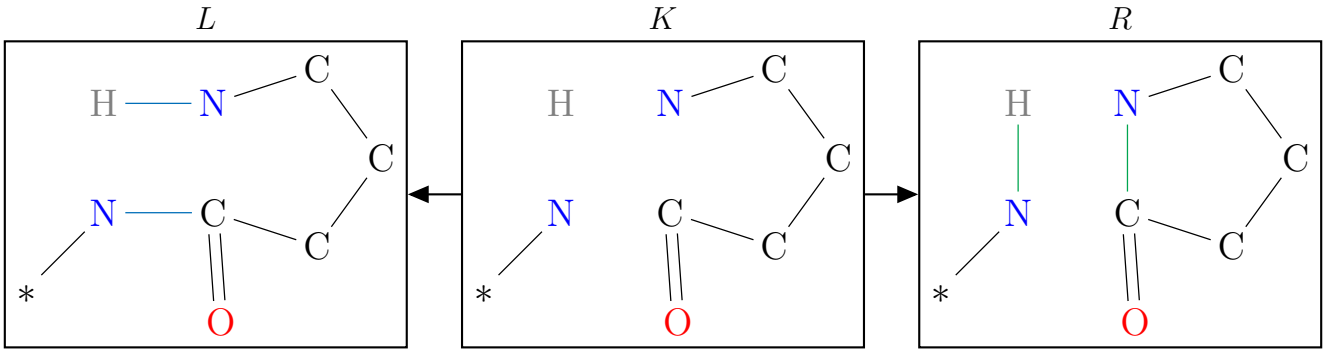
File: out/637_r_130_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

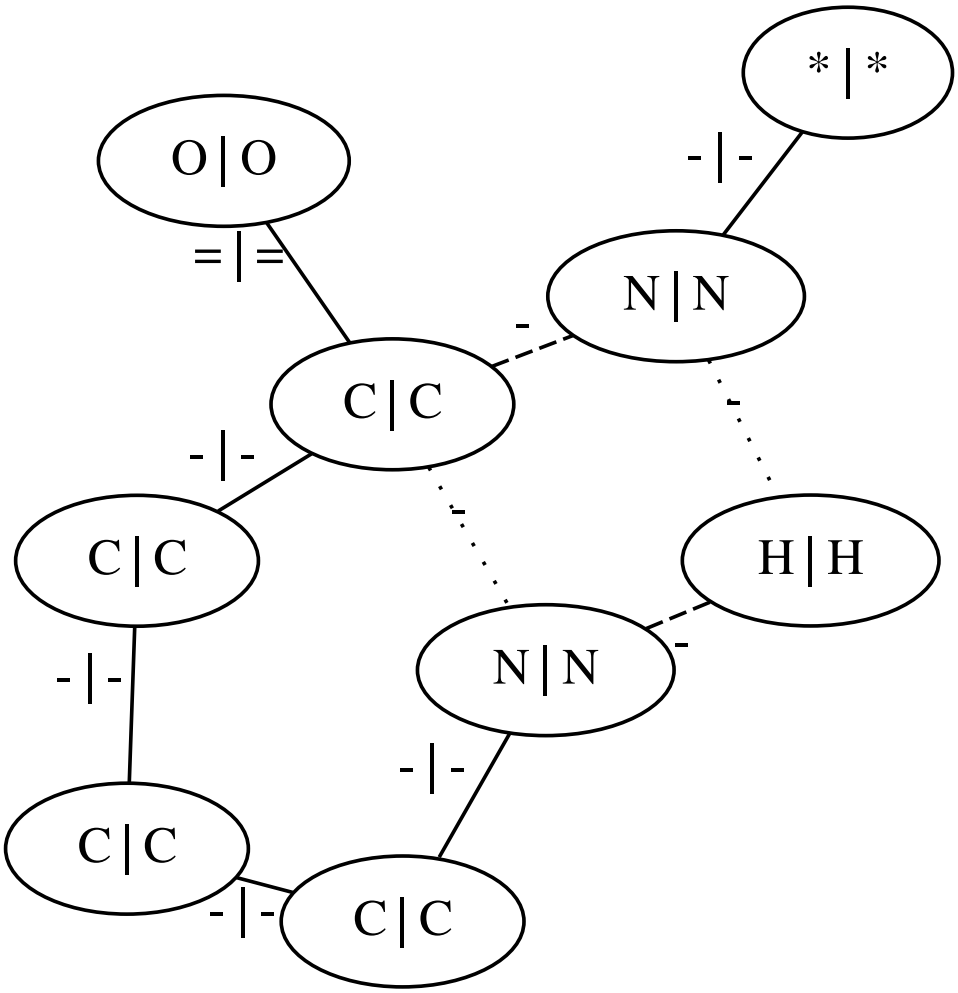
0.0.129 Ring Closure 5 membered N, N



Files: out/640_r_131_10300000_{L, K, R}



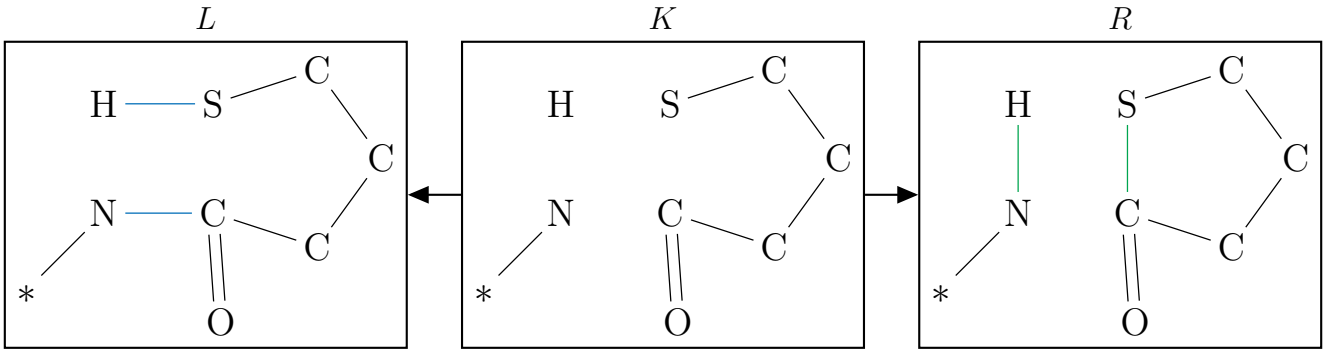
Files: out/641_r_131_11300100_{L, K, R}



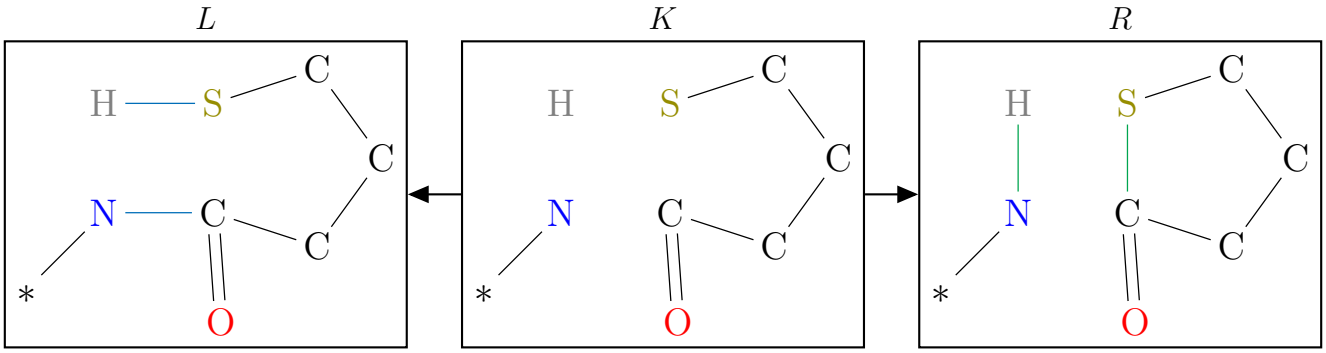
File: out/642_r_131_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

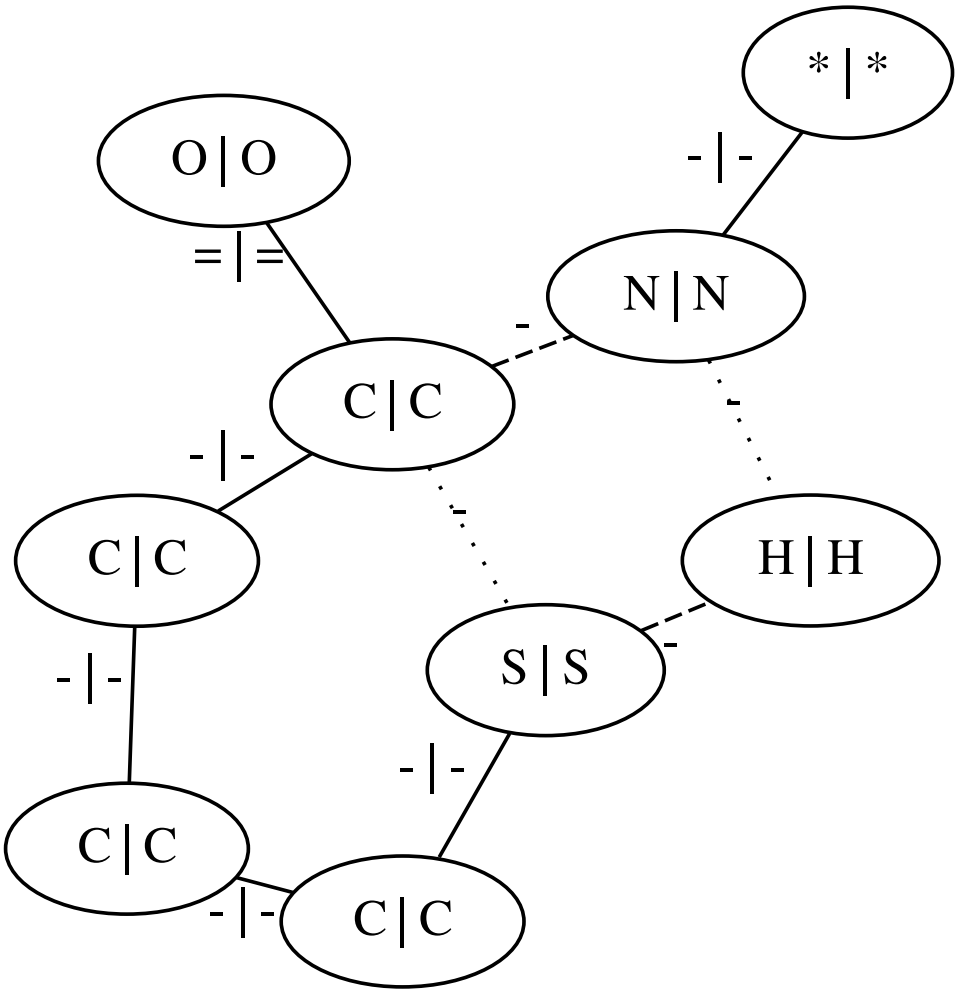
0.0.130 Ring Closure 5 membered N, S



Files: out/645_r_132_10300000_{L, K, R}



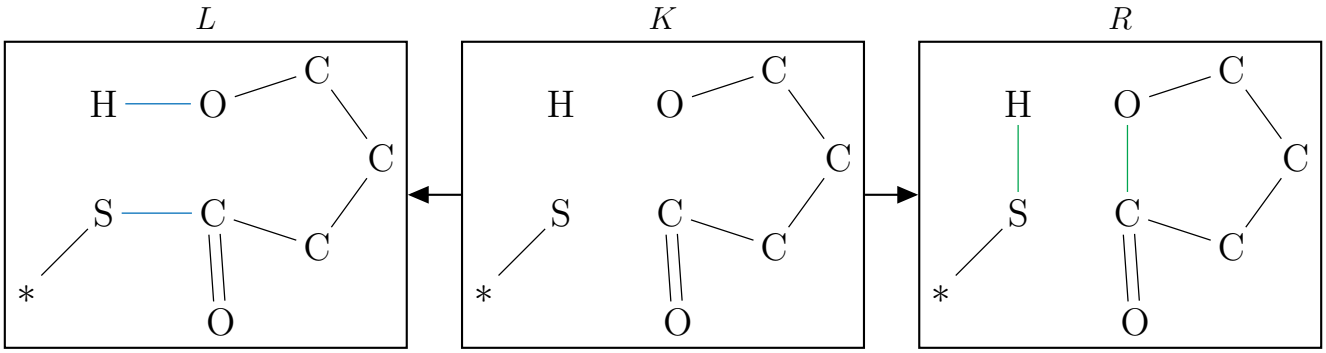
Files: out/646_r_132_11300100_{L, K, R}



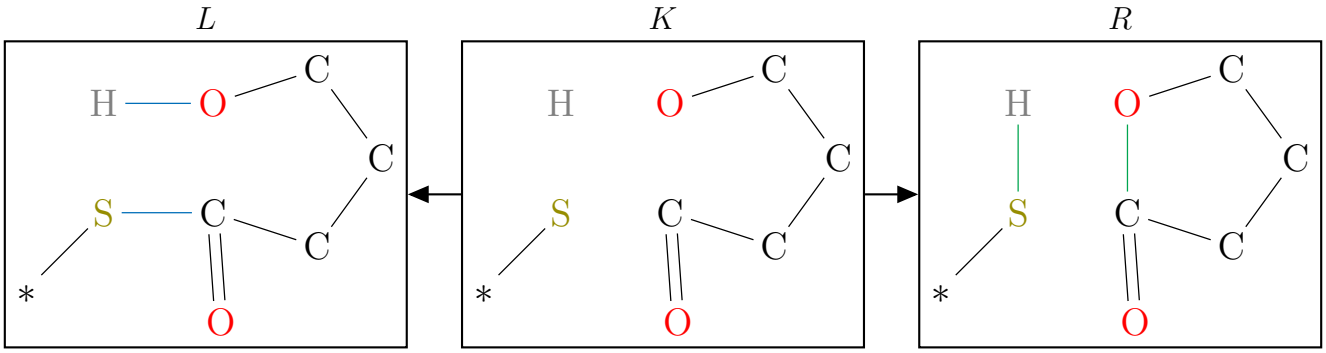
File: out/647_r_132_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

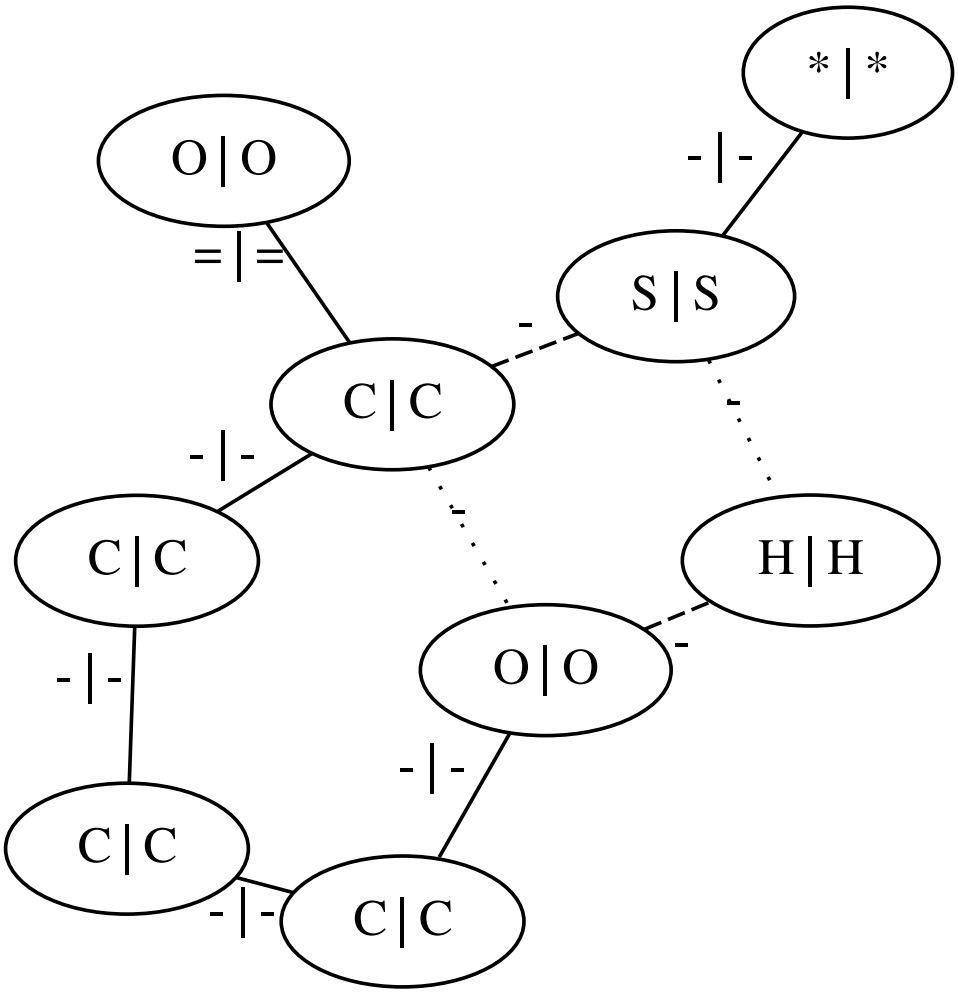
0.0.131 Ring Closure 5 membered S, O



Files: out/650_r_133_10300000_{L, K, R}



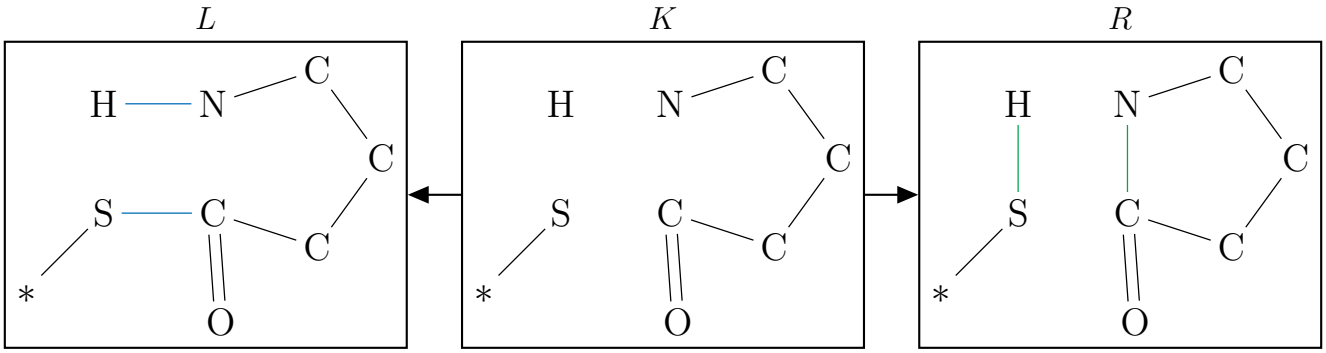
Files: out/651_r_133_11300100_{L, K, R}



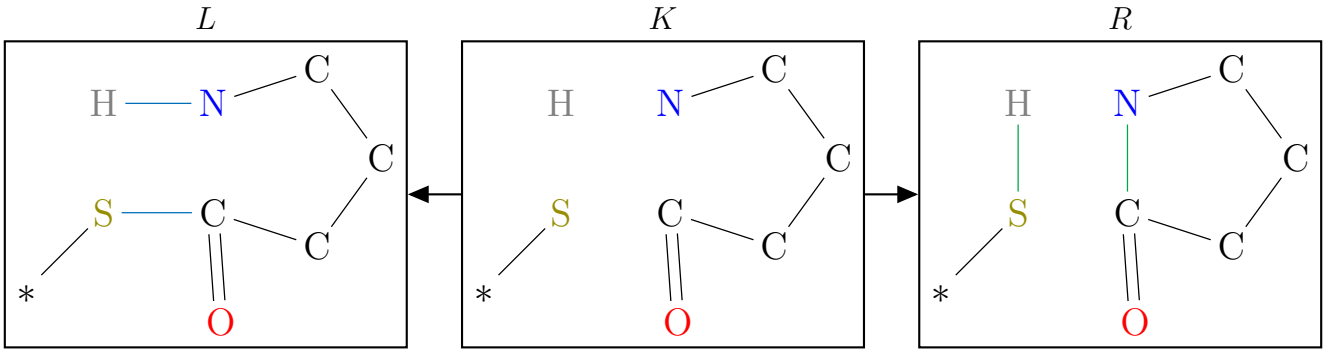
File: out/652_r_133_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

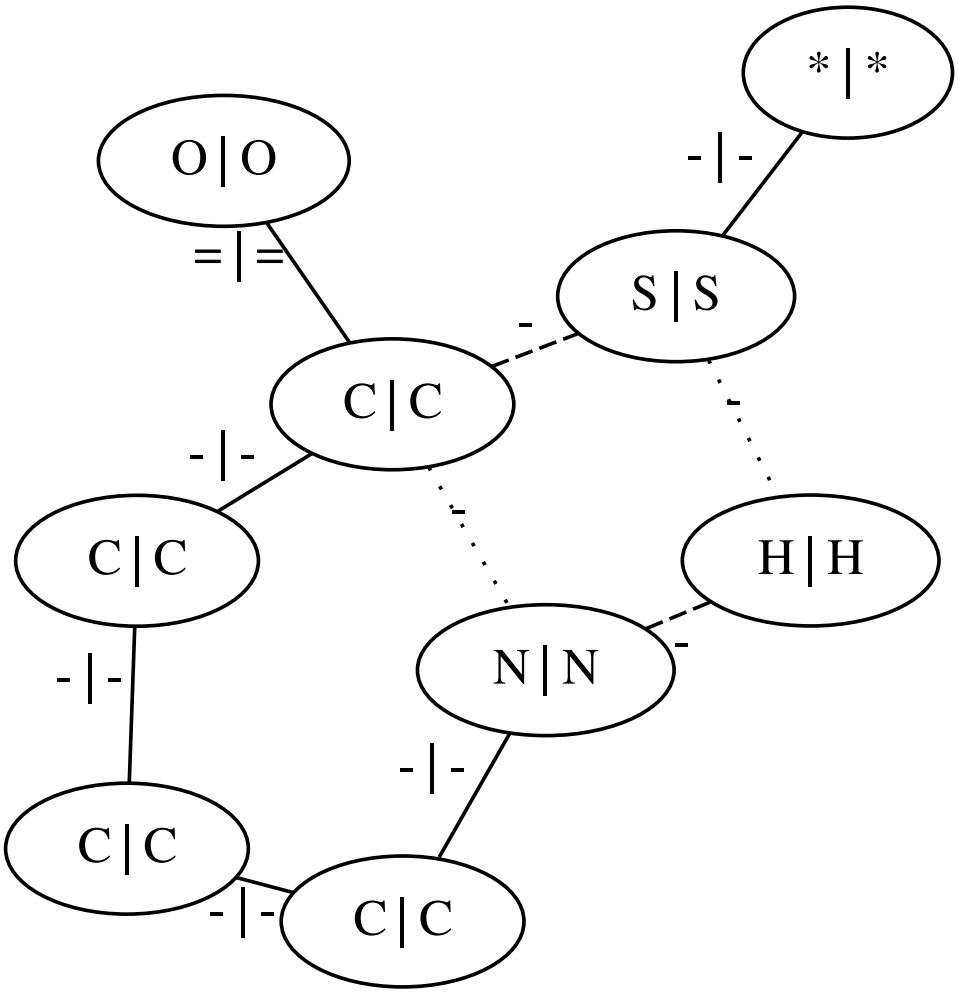
0.0.132 Ring Closure 5 membered S, N



Files: out/655_r_134_10300000_{L, K, R}



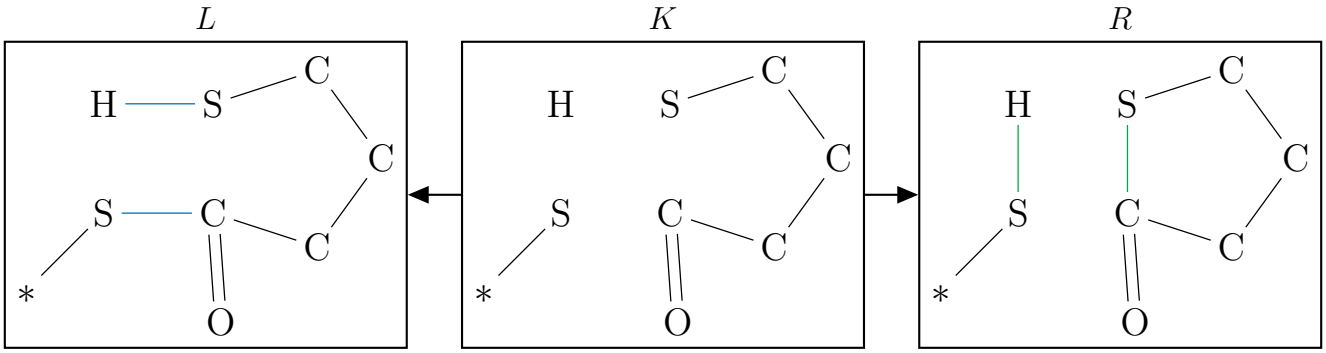
Files: out/656_r_134_11300100_{L, K, R}



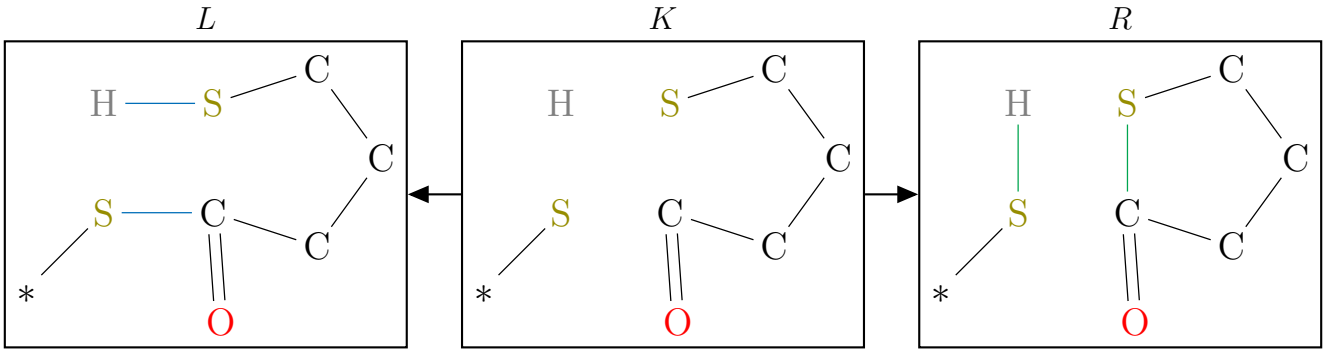
File: out/657_r_134_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

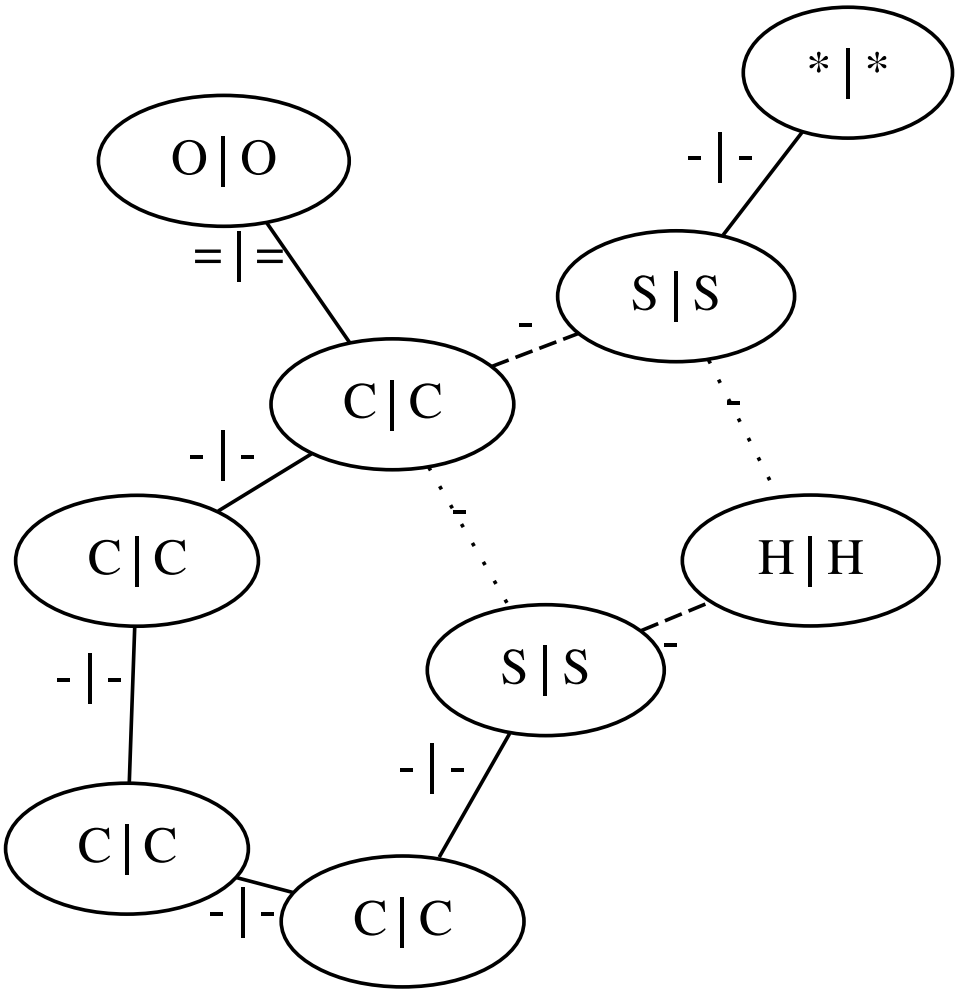
0.0.133 Ring Closure 5 membered S, S



Files: out/660_r_135_10300000_{L, K, R}



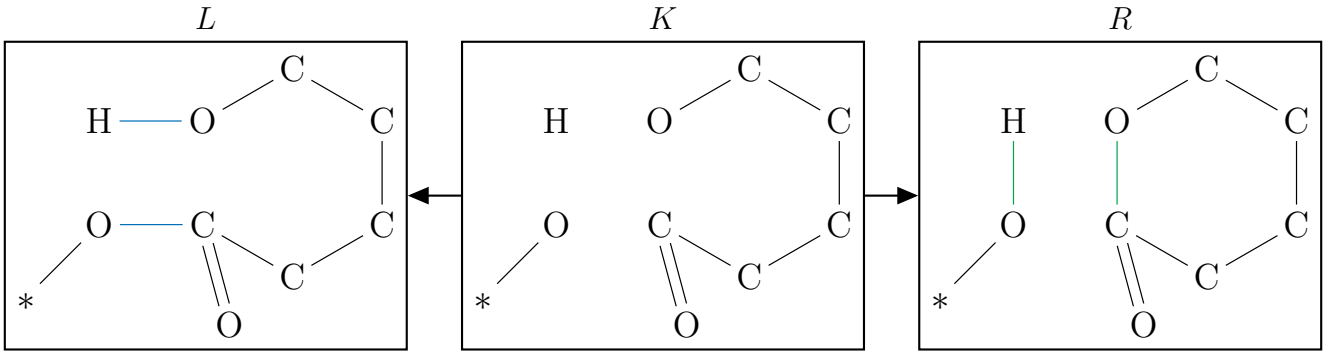
Files: out/661_r_135_11300100_{L, K, R}



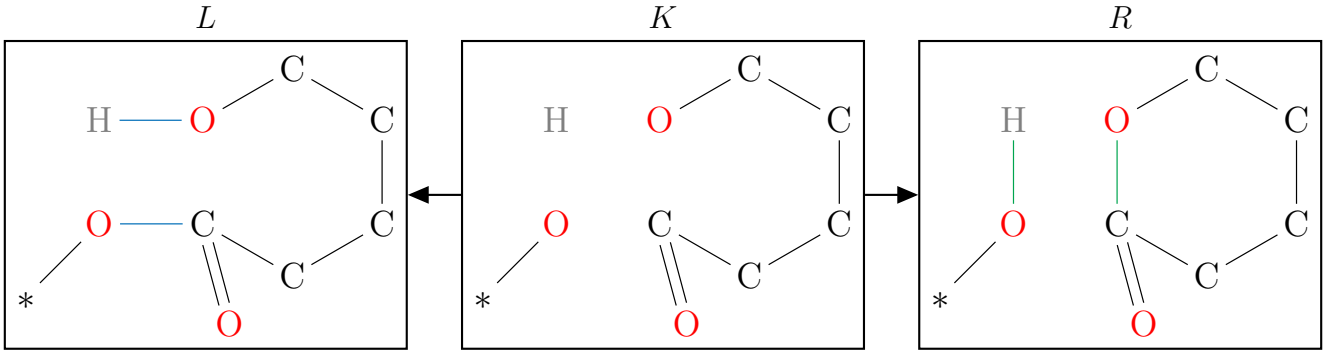
File: out/662_r_135_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

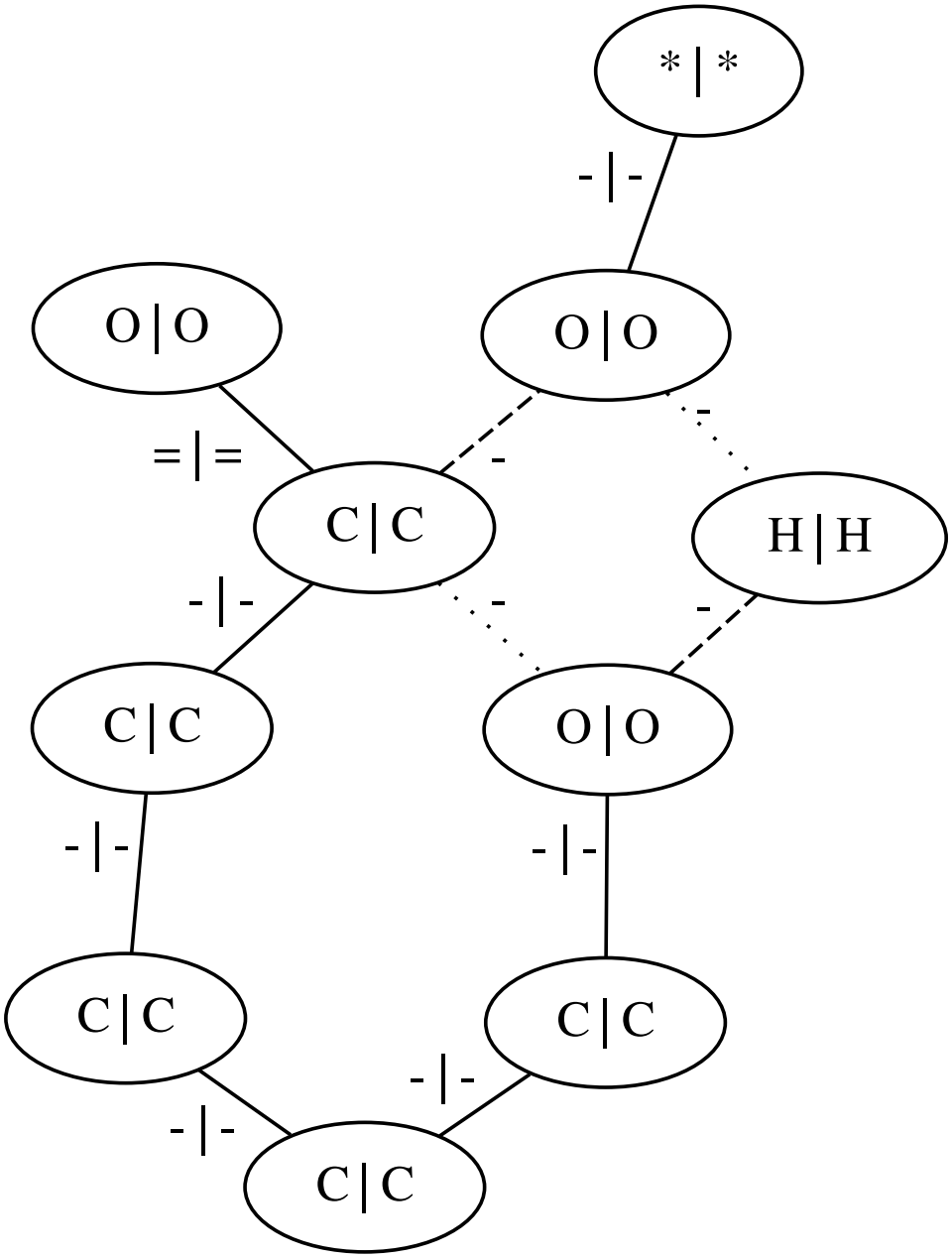
0.0.134 Ring Closure 6 membered O, O



Files: out/665_r_136_10300000_{L, K, R}



Files: out/666_r_136_11300100_{L, K, R}

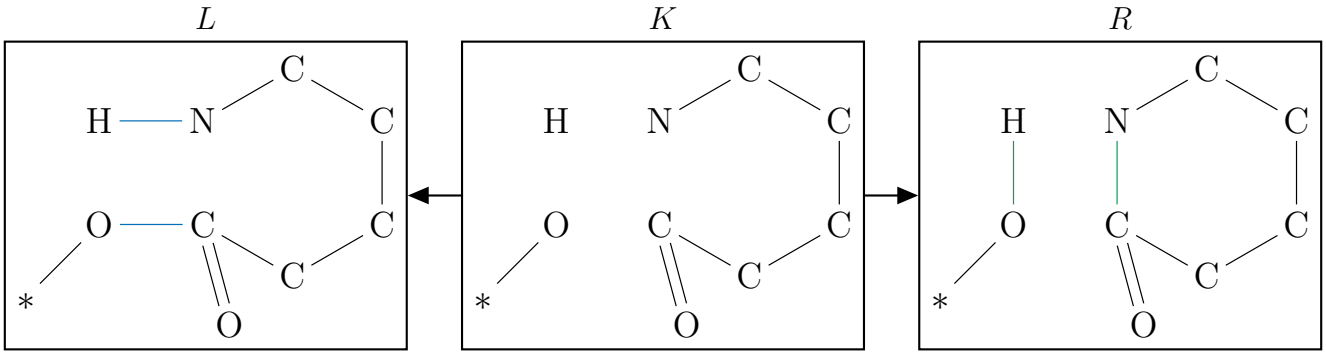


File: out/667_r_136_combined

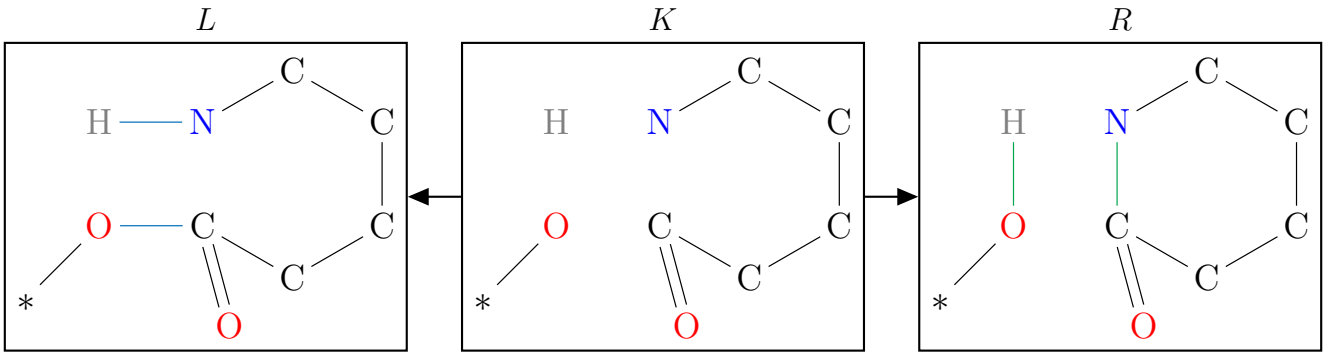
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

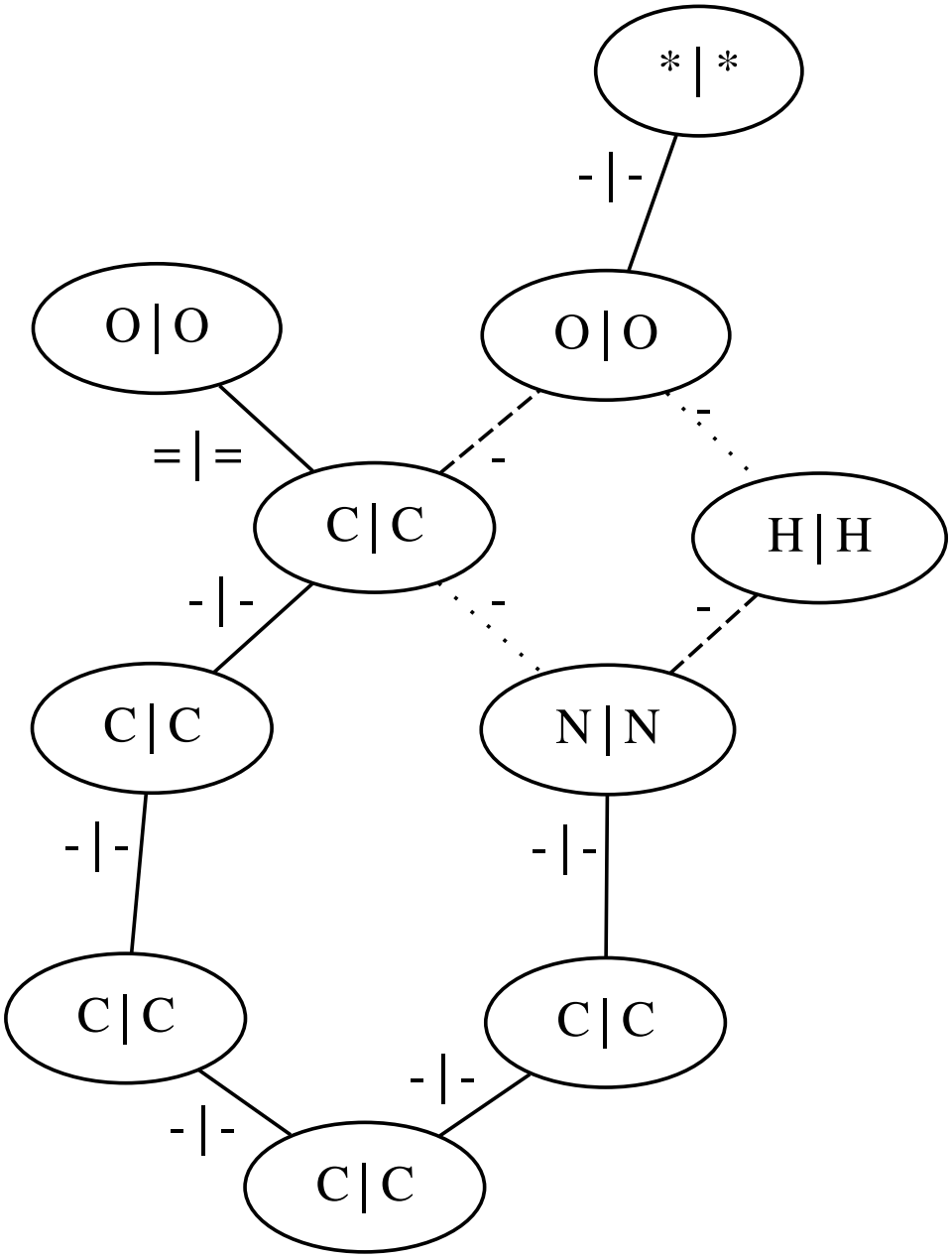
0.0.135 Ring Closure 6 membered O, N



Files: out/670_r_137_10300000_{L, K, R}



Files: out/671_r_137_11300100_{L, K, R}

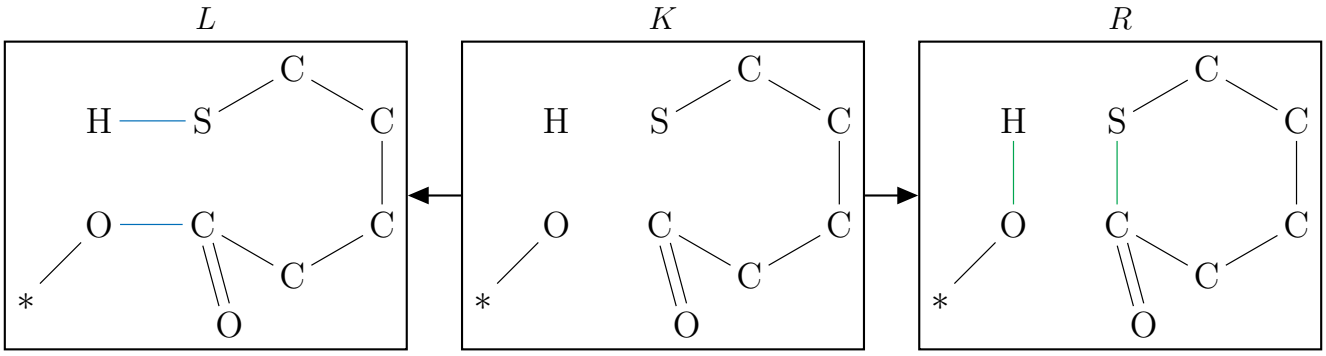


File: out/672_r_137_combined

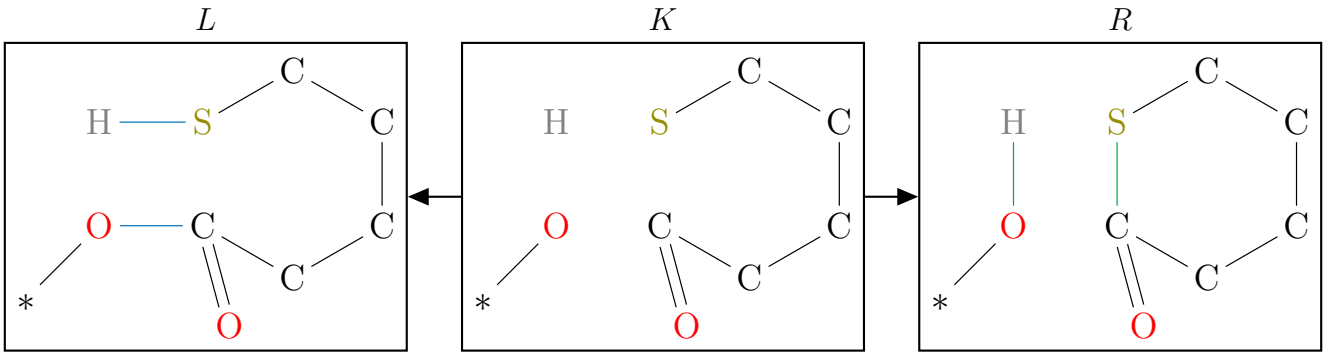
$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

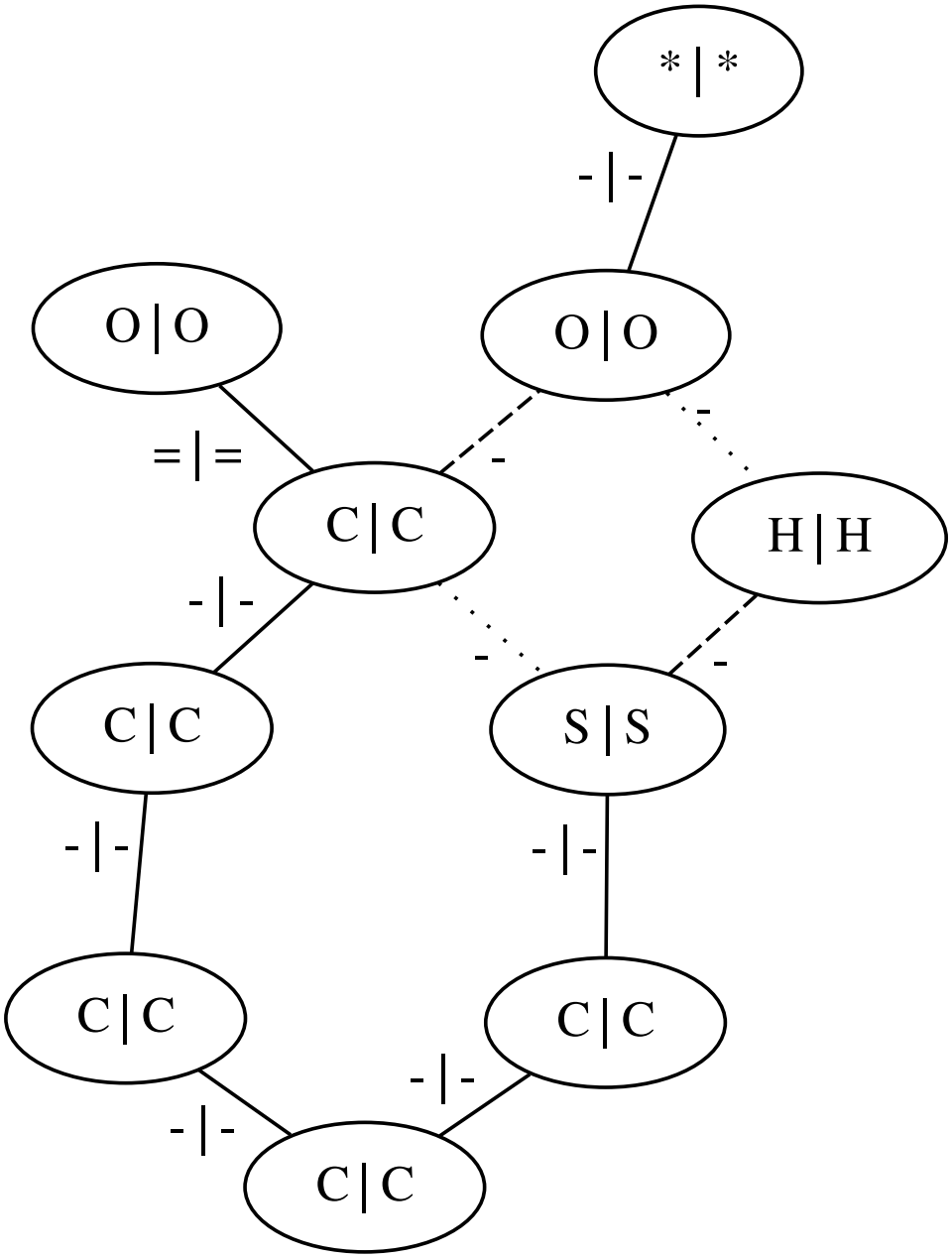
0.0.136 Ring Closure 6 membered O, S



Files: out/675_r_138_10300000_{L, K, R}



Files: out/676_r_138_11300100_{L, K, R}

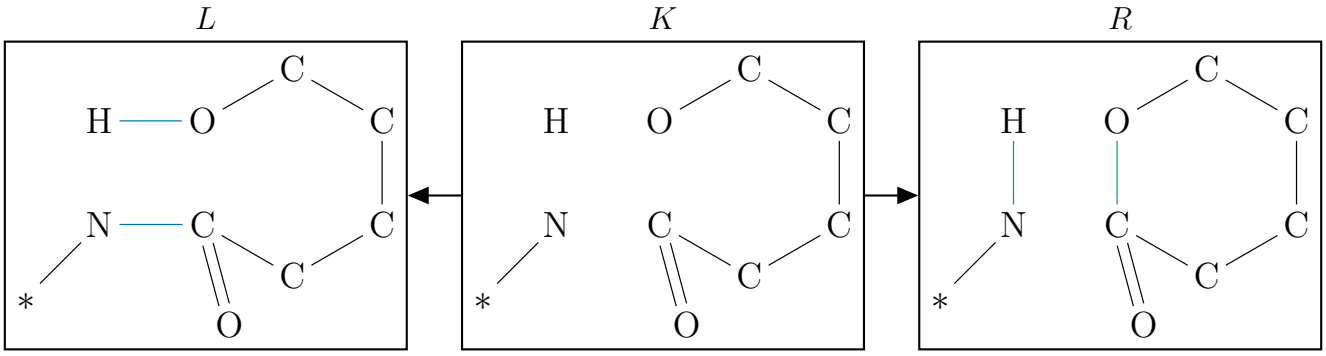


File: out/677_r_138_combined

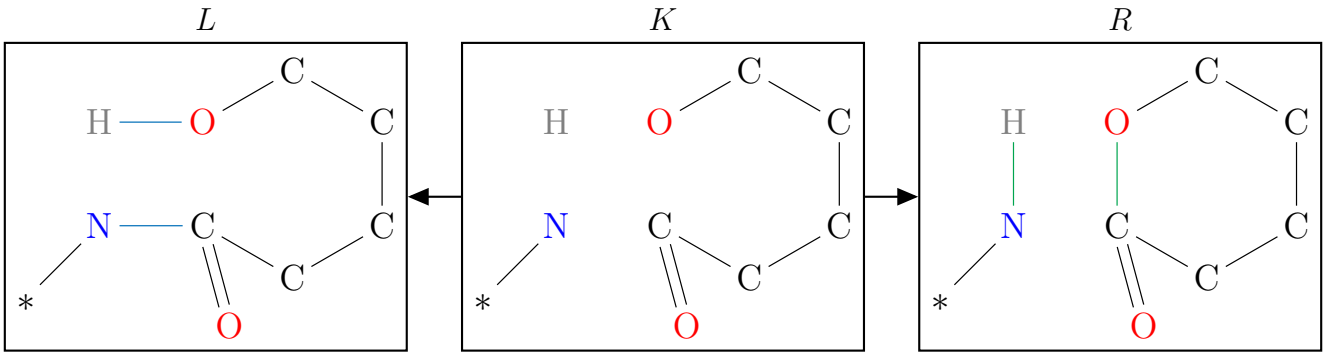
$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

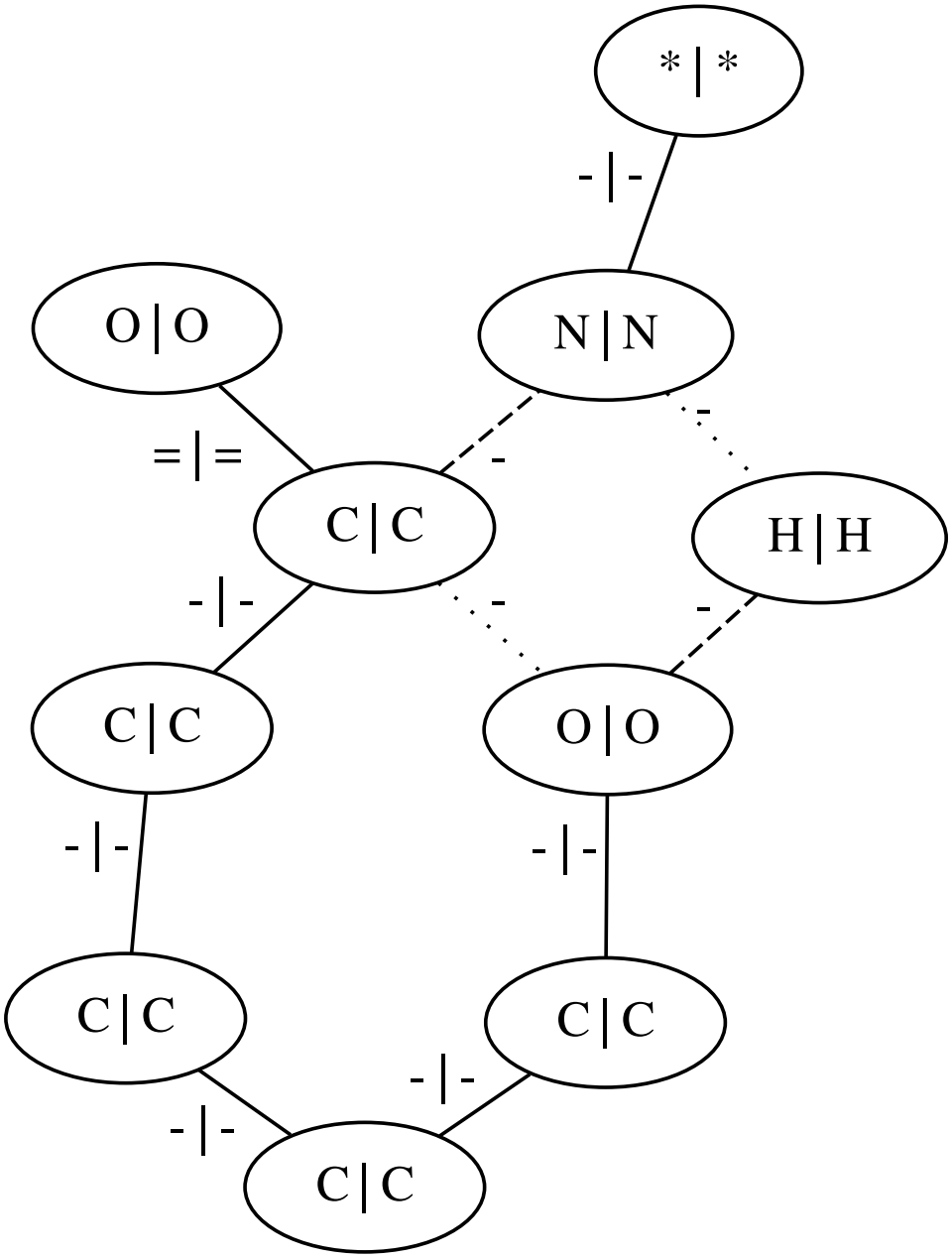
0.0.137 Ring Closure 6 membered N, O



Files: out/680_r_139_10300000_{L, K, R}



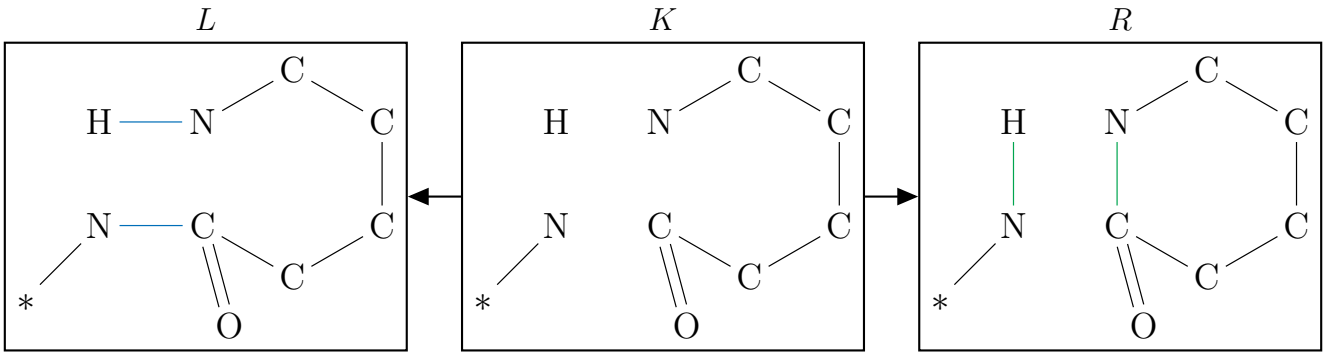
Files: out/681_r_139_11300100_{L, K, R}



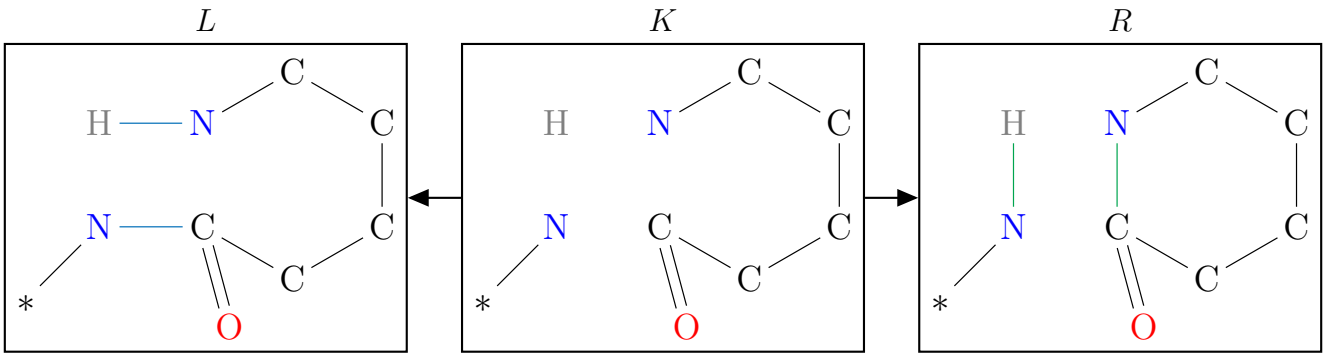
File: out/682_r_139_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

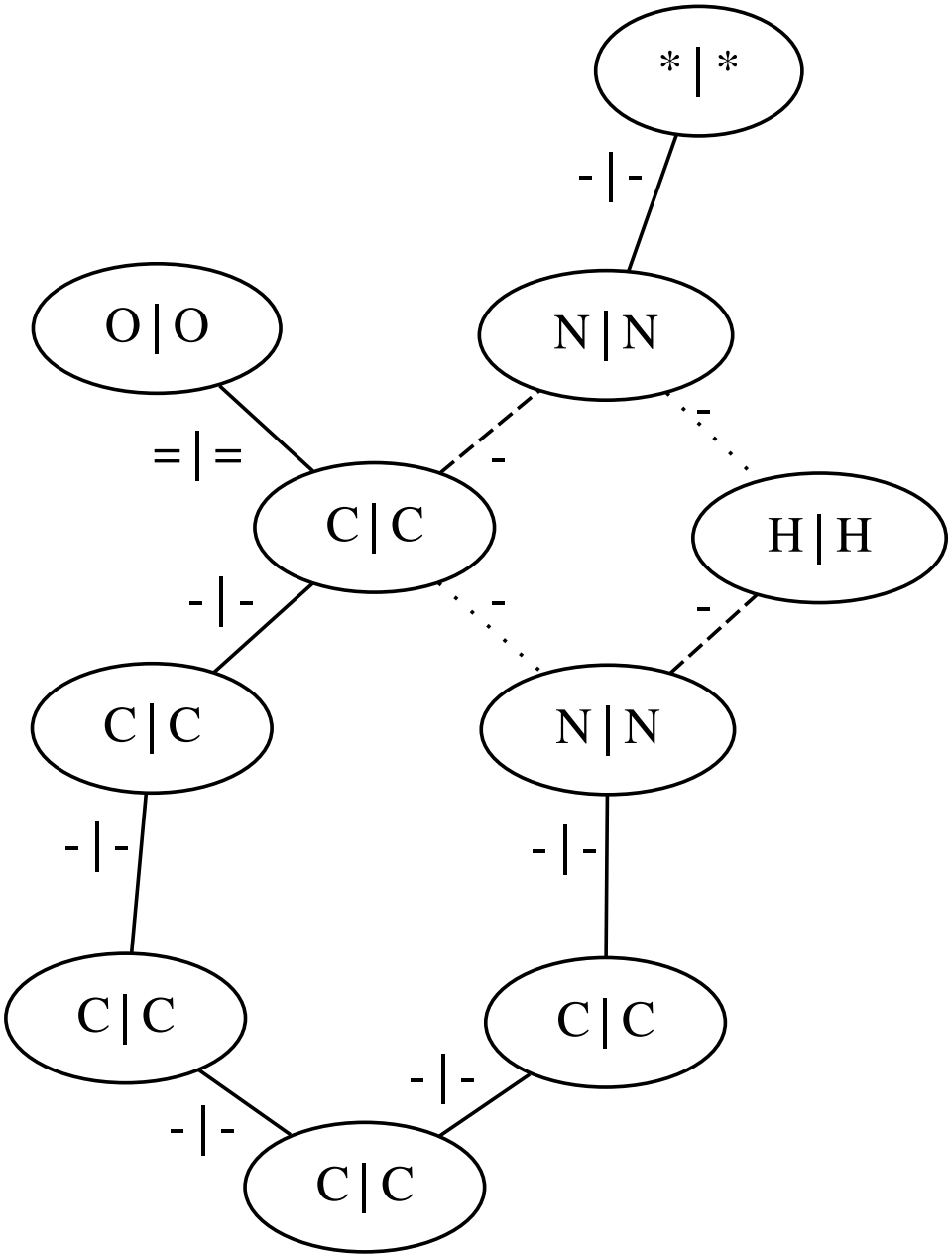
0.0.138 Ring Closure 6 membered N, N



Files: out/685_r_140_10300000_{L, K, R}



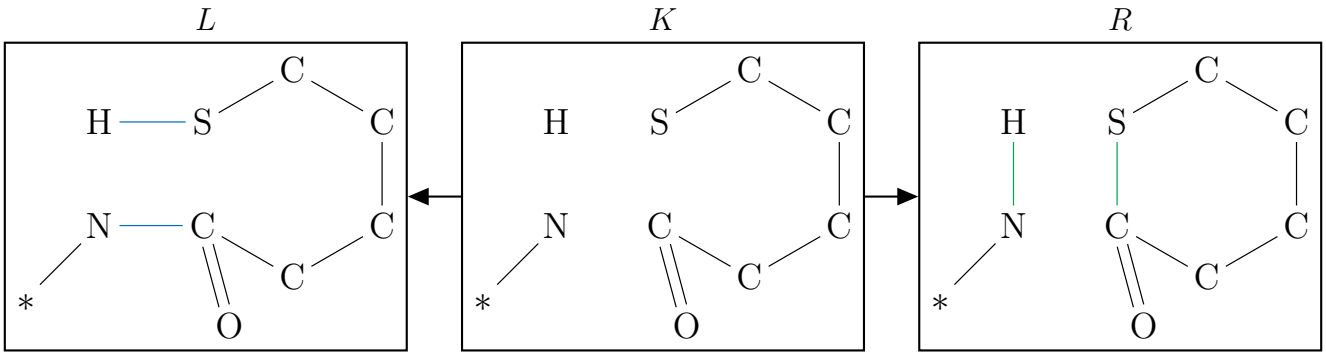
Files: out/686_r_140_11300100_{L, K, R}



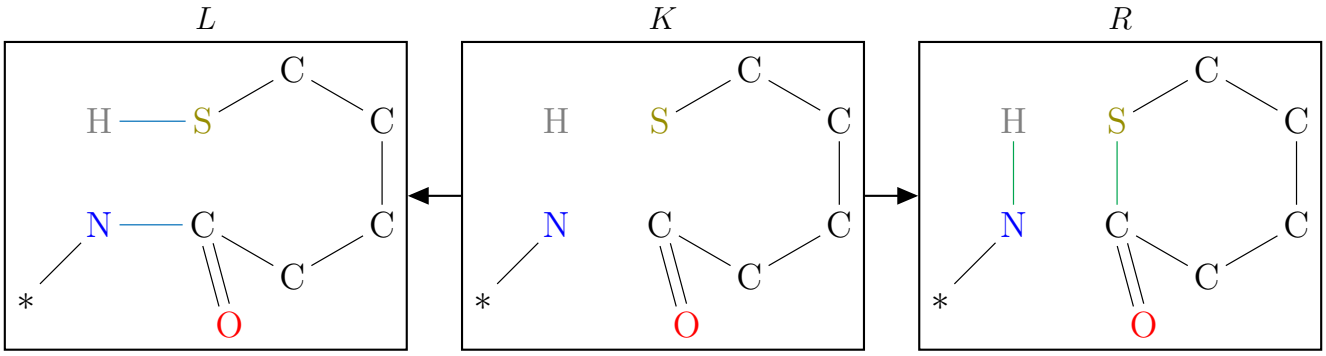
File: out/687_r_140_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

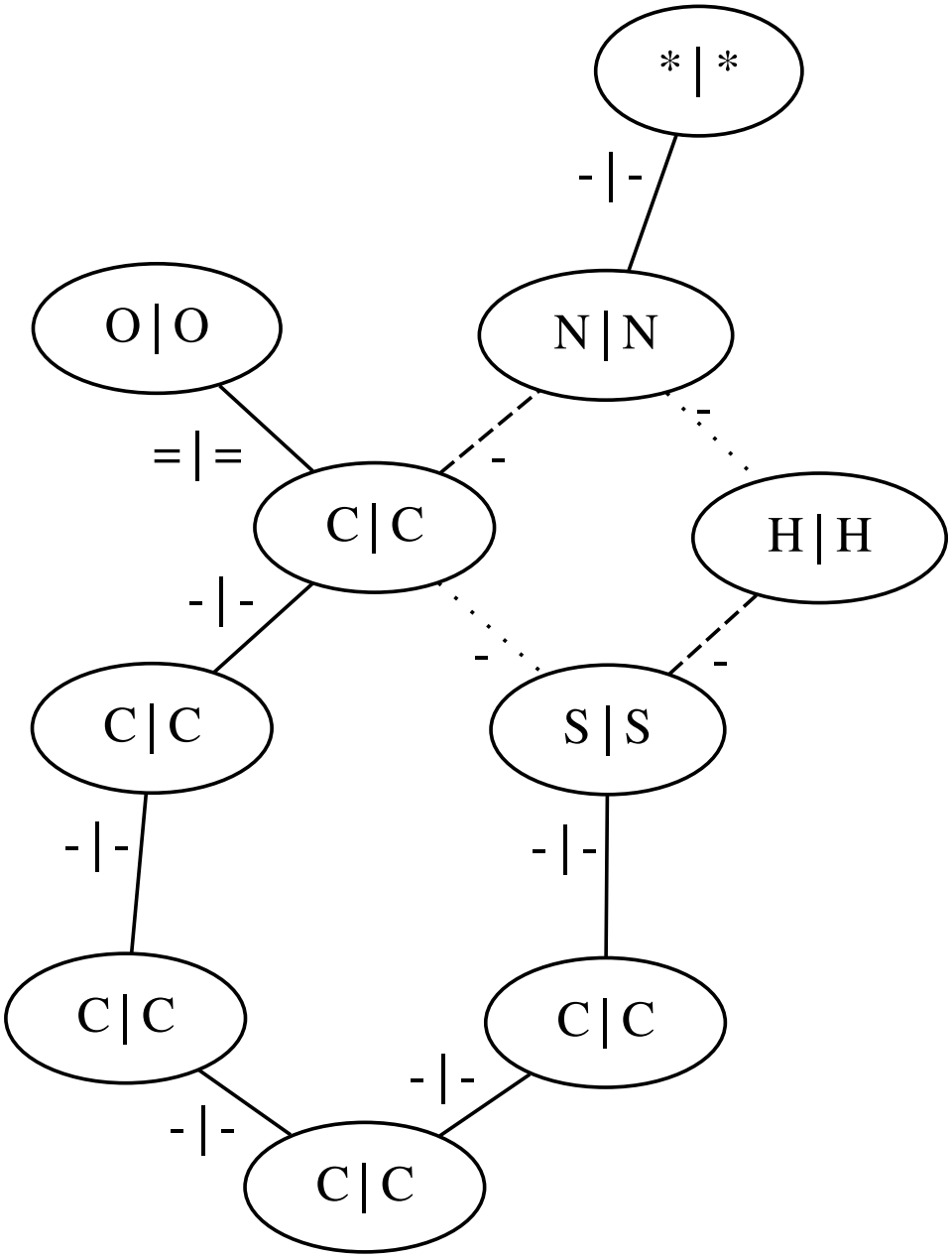
0.0.139 Ring Closure 6 membered N, S



Files: out/690_r_141_10300000_{L, K, R}



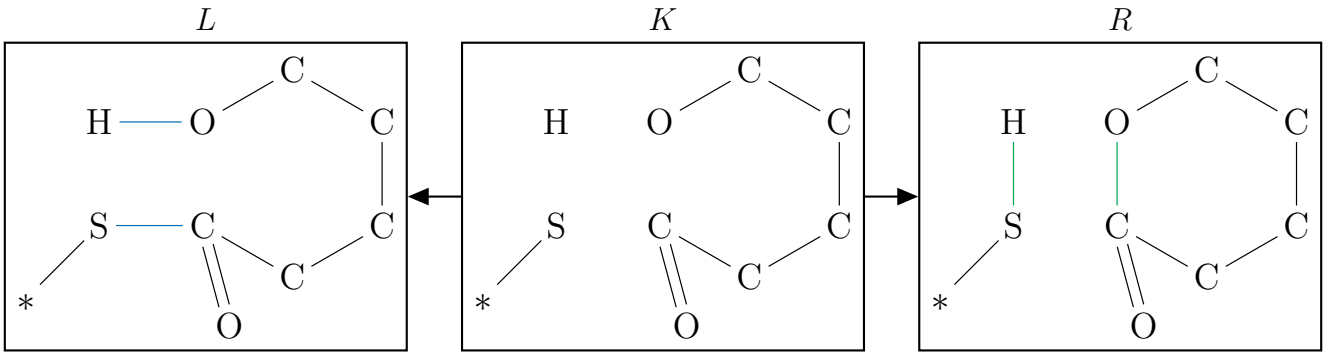
Files: out/691_r_141_11300100_{L, K, R}



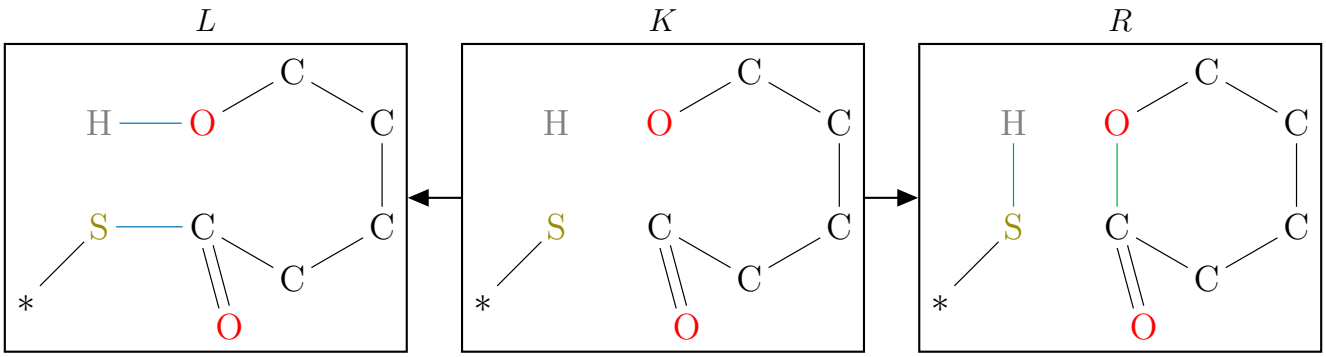
File: out/692_r_141_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

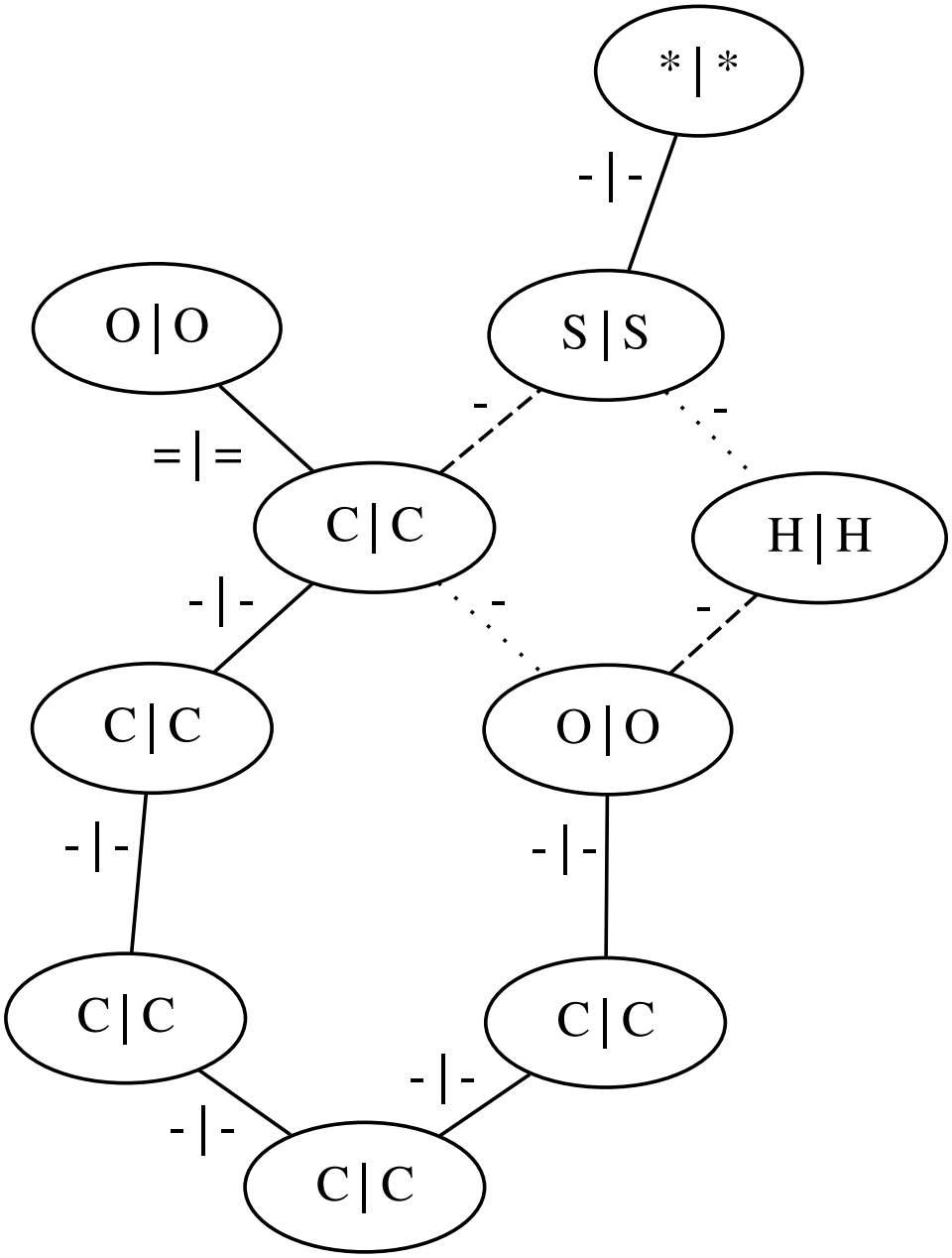
0.0.140 Ring Closure 6 membered S, O



Files: out/695_r_142_10300000_{L, K, R}



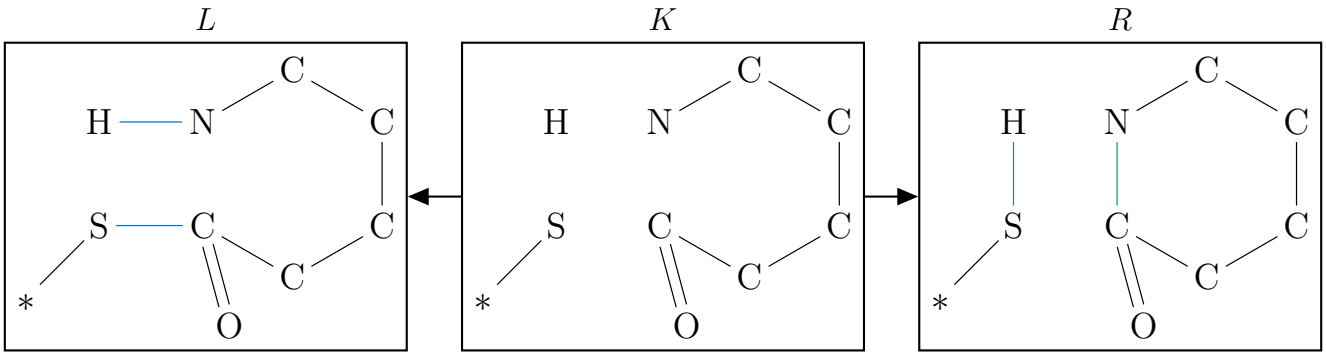
Files: out/696_r_142_11300100_{L, K, R}



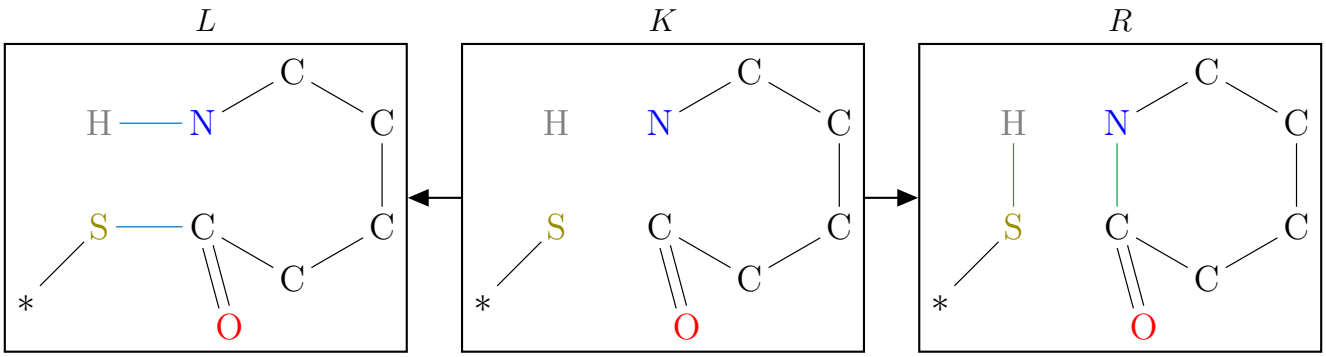
File: out/697_r_142_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

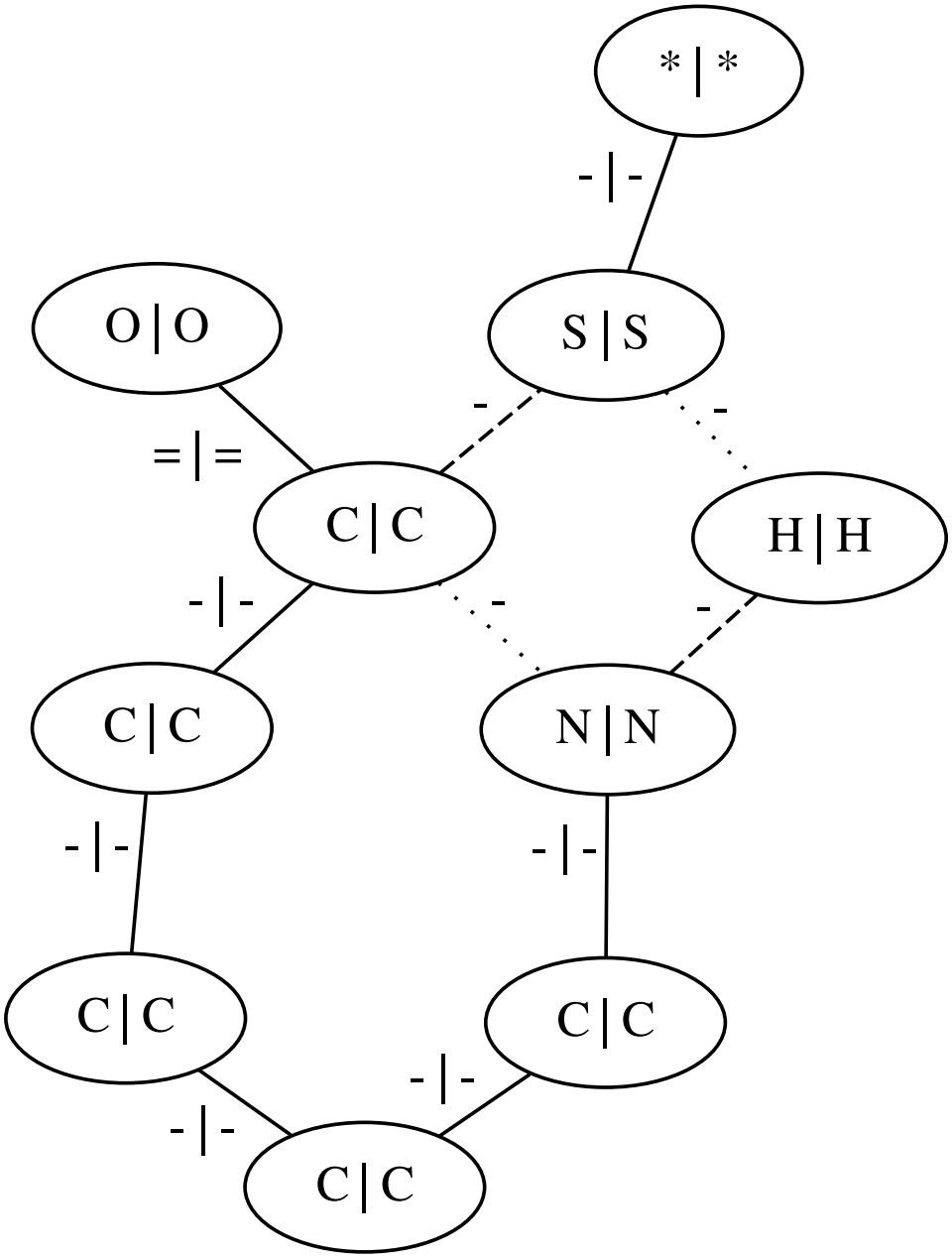
0.0.141 Ring Closure 6 membered S, N



Files: out/700_r_143_10300000_{L, K, R}



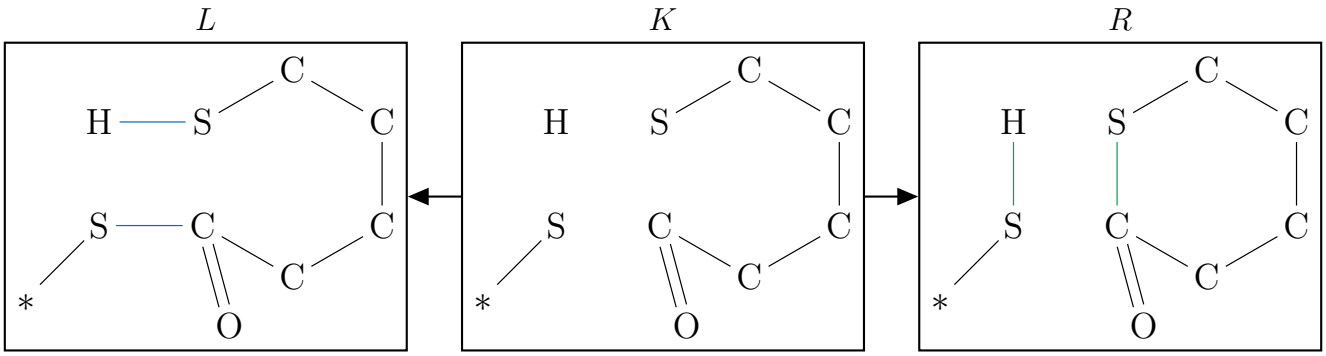
Files: out/701_r_143_11300100_{L, K, R}



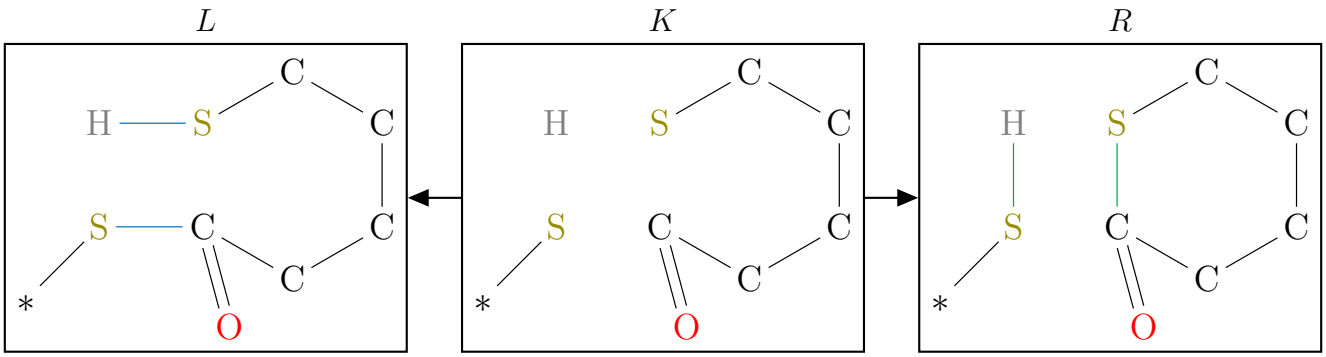
File: out/702_r_143_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

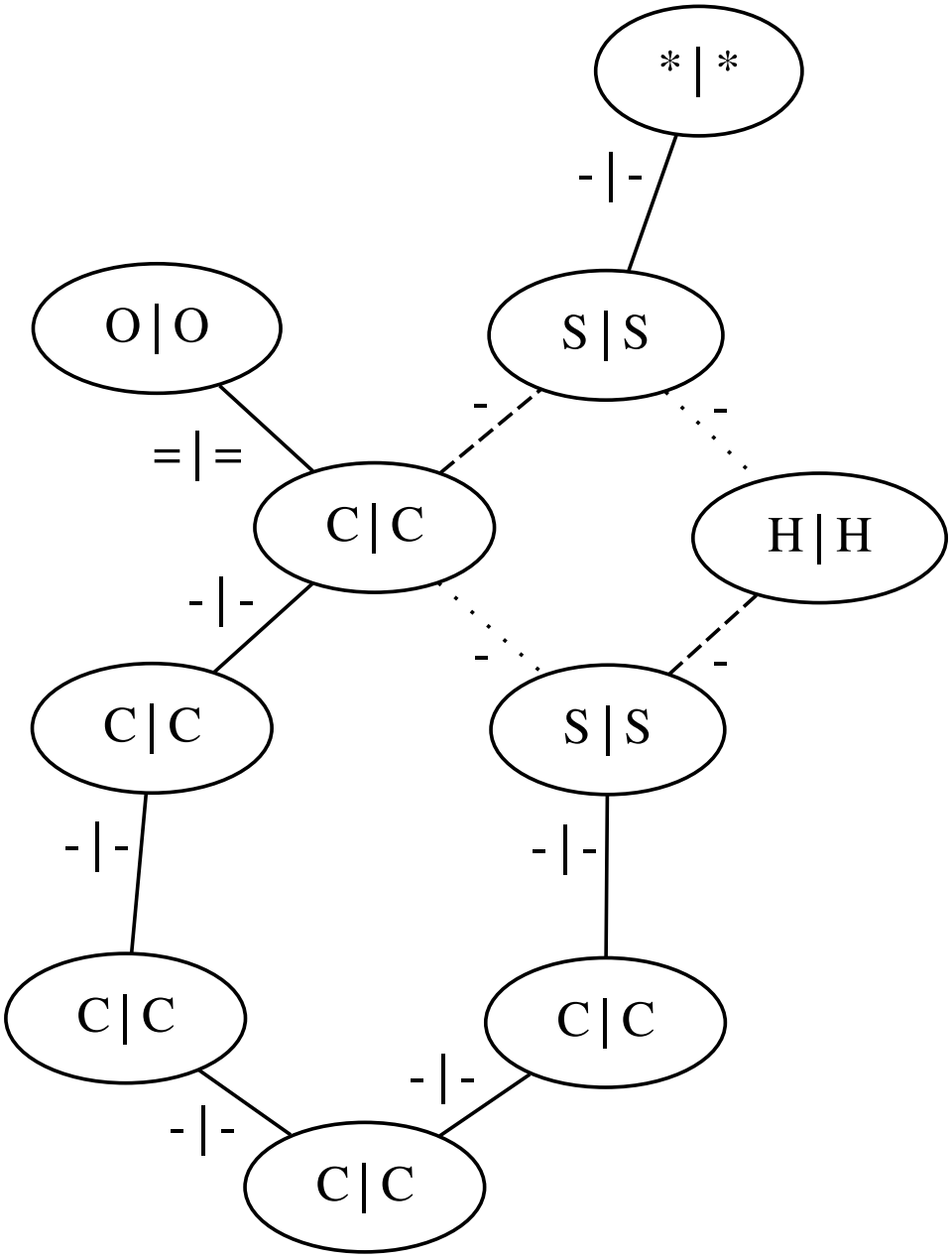
0.0.142 Ring Closure 6 membered S, S



Files: out/705_r_144_10300000_{L, K, R}



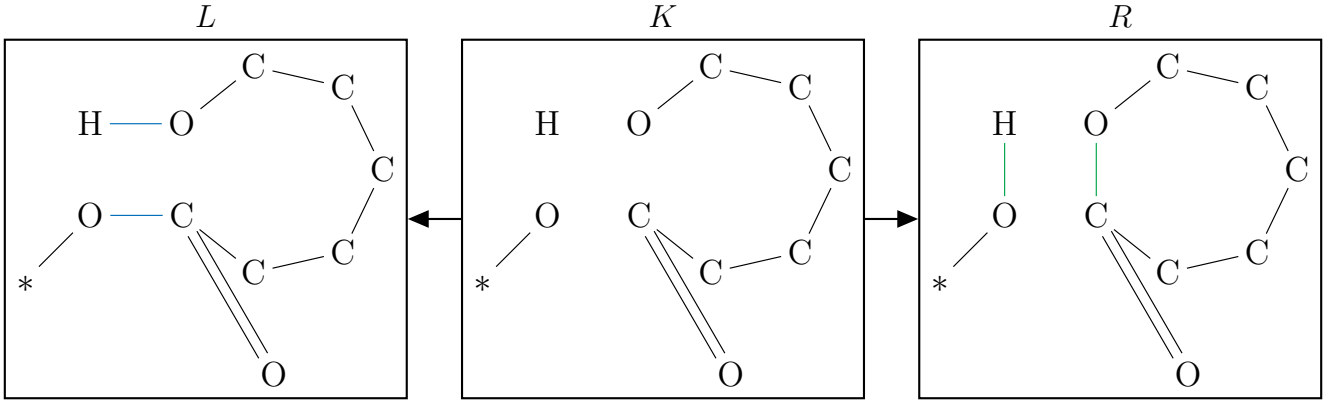
Files: out/706_r_144_11300100_{L, K, R}



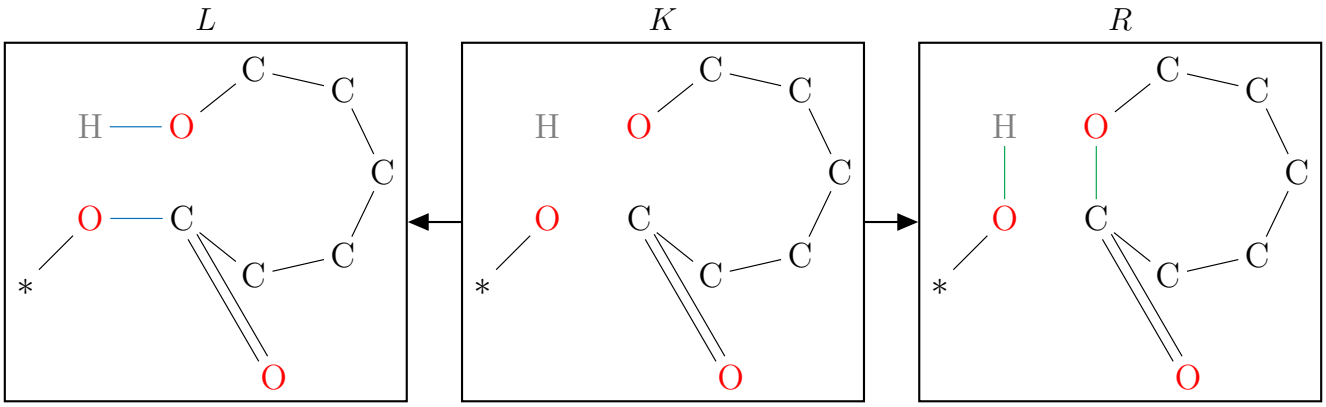
File: out/707_r_144_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

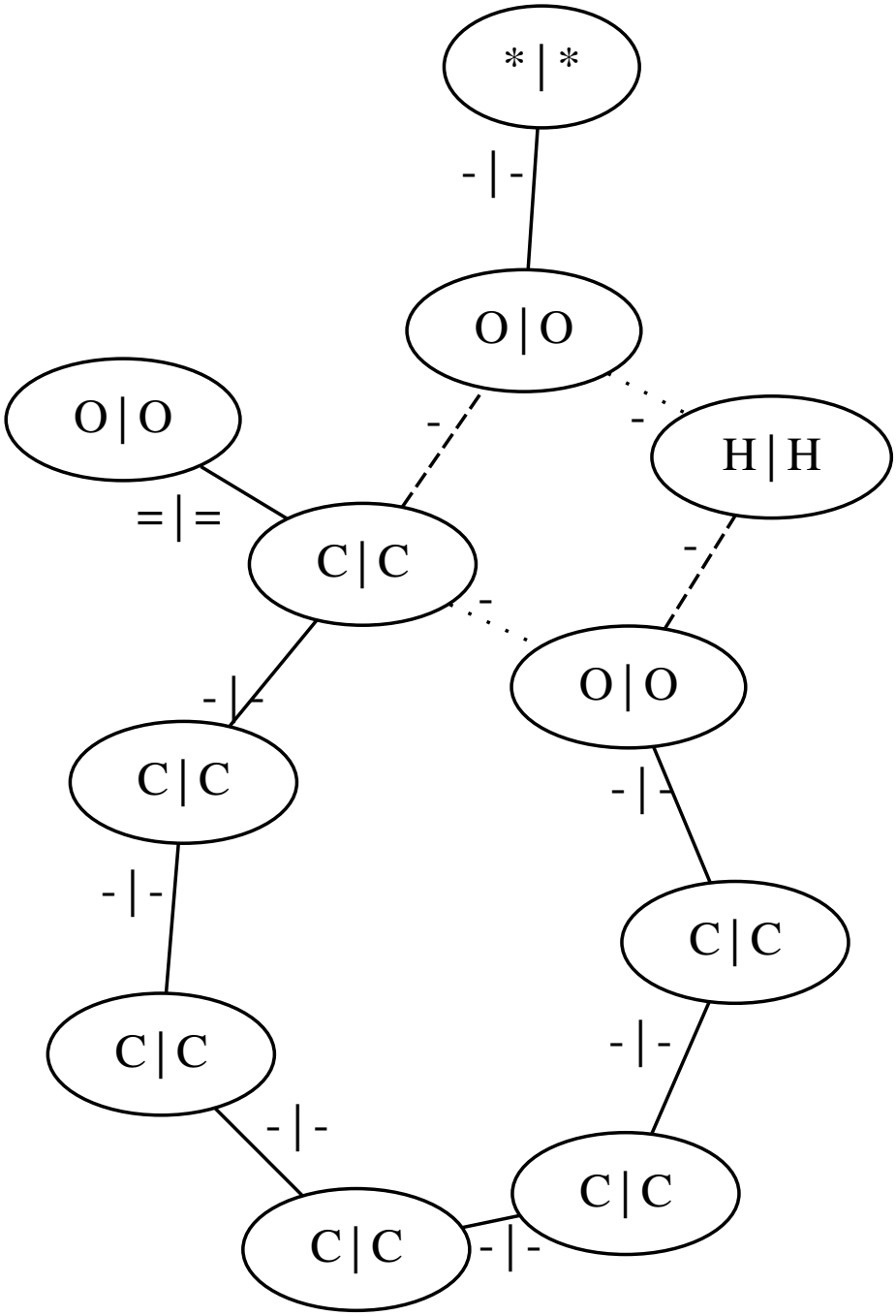
0.0.143 Ring Closure 7 membered O, O



Files: out/710_r_145_10300000_{L, K, R}



Files: out/711_r_145_11300100_{L, K, R}

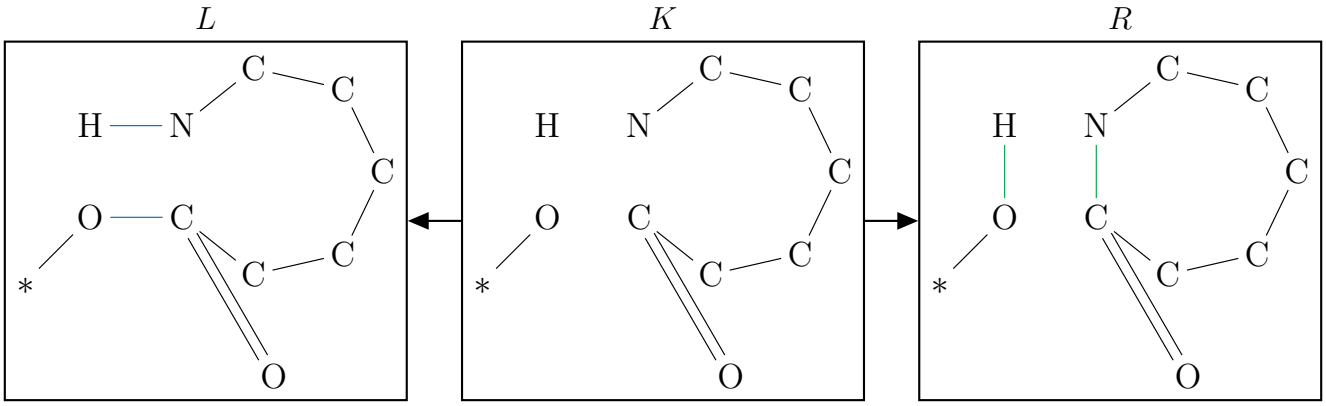


File: out/712_r_145_combined

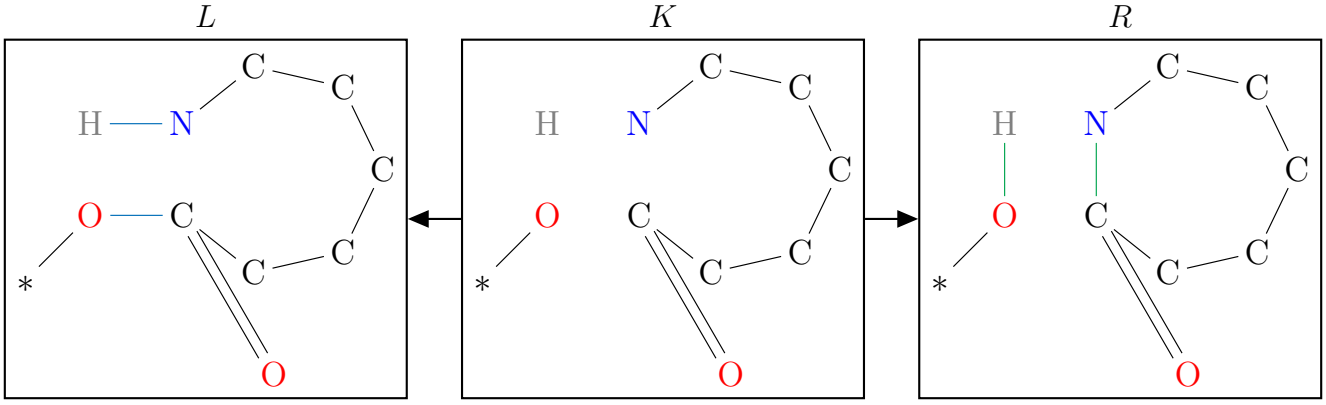
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

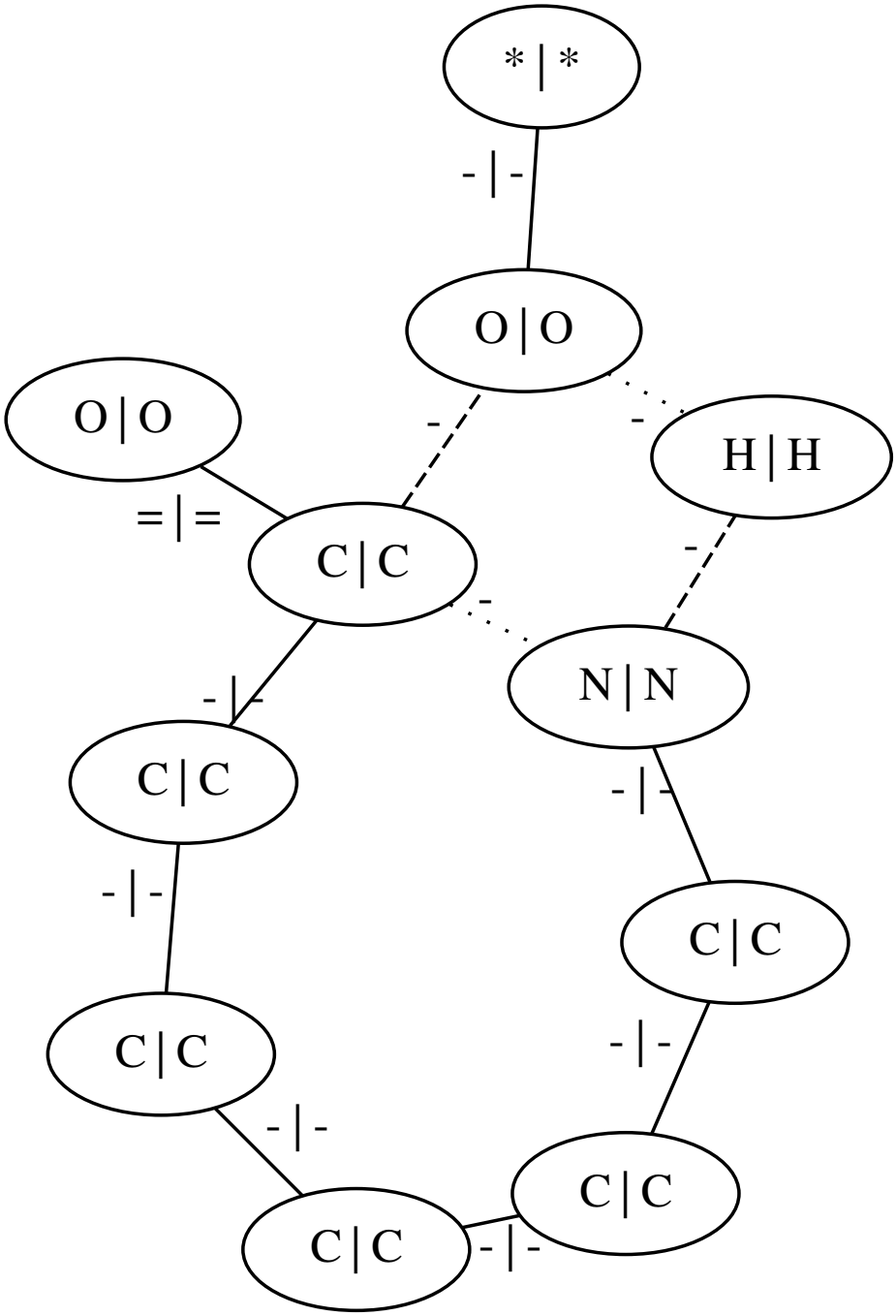
0.0.144 Ring Closure 7 membered O, N



Files: out/715_r_146_10300000_{L, K, R}



Files: out/716_r_146_11300100_{L, K, R}

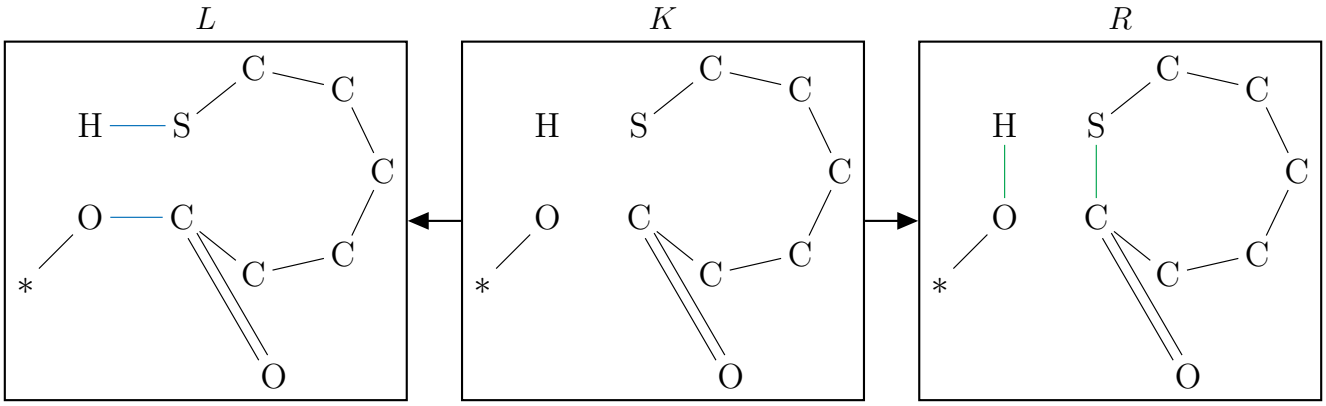


File: out/717_r_146_combined

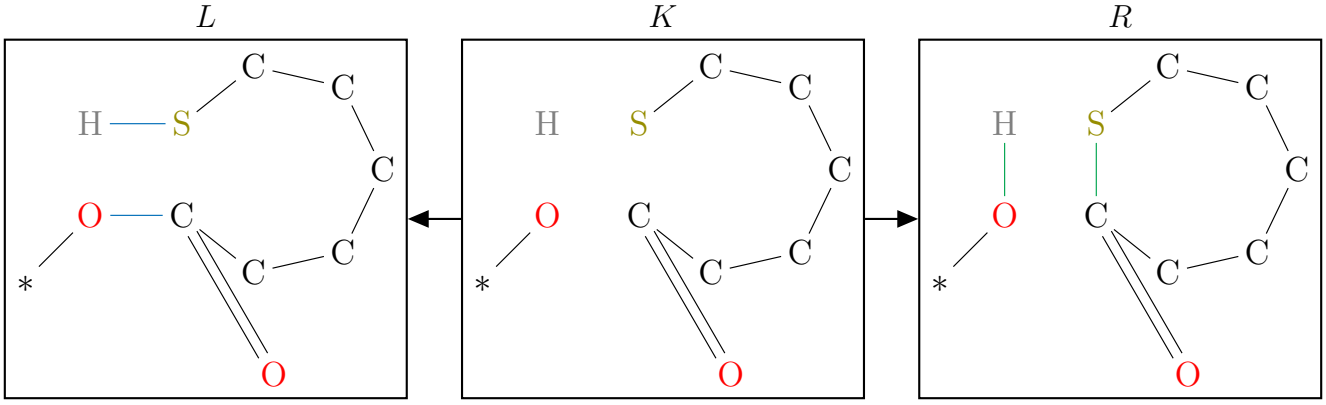
$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

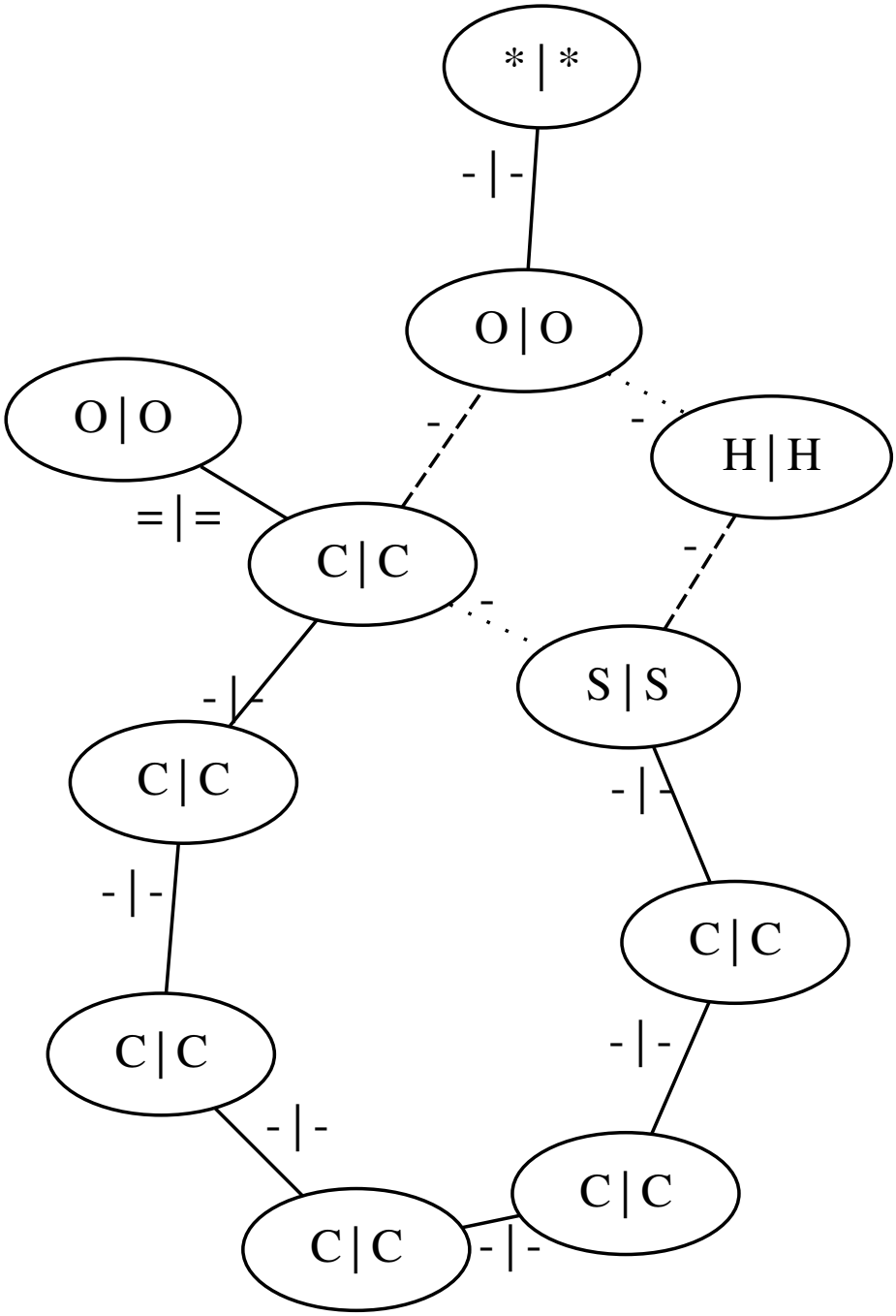
0.0.145 Ring Closure 7 membered O, S



Files: out/720_r_147_10300000_{L, K, R}



Files: out/721_r_147_11300100_{L, K, R}

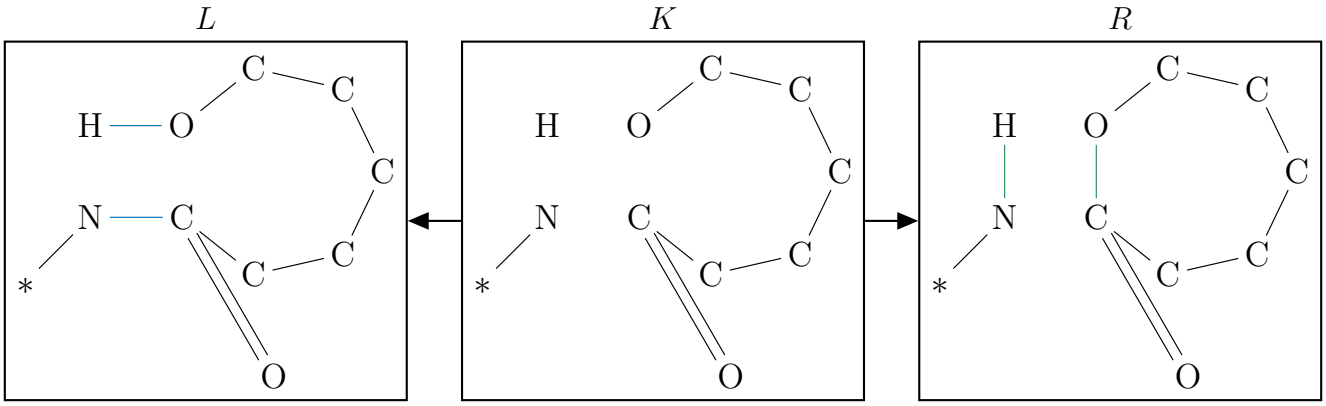


File: out/722_r_147_combined

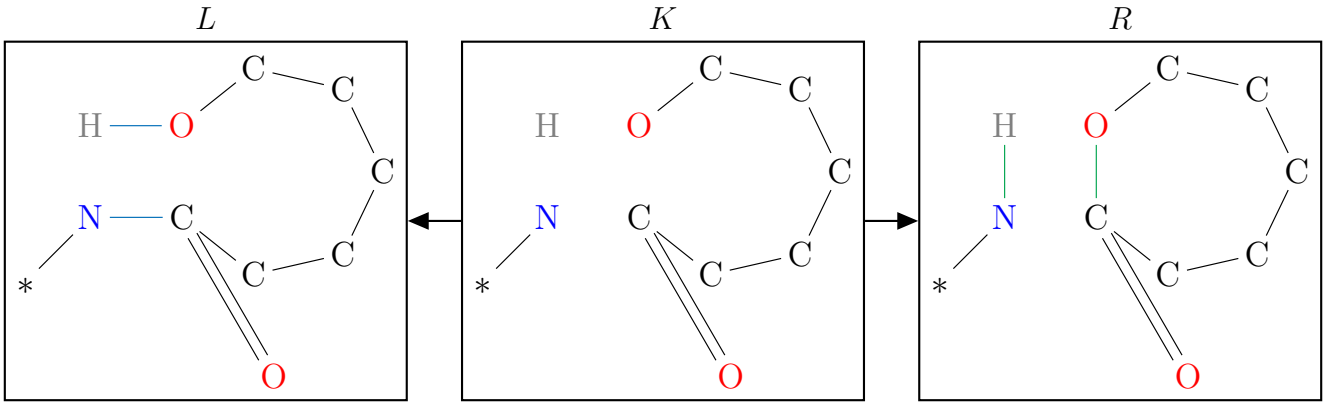
$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

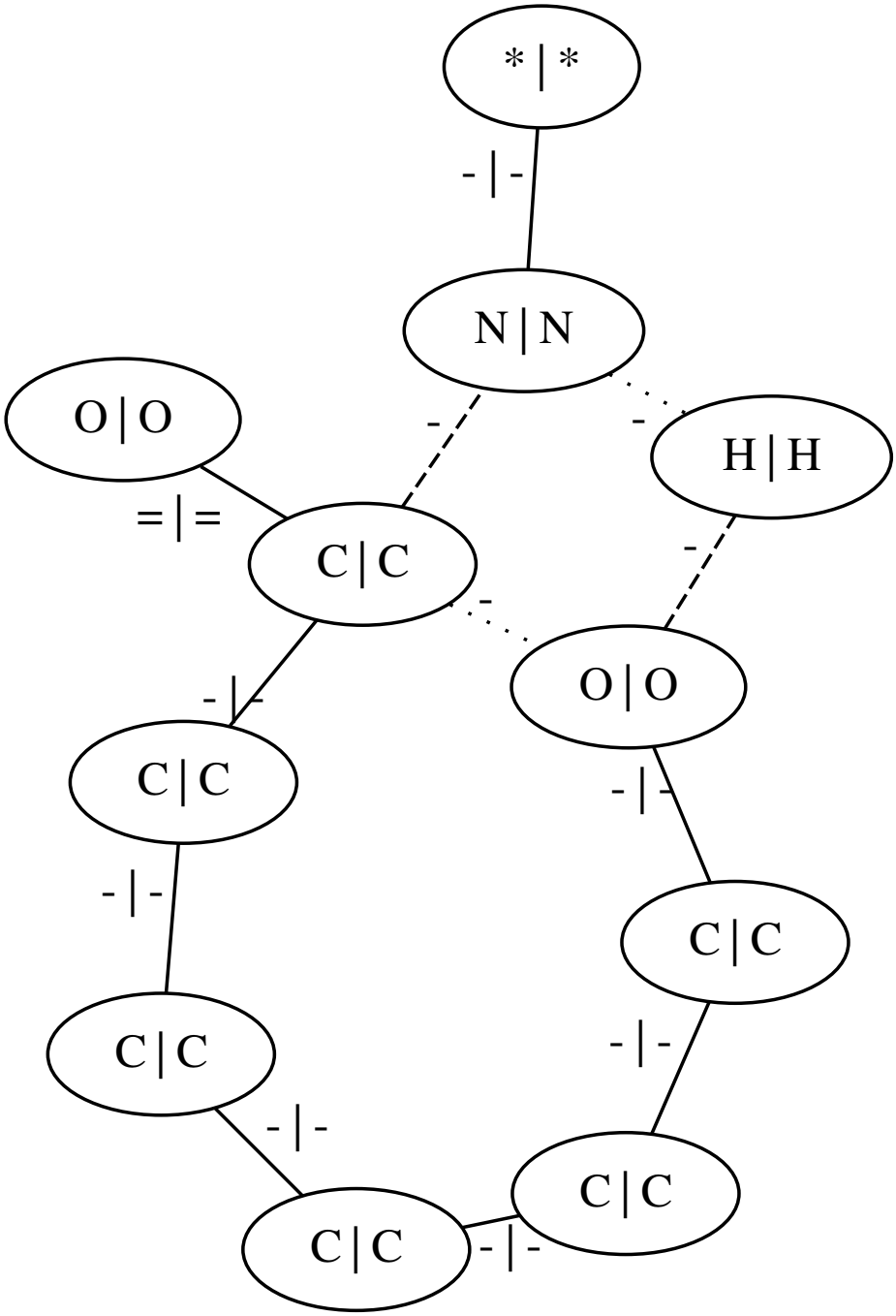
0.0.146 Ring Closure 7 membered N, O



Files: out/725_r_148_10300000_{L, K, R}



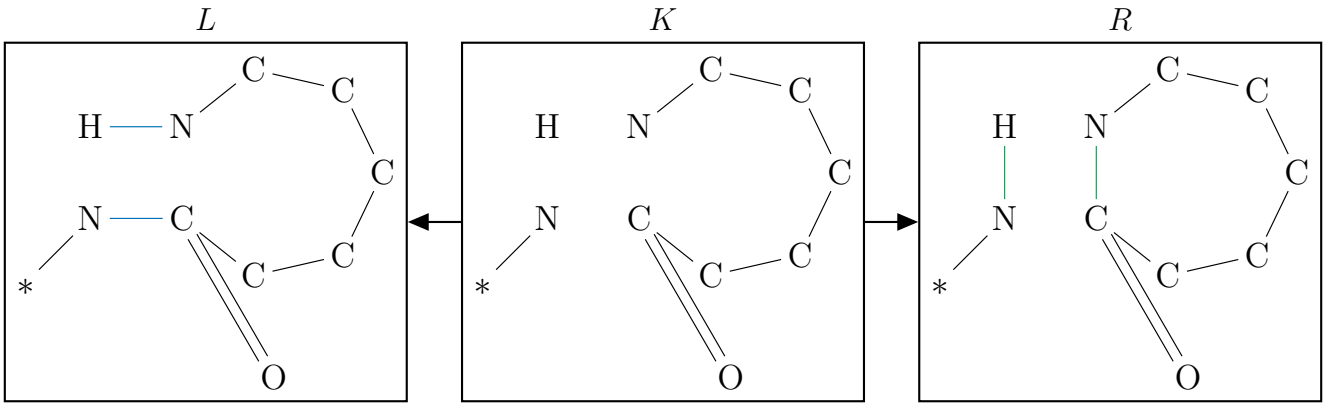
Files: out/726_r_148_11300100_{L, K, R}



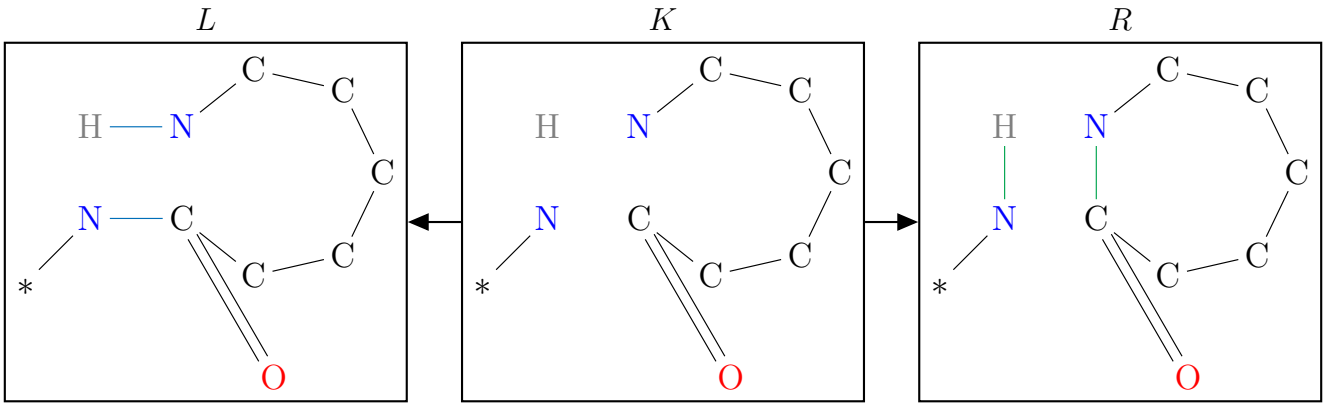
File: out/727_r_148_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

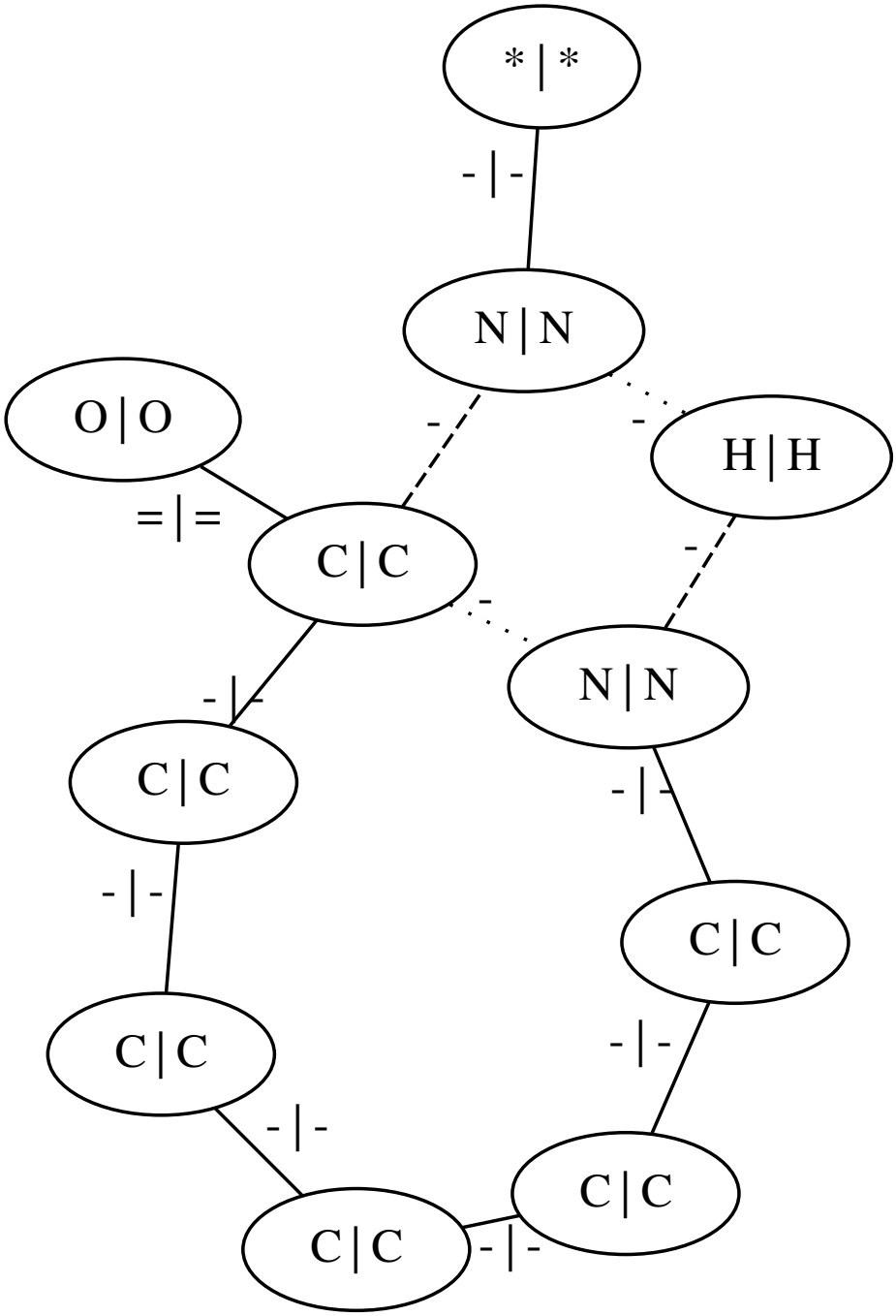
0.0.147 Ring Closure 7 membered N, N



Files: out/730_r_149_10300000_{L, K, R}



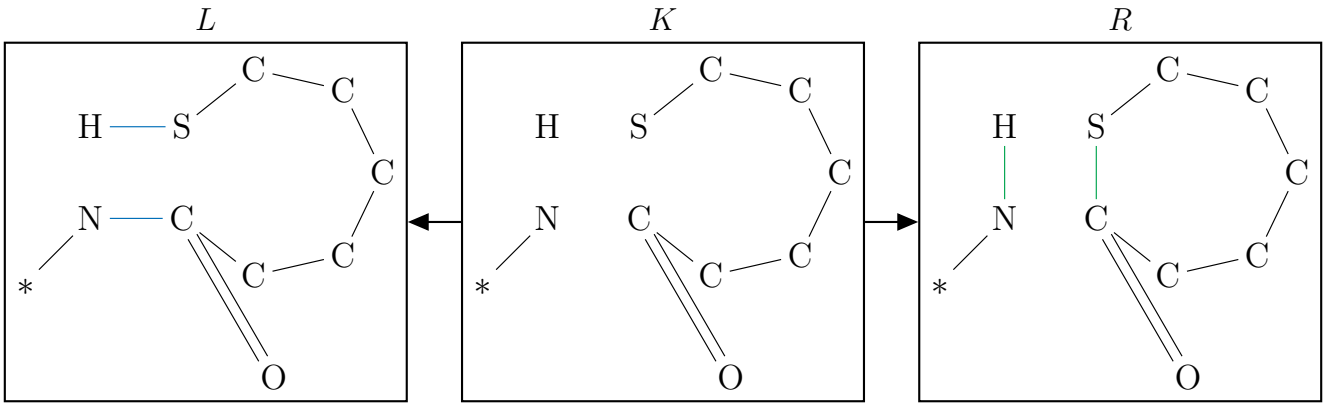
Files: out/731_r_149_11300100_{L, K, R}



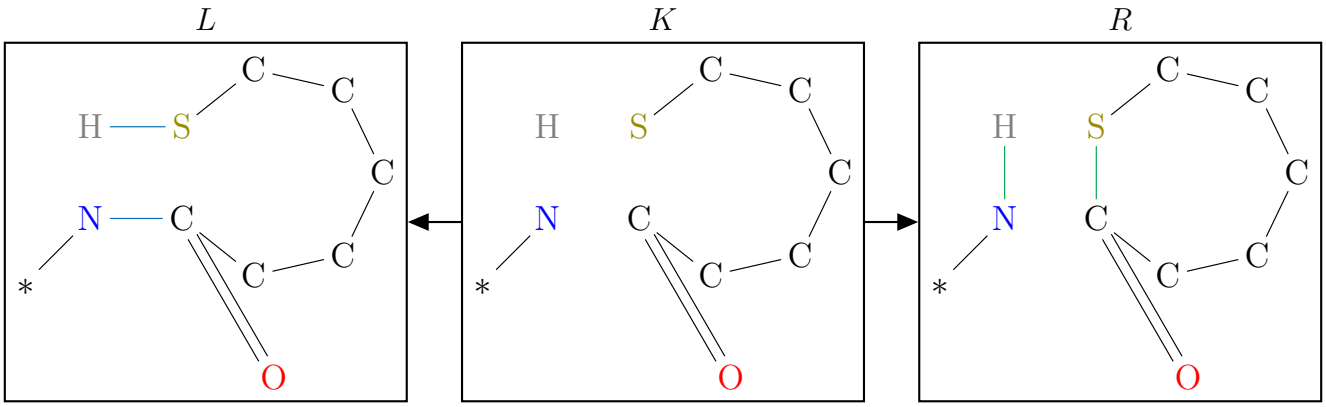
File: out/732_r_149_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

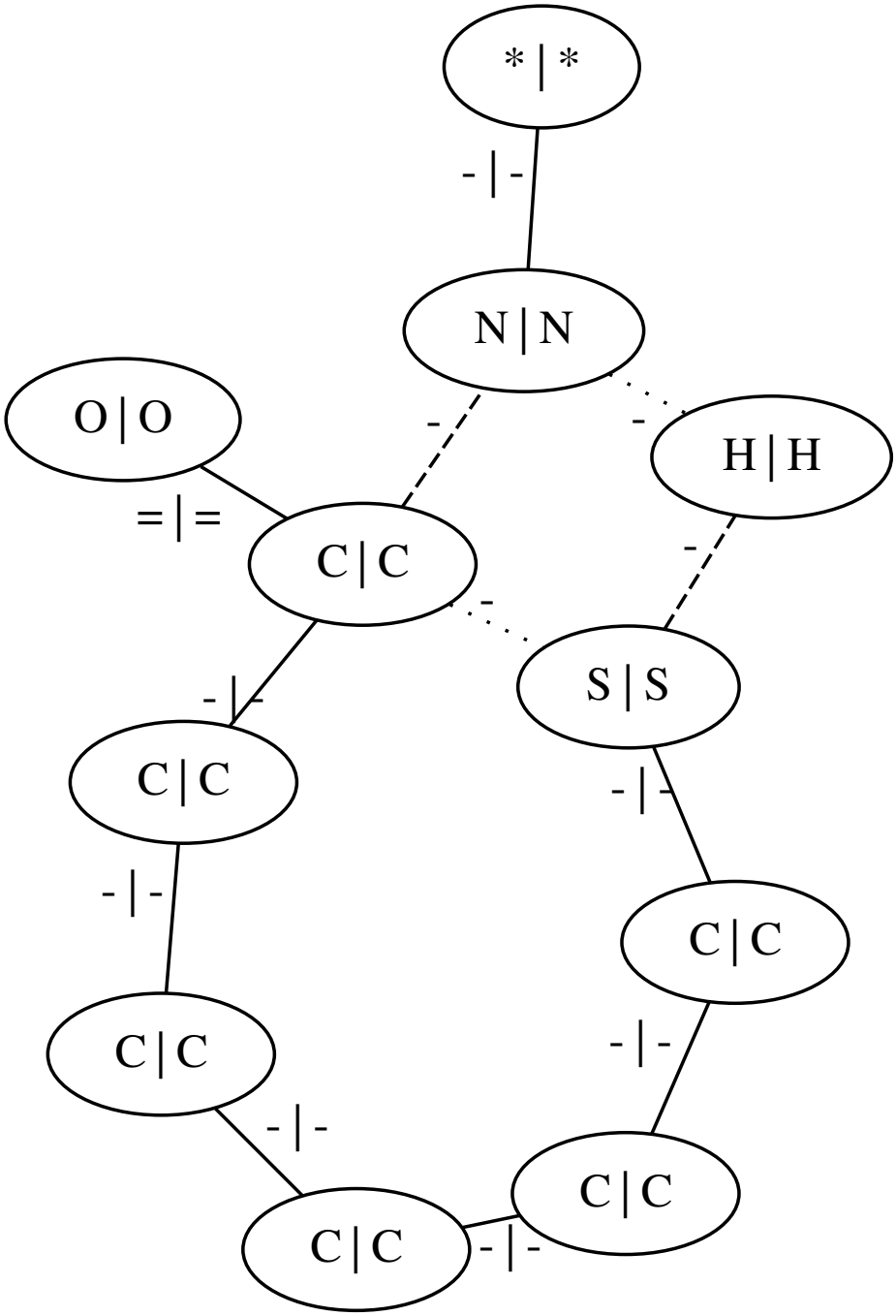
0.0.148 Ring Closure 7 membered N, S



Files: out/735_r_150_10300000_{L, K, R}



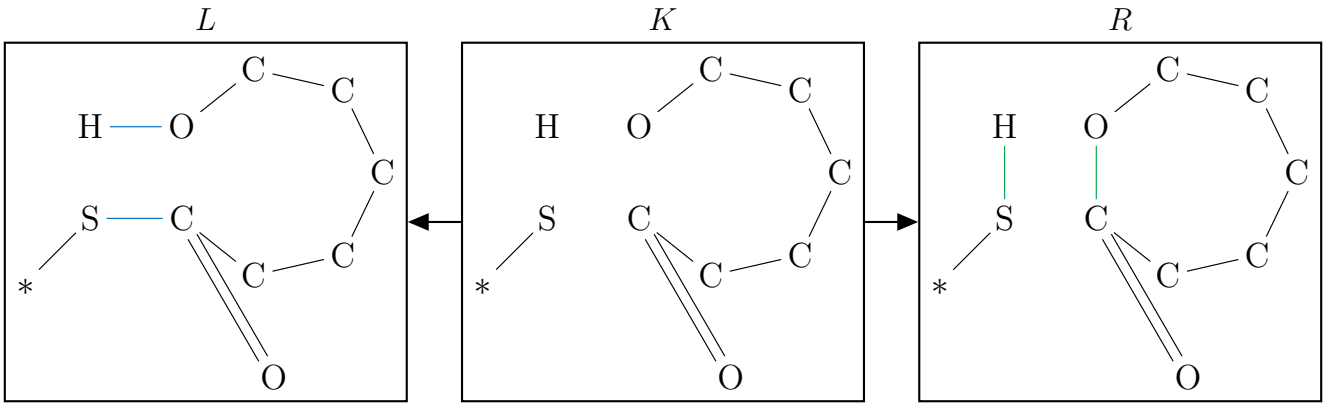
Files: out/736_r_150_11300100_{L, K, R}



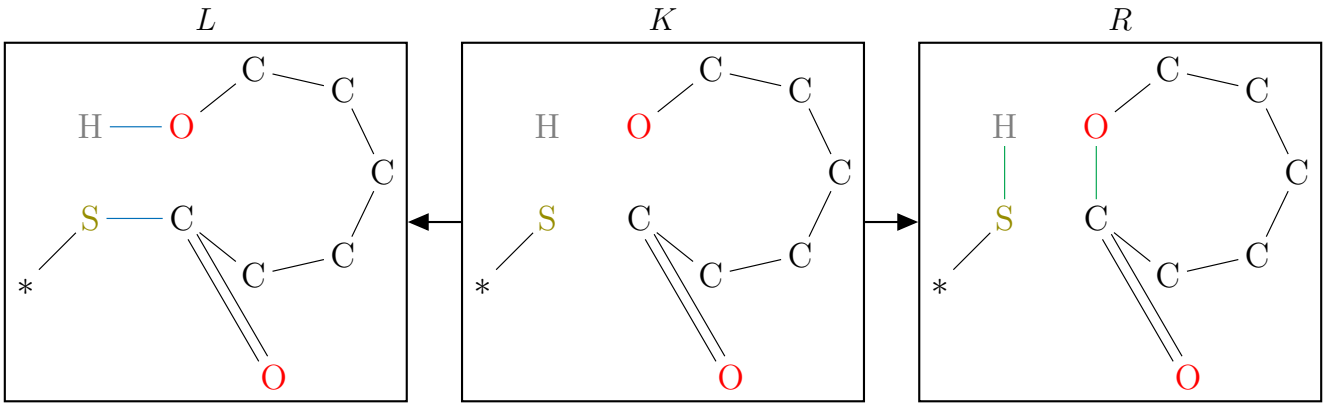
File: out/737_r_150_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

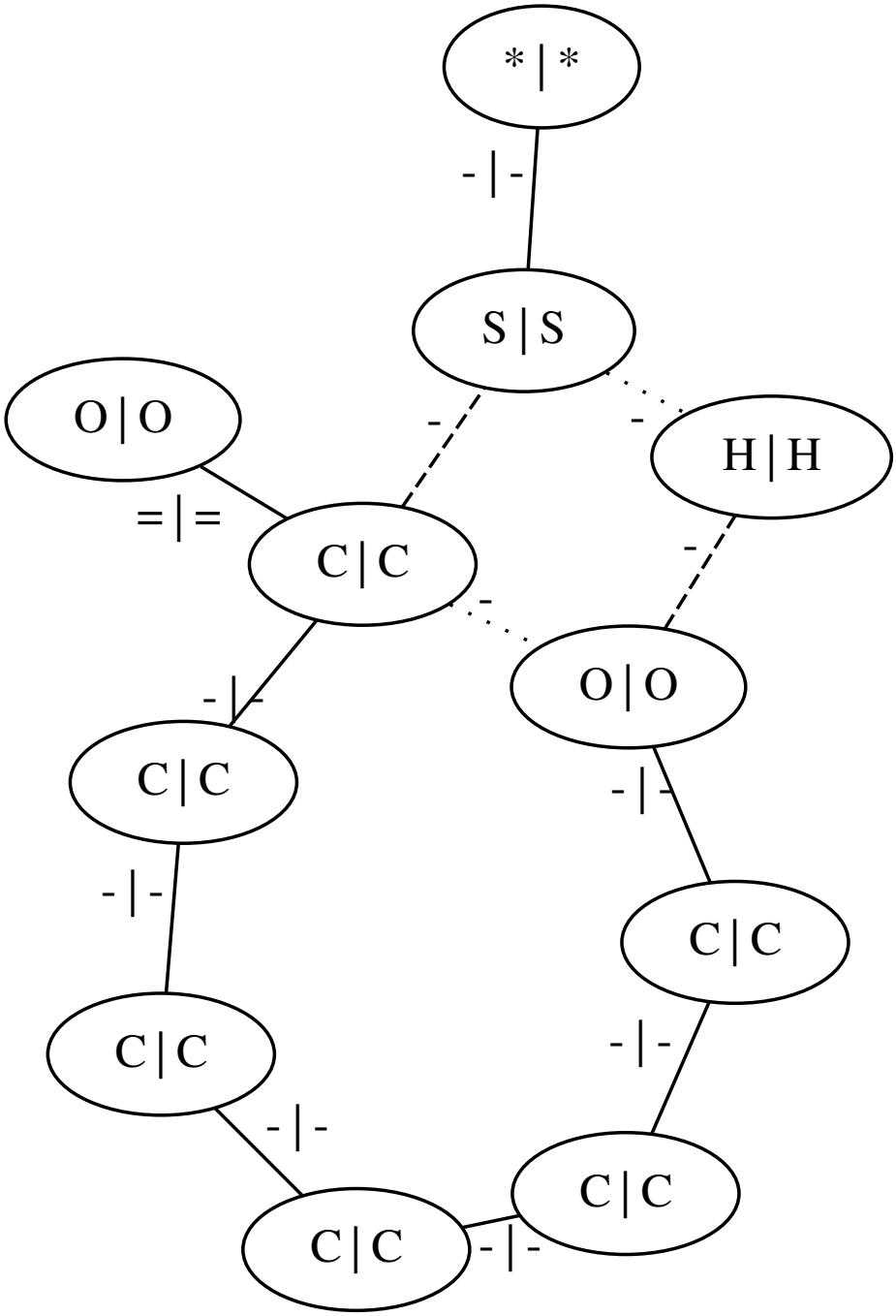
0.0.149 Ring Closure 7 membered S, O



Files: out/740_r_151_10300000_{L, K, R}



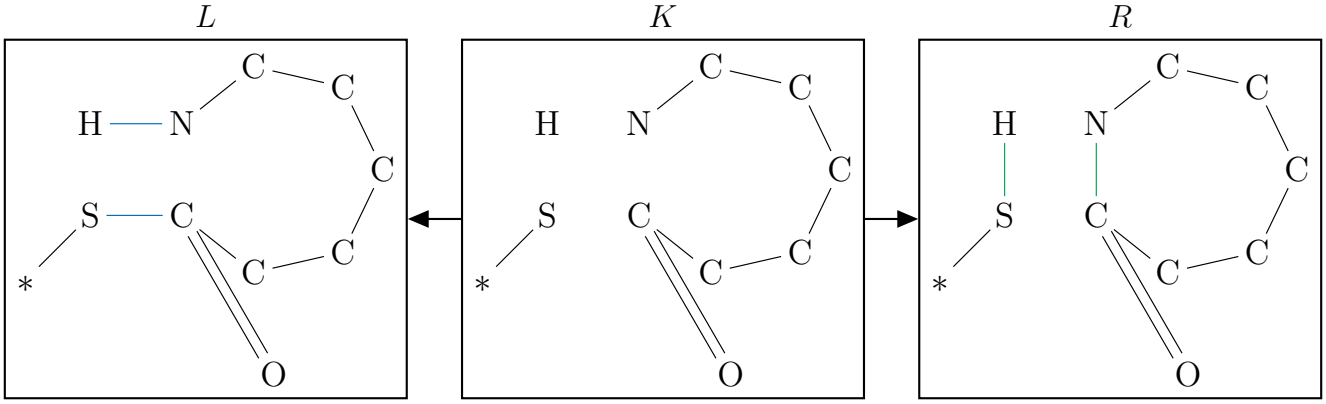
Files: out/741_r_151_11300100_{L, K, R}



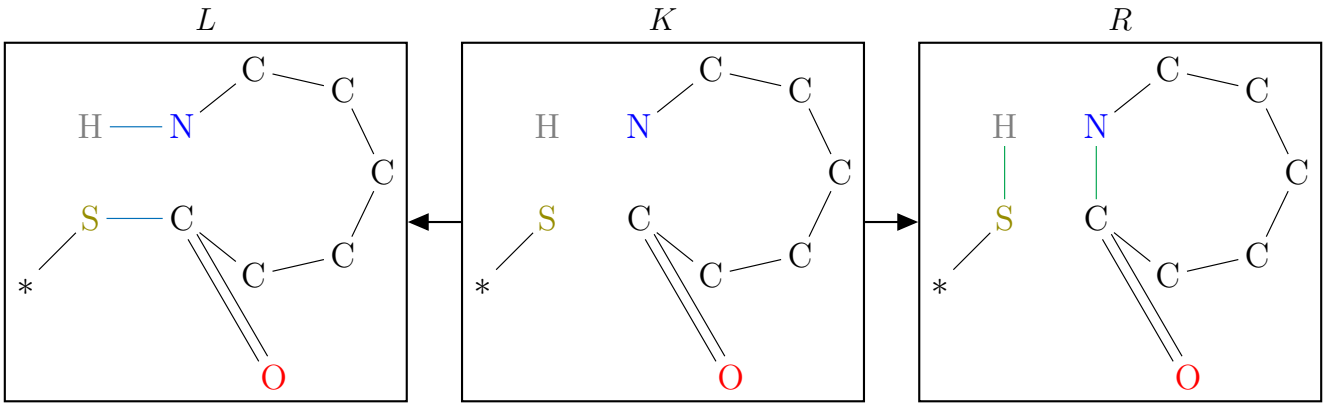
File: out/742_r_151_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

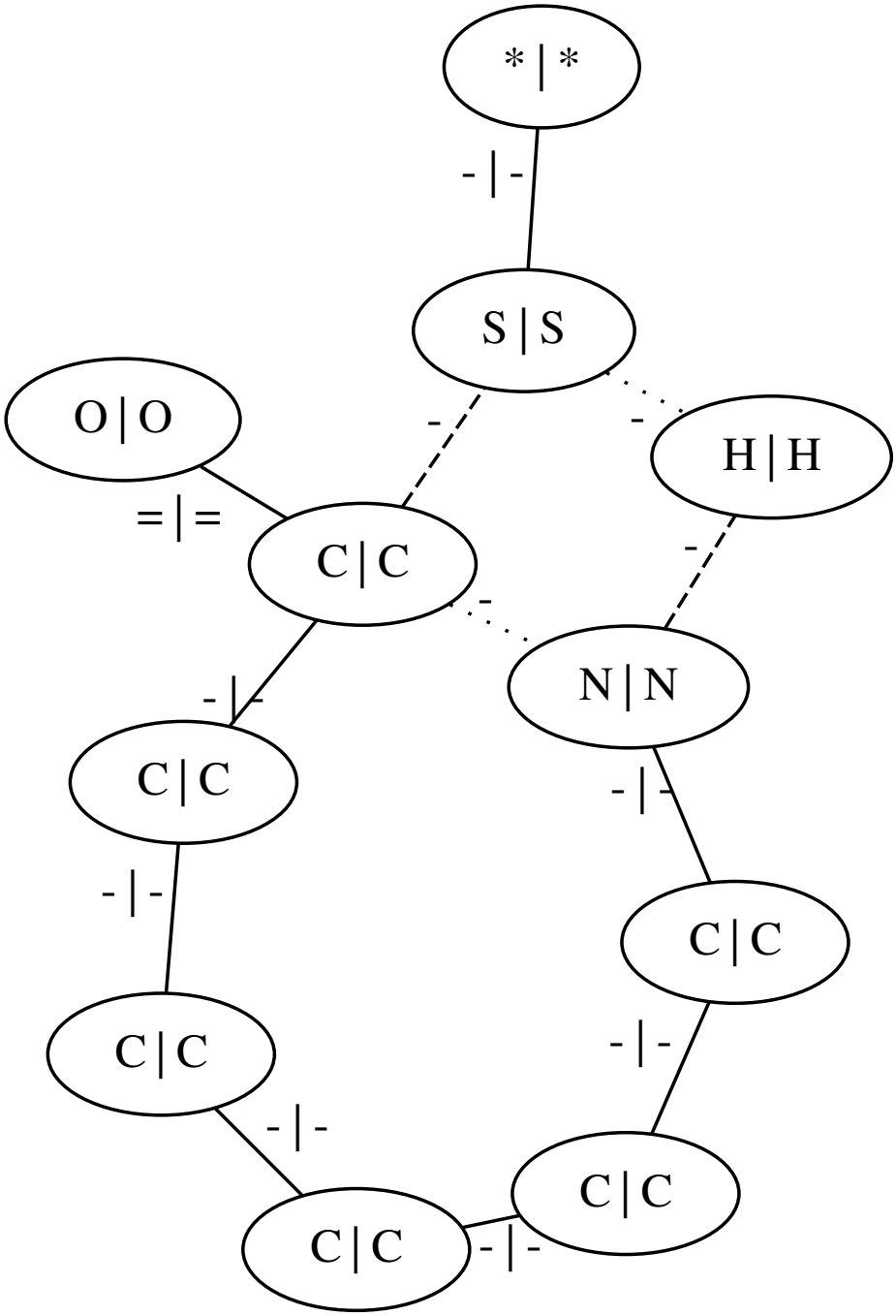
0.0.150 Ring Closure 7 membered S, N



Files: out/745_r_152_10300000_{L, K, R}



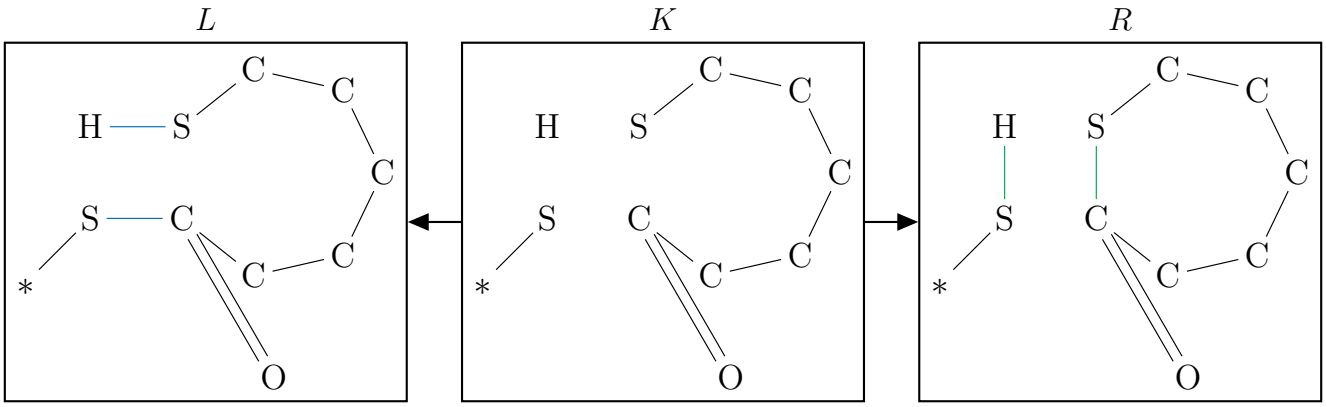
Files: out/746_r_152_11300100_{L, K, R}



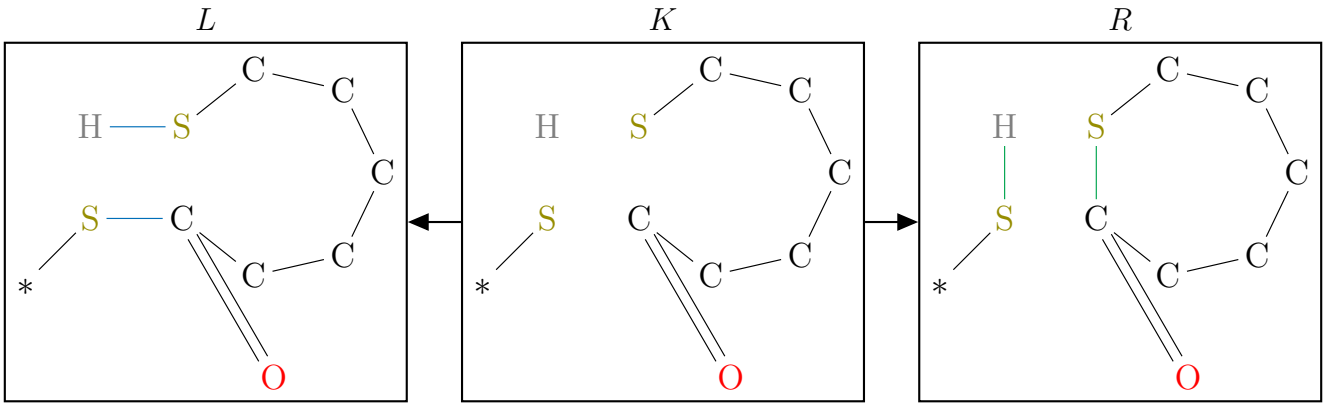
File: out/747_r_152_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

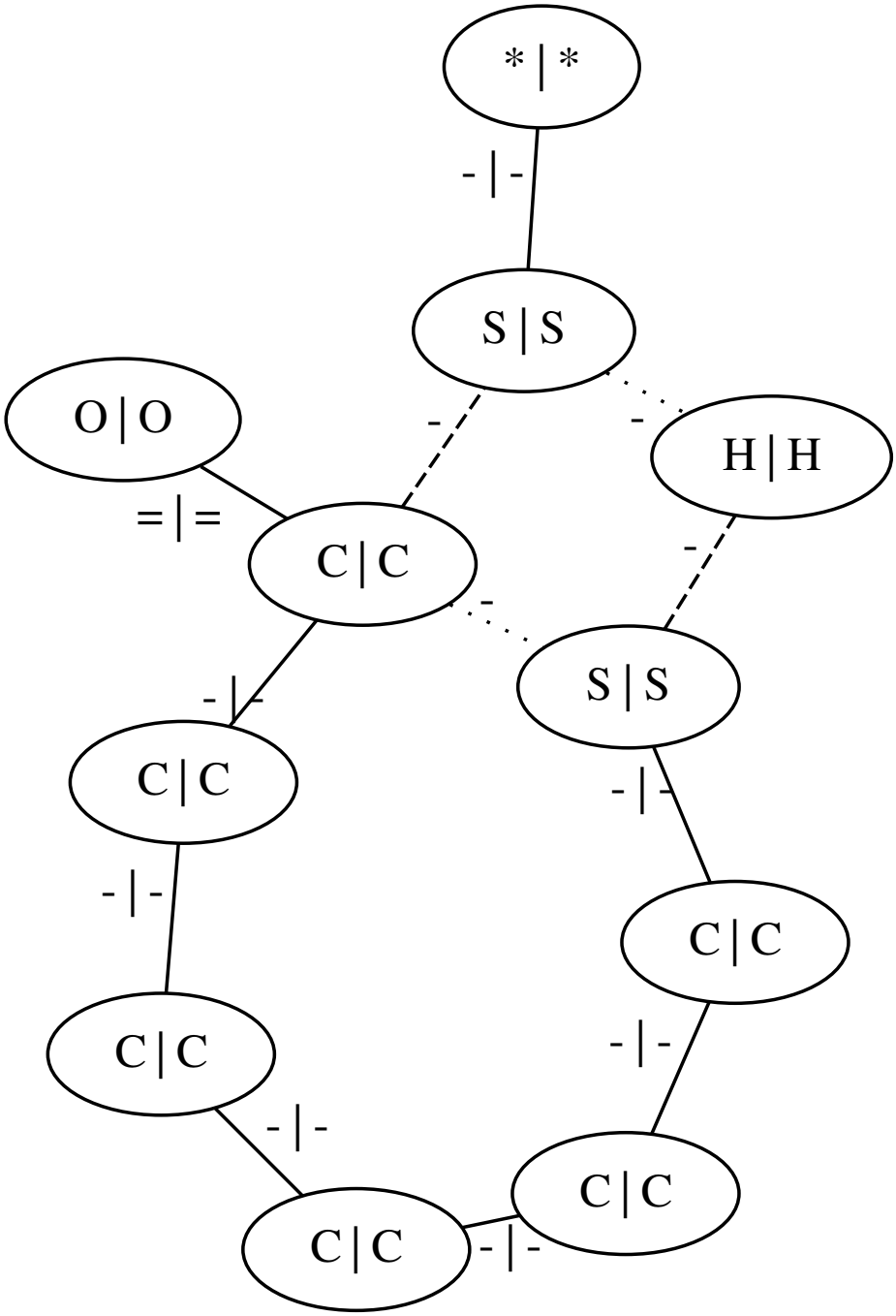
0.0.151 Ring Closure 7 membered S, S



Files: out/750_r_153_10300000_{L, K, R}



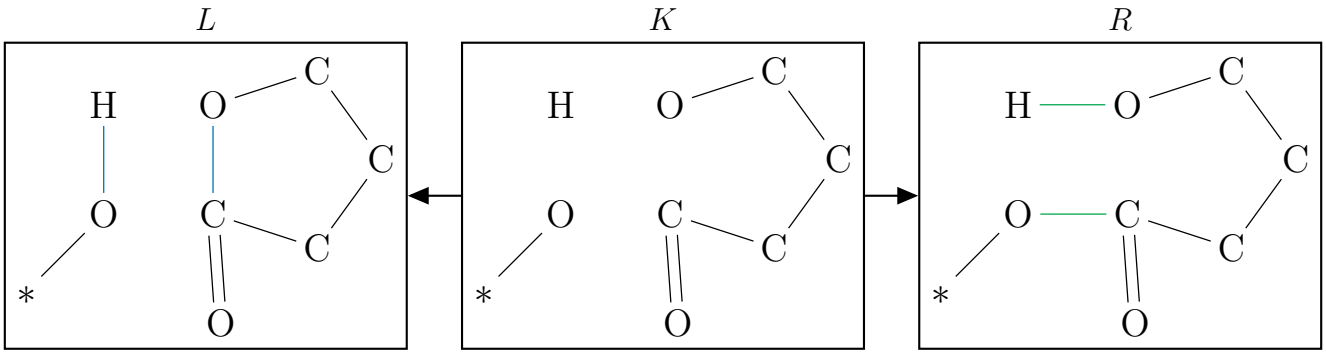
Files: out/751_r_153_11300100_{L, K, R}



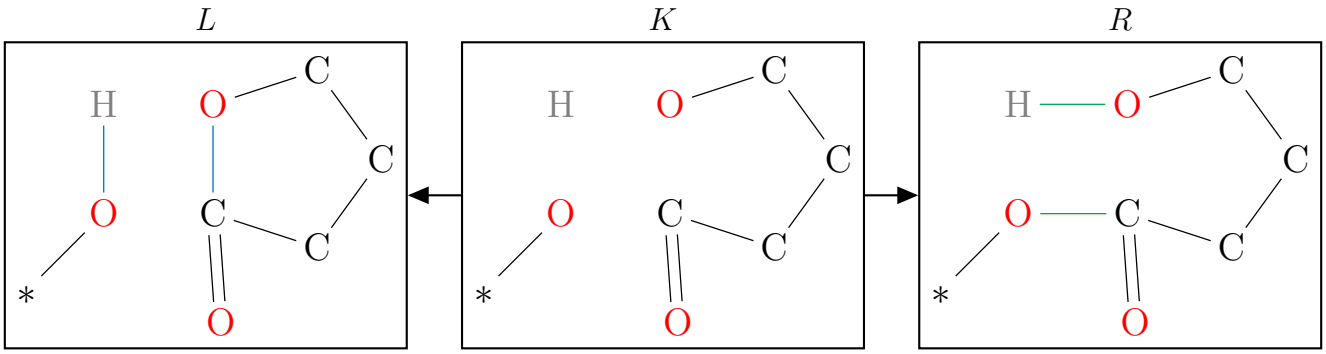
File: out/752_r_153_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

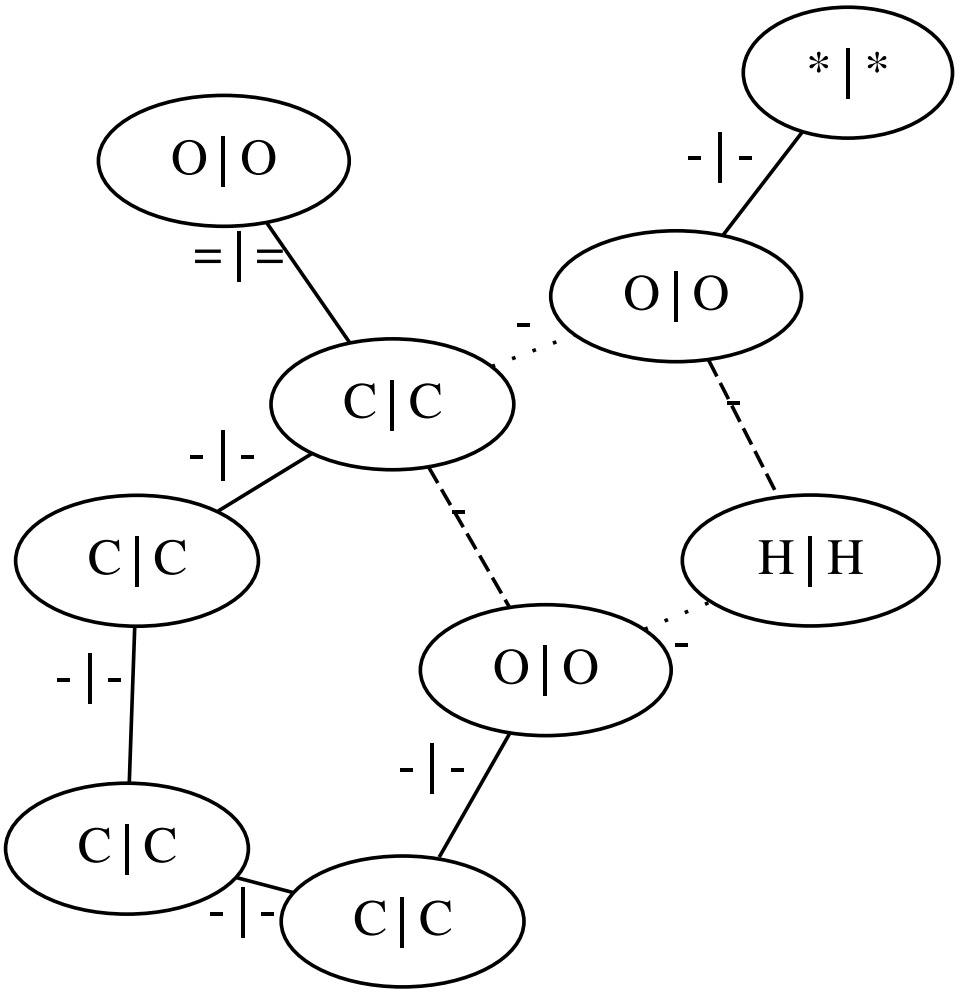
0.0.152 Ring Closure 5 membered, inverse O, O



Files: out/755_r_154_10300000_{L, K, R}



Files: out/756_r_154_11300100_{L, K, R}

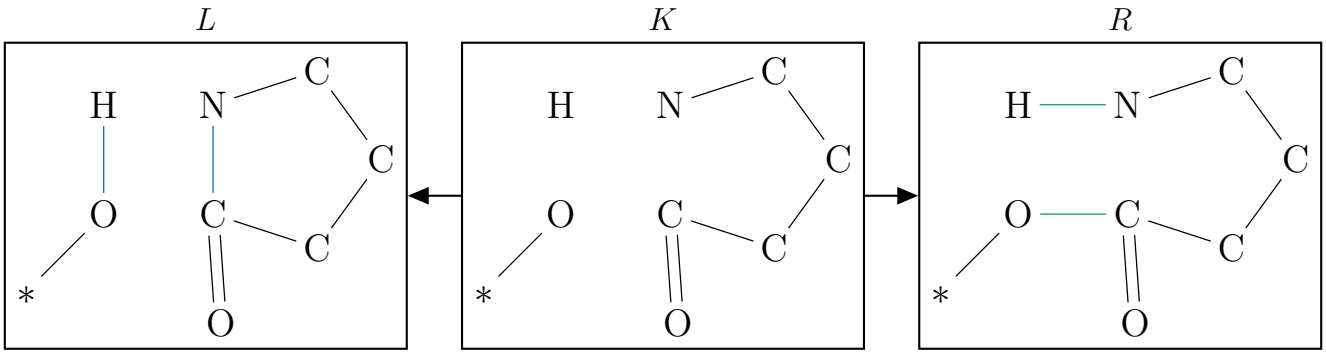


File: out/757_r_154_combined

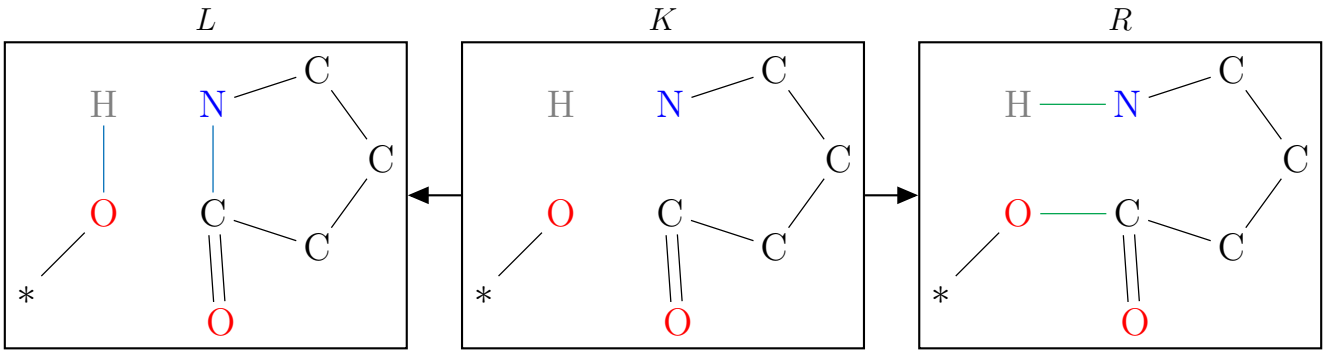
$$|\{e \in \text{outEdges}(8) \mid \\ \quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\ \quad \wedge \\ \quad \text{label}(e) \in \{\text{`-'}\} \\ \}| \leq 1$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 1
\end{aligned}
$$

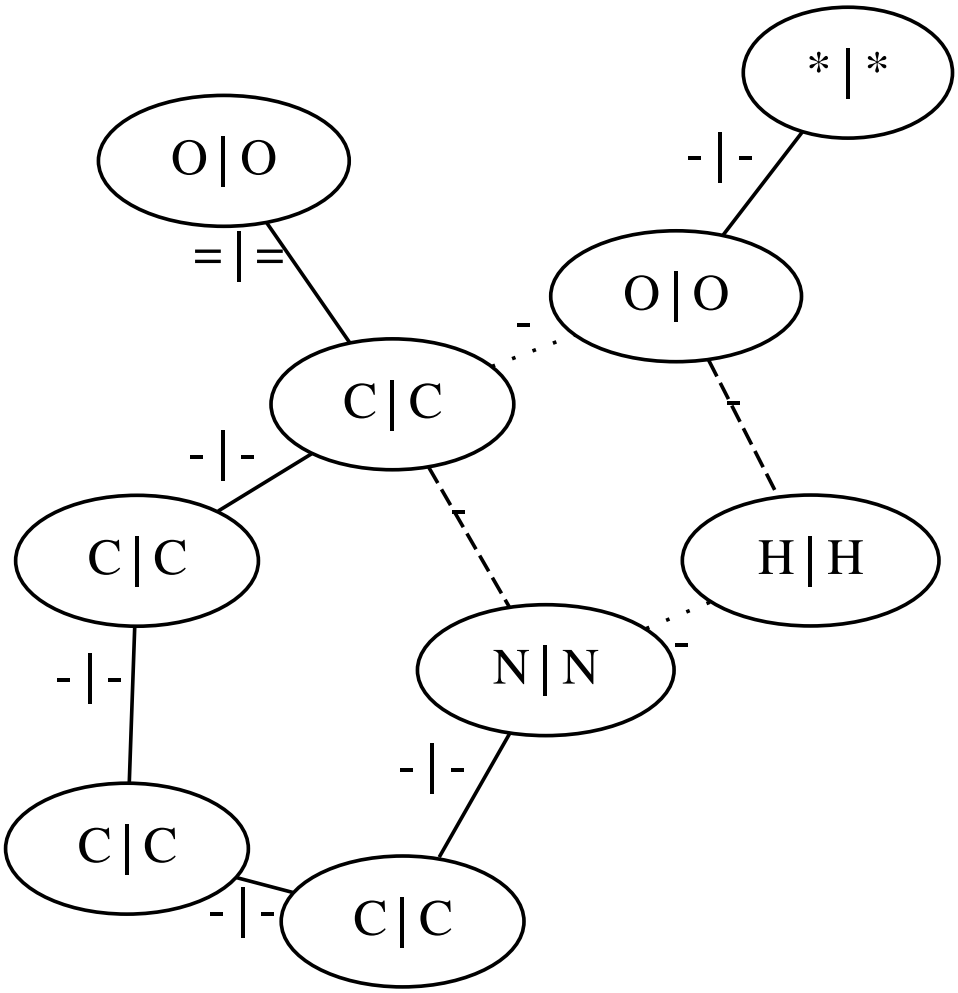
0.0.153 Ring Closure 5 membered, inverse O, N



Files: out/760_r_155_10300000_{L, K, R}



Files: out/761_r_155_11300100_{L, K, R}

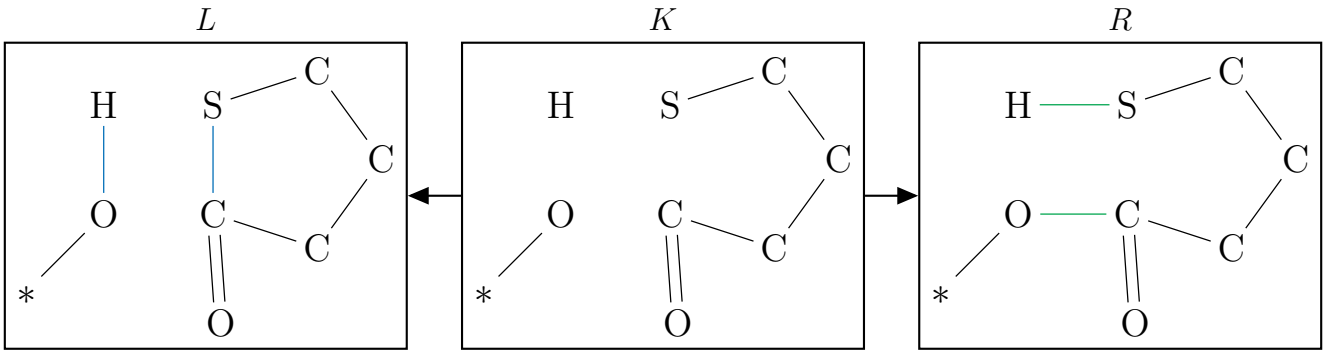


File: out/762_r_155_combined

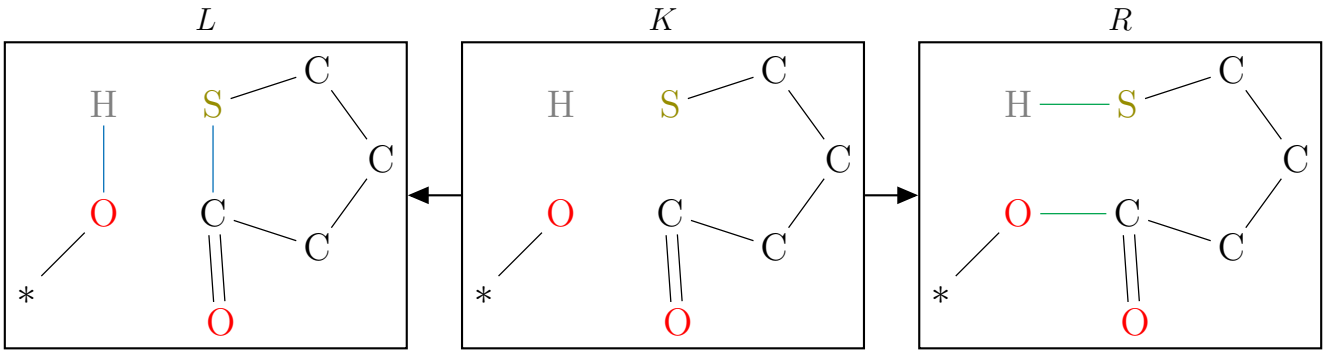
$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 1
\end{aligned}
$$

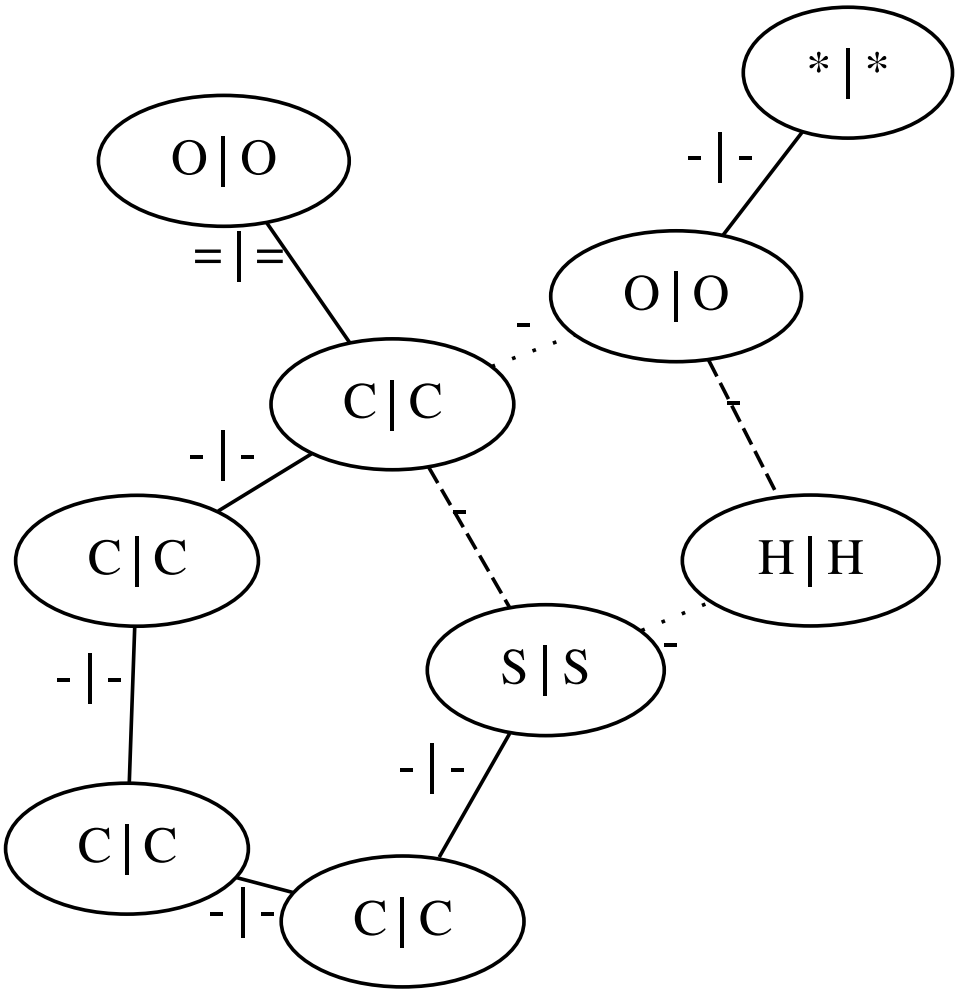
0.0.154 Ring Closure 5 membered, inverse O, S



Files: out/765_r_156_10300000_{L, K, R}



Files: out/766_r_156_11300100_{L, K, R}

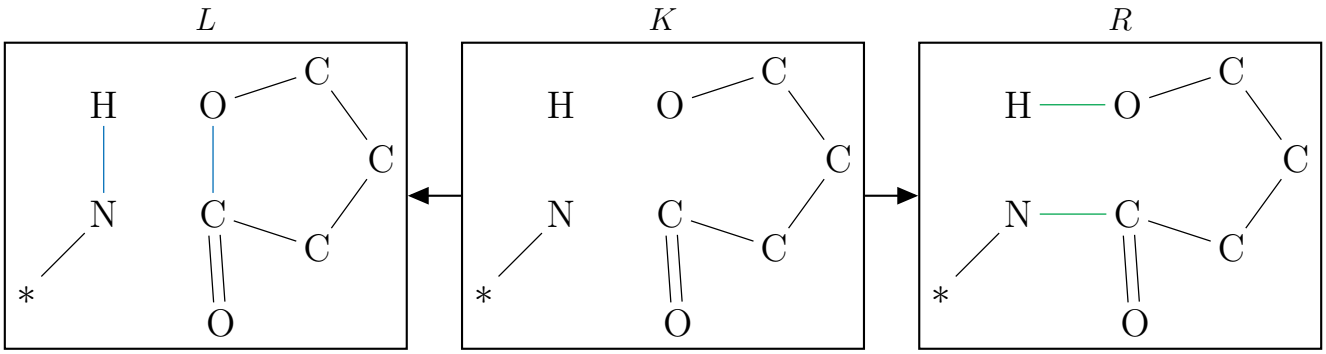


File: out/767_r_156_combined

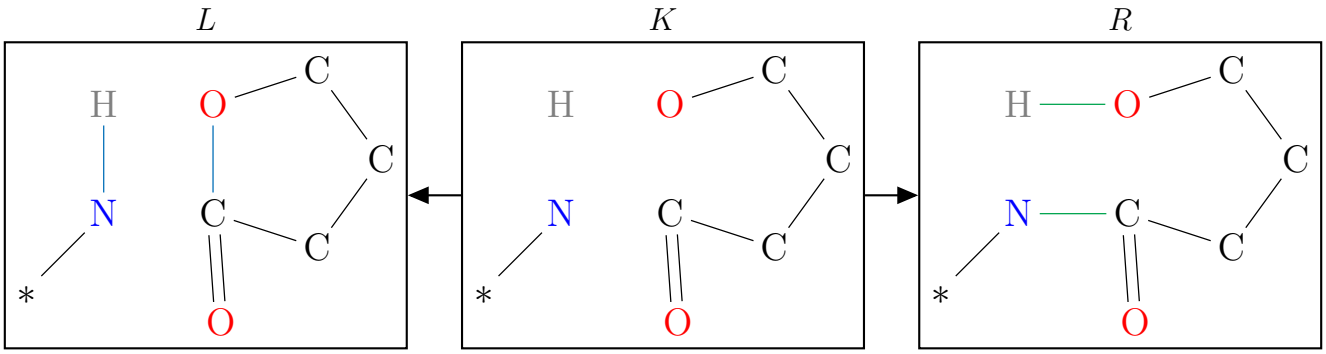
$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 1
\end{aligned}
$$

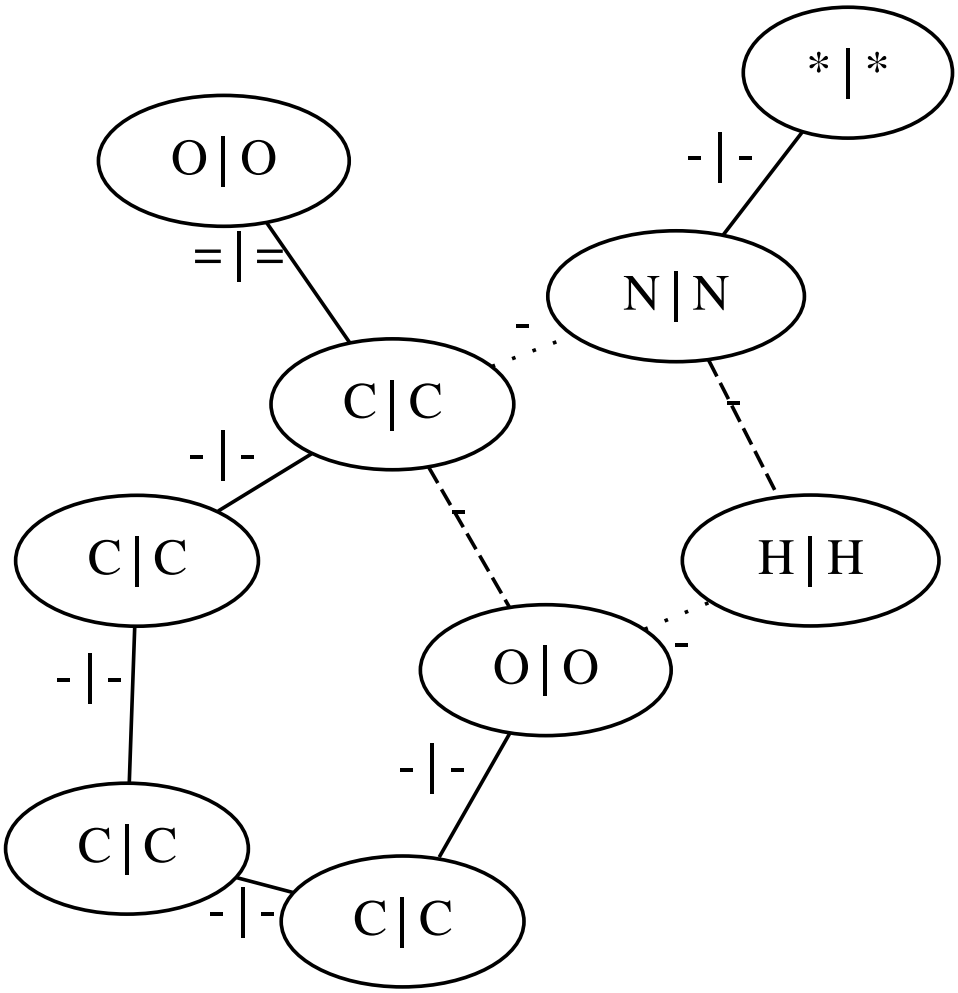
0.0.155 Ring Closure 5 membered, inverse N, O



Files: out/770_r_157_10300000_{L, K, R}



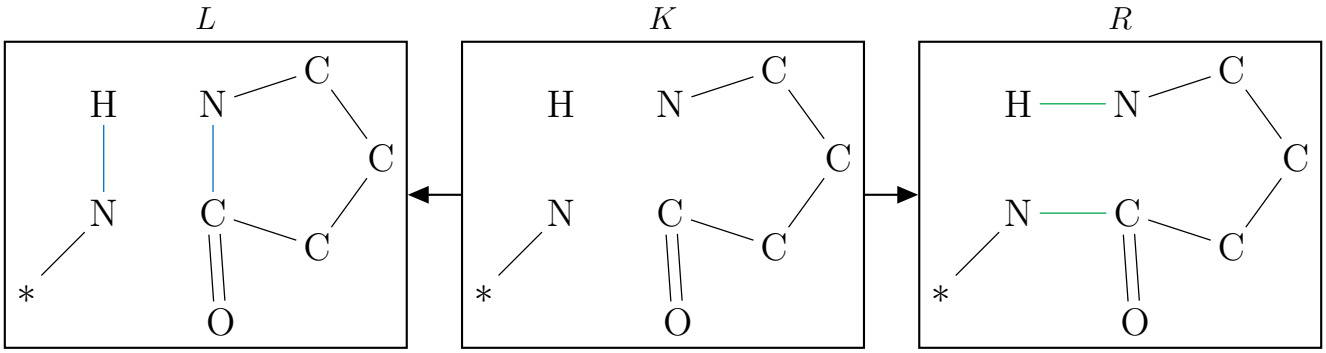
Files: out/771_r_157_11300100_{L, K, R}



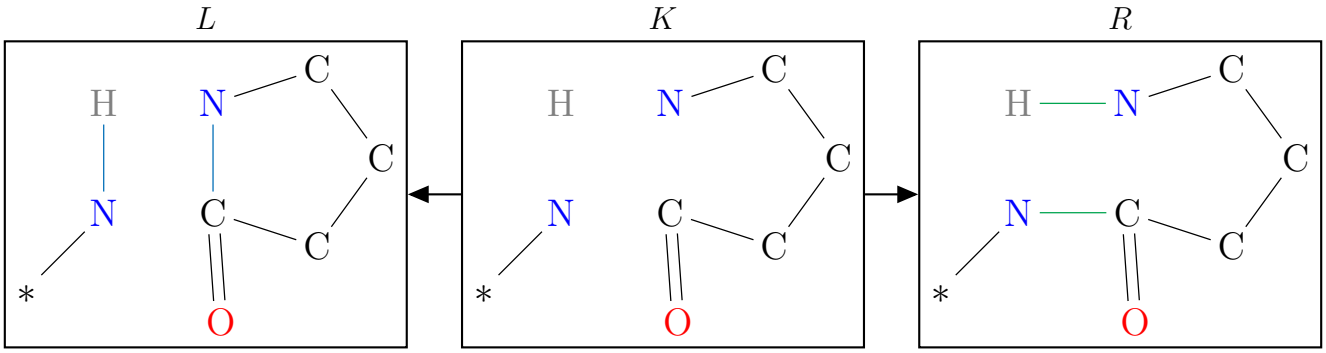
File: out/772_r_157_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

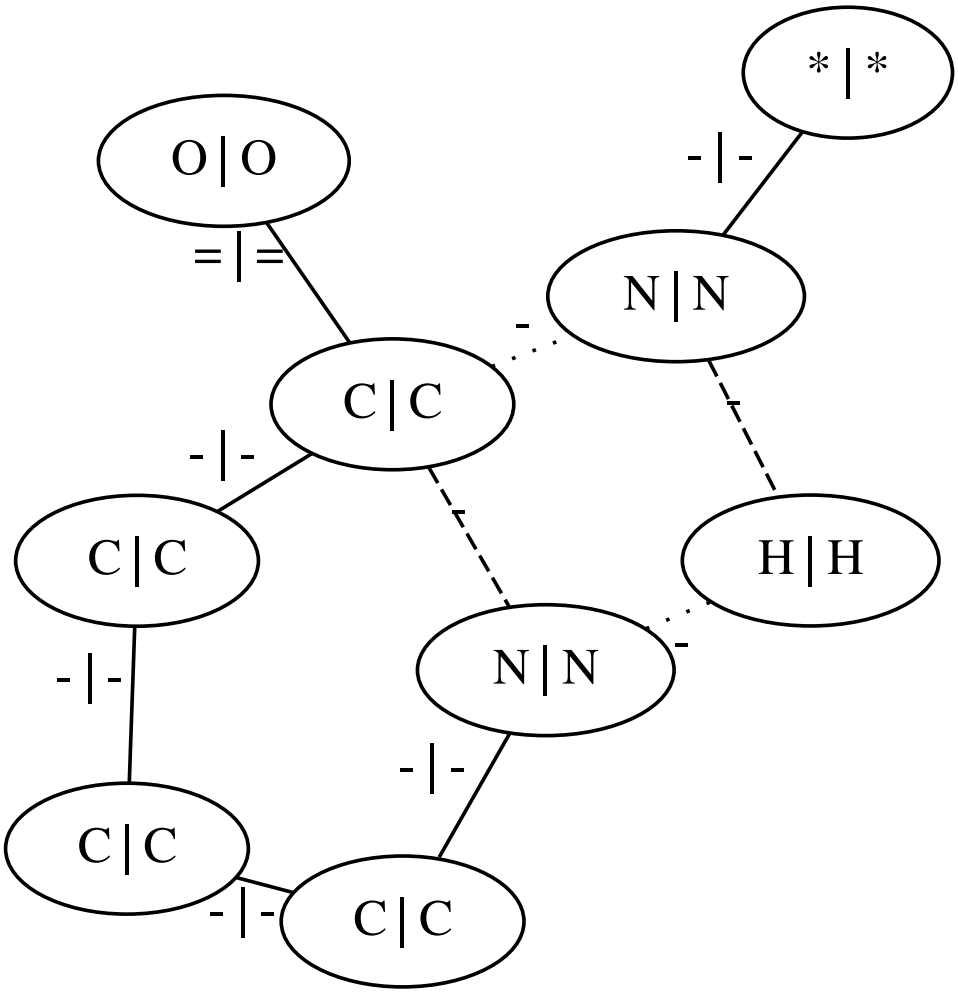
0.0.156 Ring Closure 5 membered, inverse N, N



Files: out/775_r_158_10300000_{L, K, R}



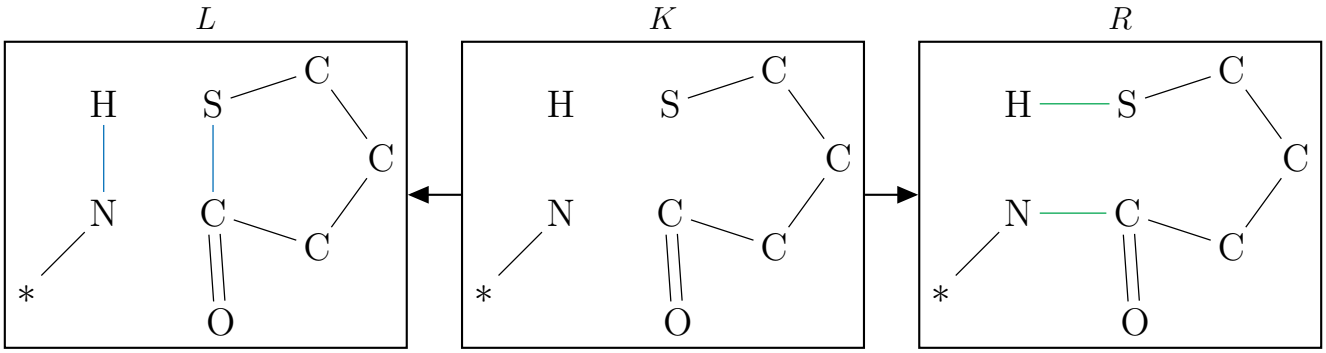
Files: out/776_r_158_11300100_{L, K, R}



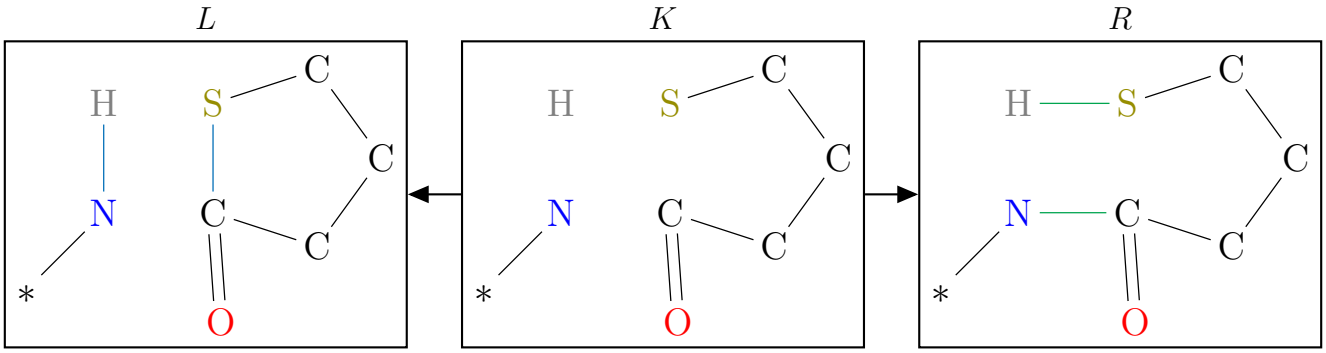
File: out/777_r_158_combined

$$|\{e \in \text{outEdges}(8) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

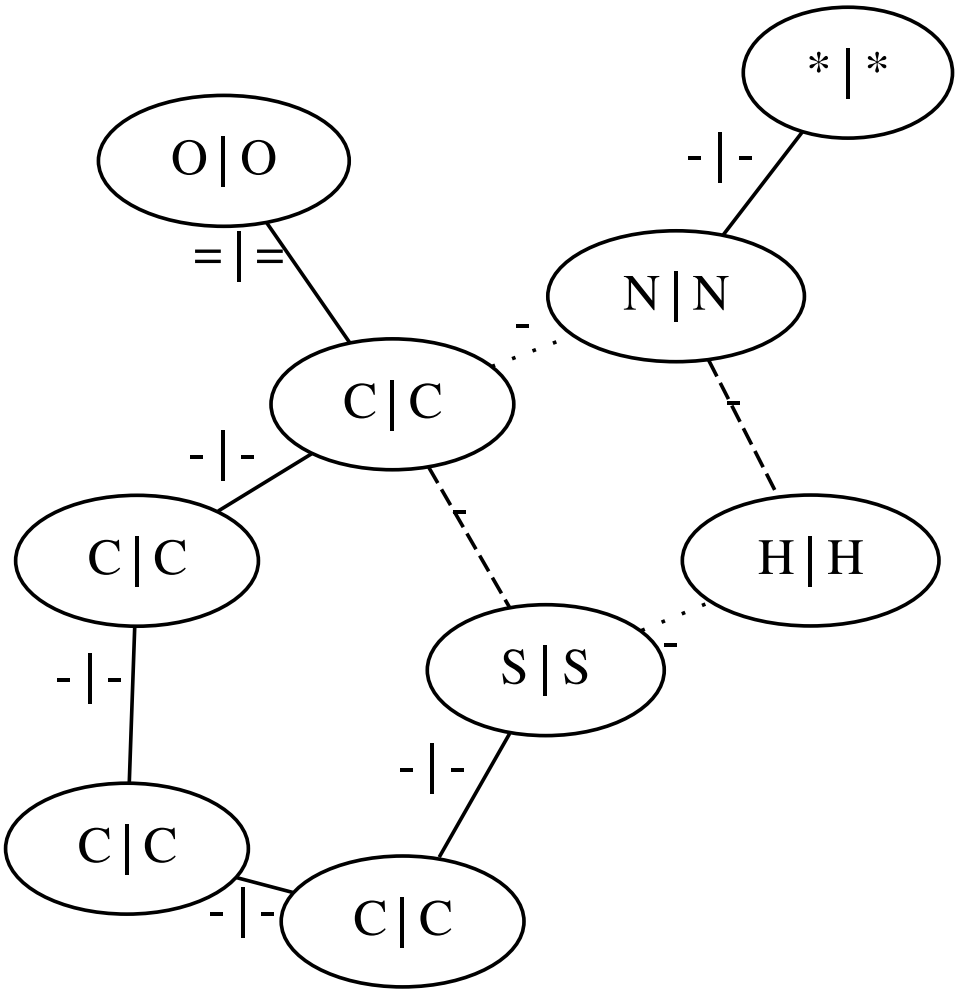
0.0.157 Ring Closure 5 membered, inverse N, S



Files: out/780_r_159_10300000_{L, K, R}



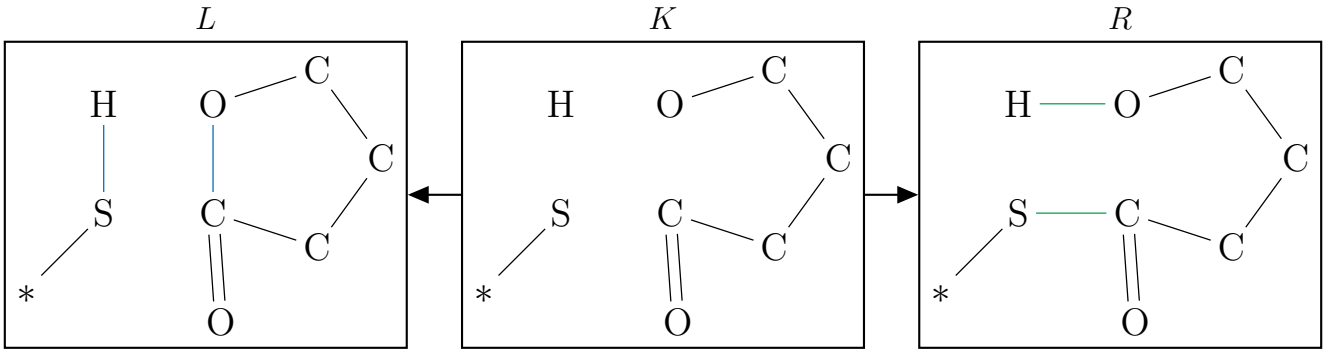
Files: out/781_r_159_11300100_{L, K, R}



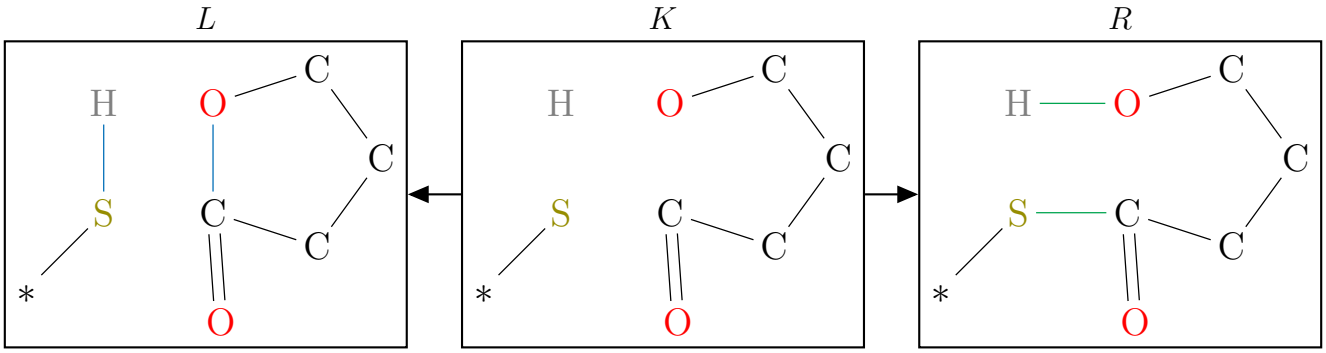
File: out/782_r_159_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

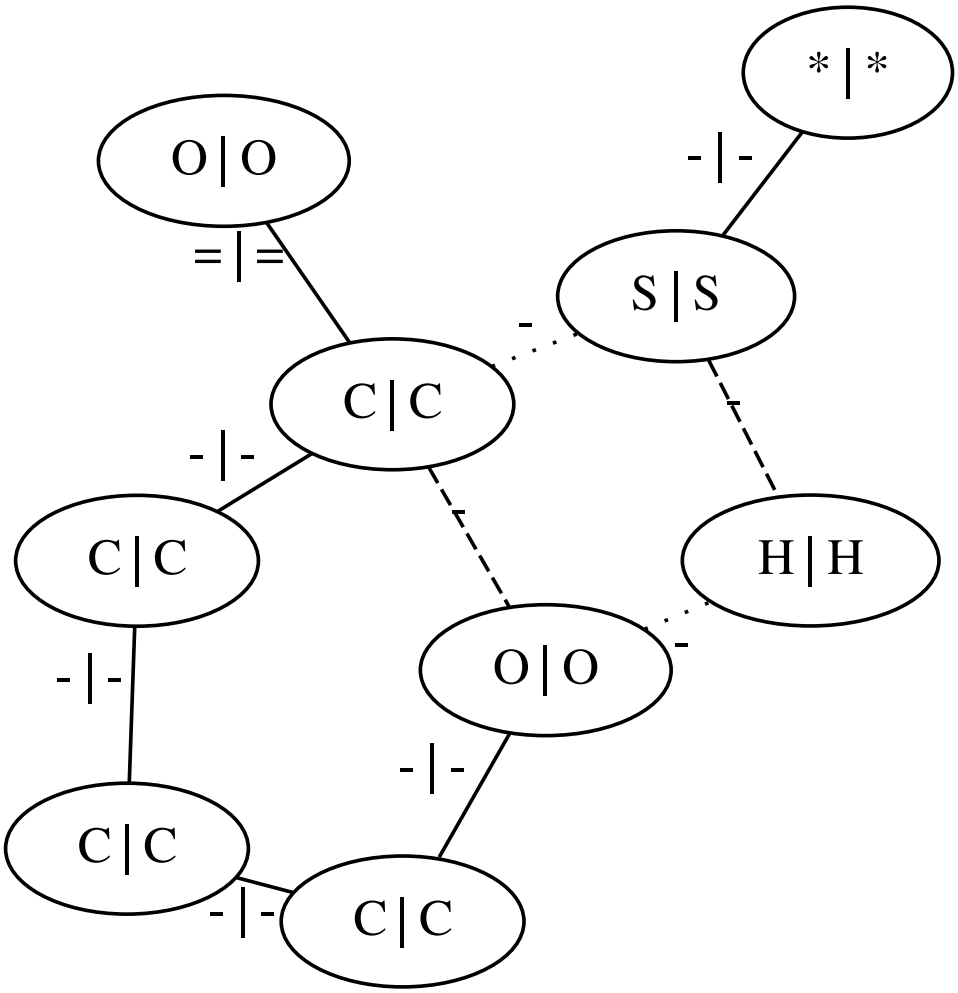
0.0.158 Ring Closure 5 membered, inverse S, O



Files: out/785_r_160_10300000_{L, K, R}



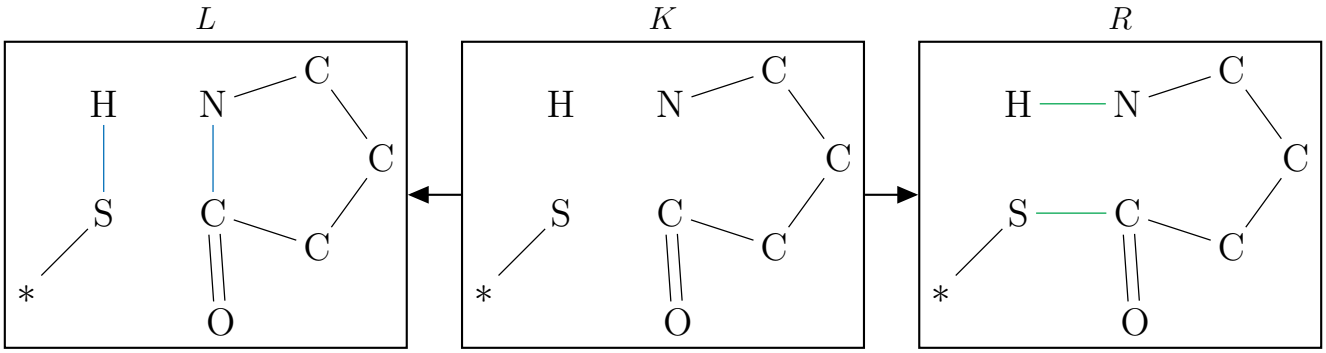
Files: out/786_r_160_11300100_{L, K, R}



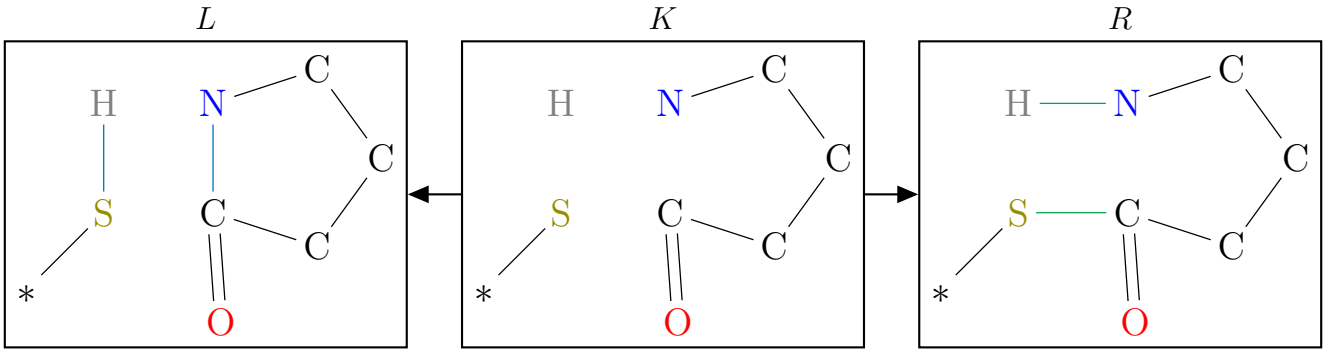
File: out/787_r_160_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

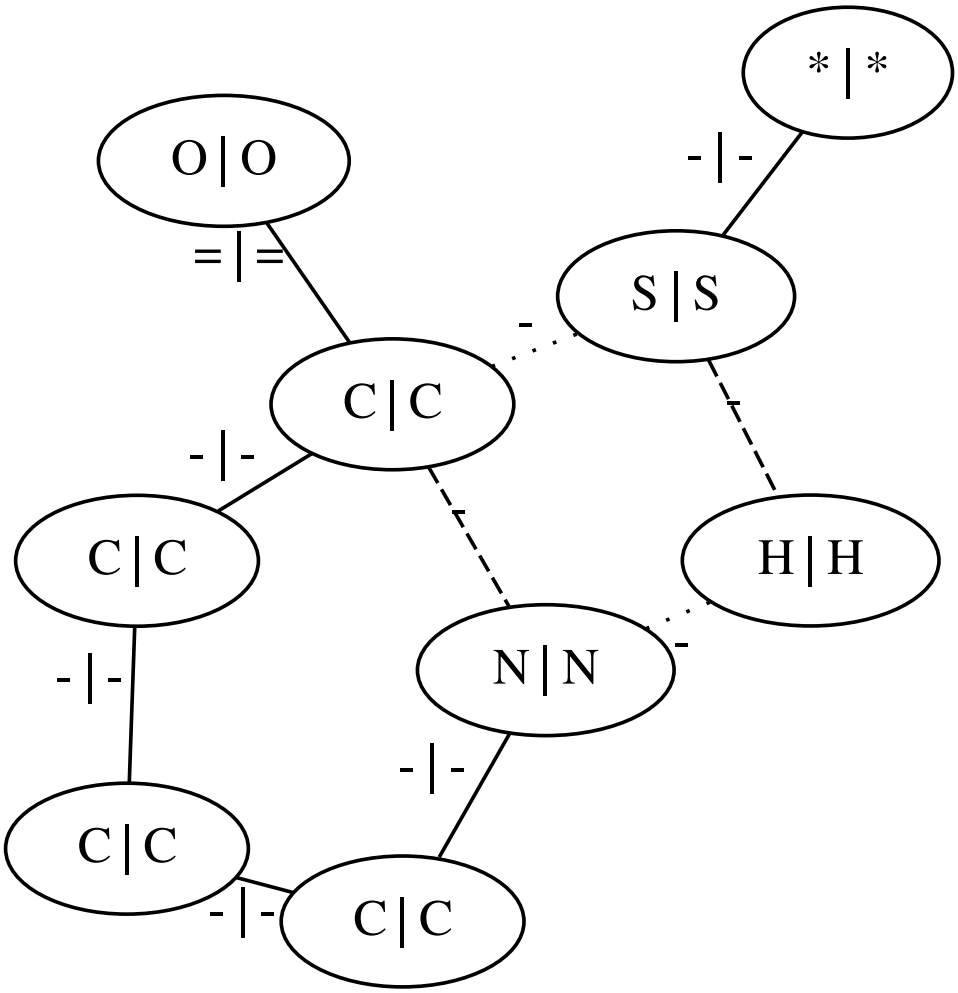
0.0.159 Ring Closure 5 membered, inverse S, N



Files: out/790_r_161_10300000_{L, K, R}



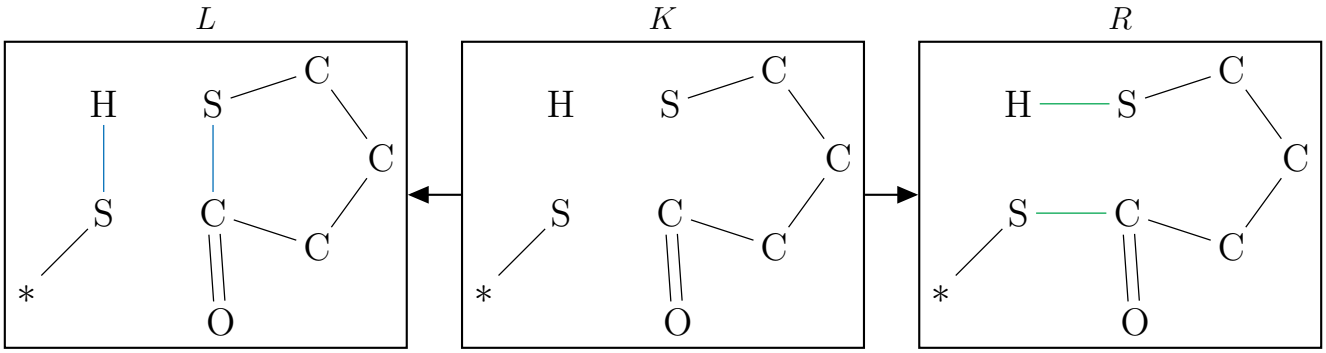
Files: out/791_r_161_11300100_{L, K, R}



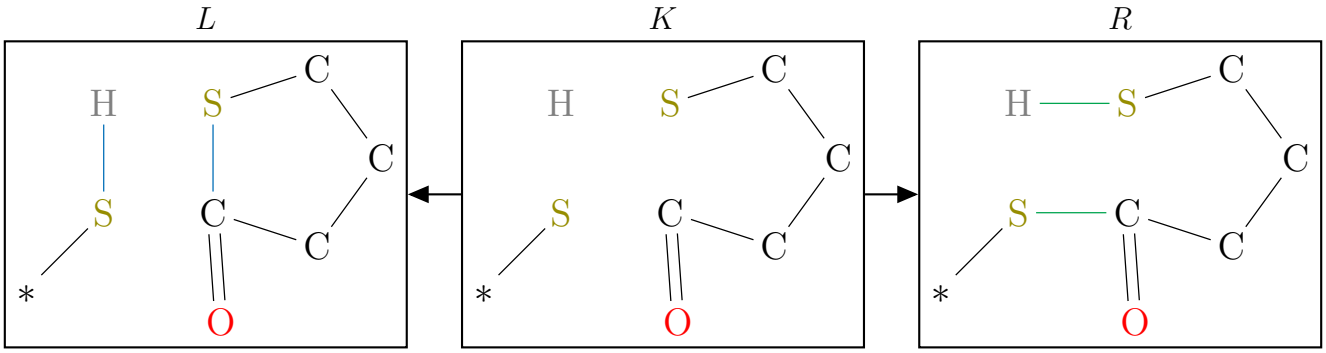
File: out/792_r_161_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

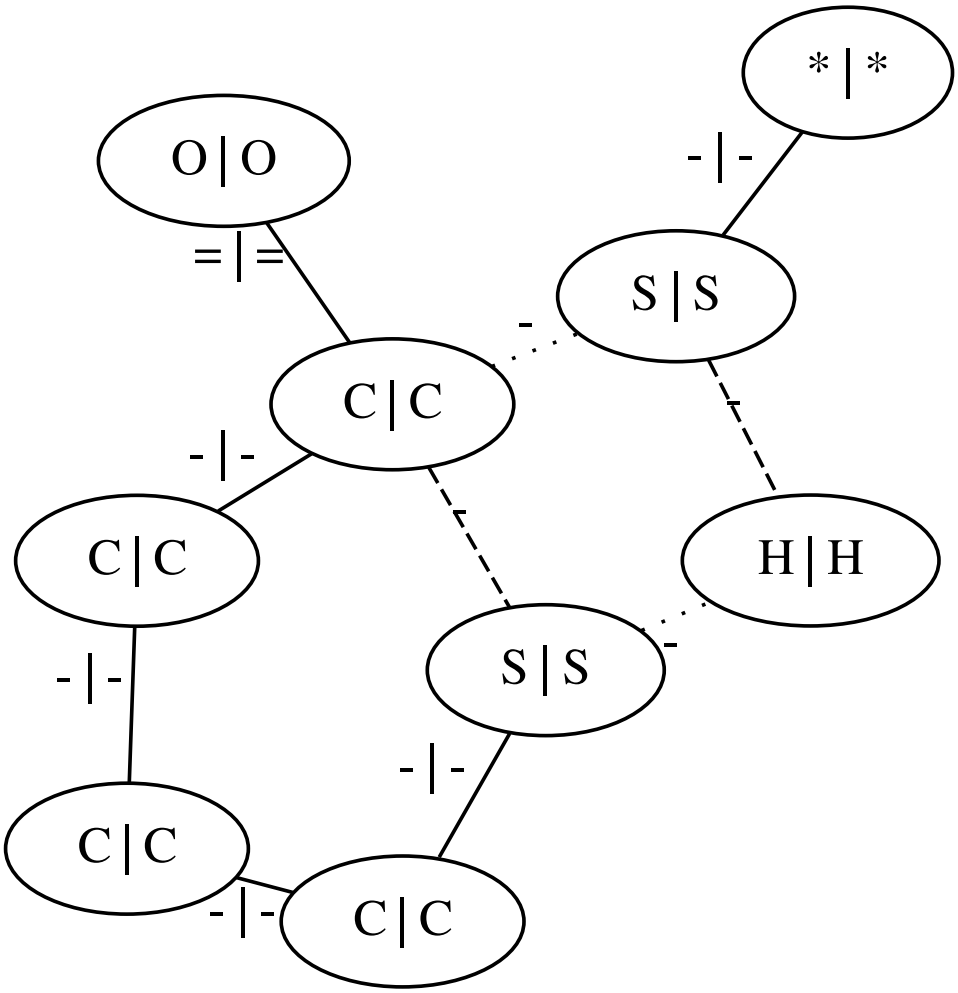
0.0.160 Ring Closure 5 membered, inverse S, S



Files: out/795_r_162_10300000_{L, K, R}



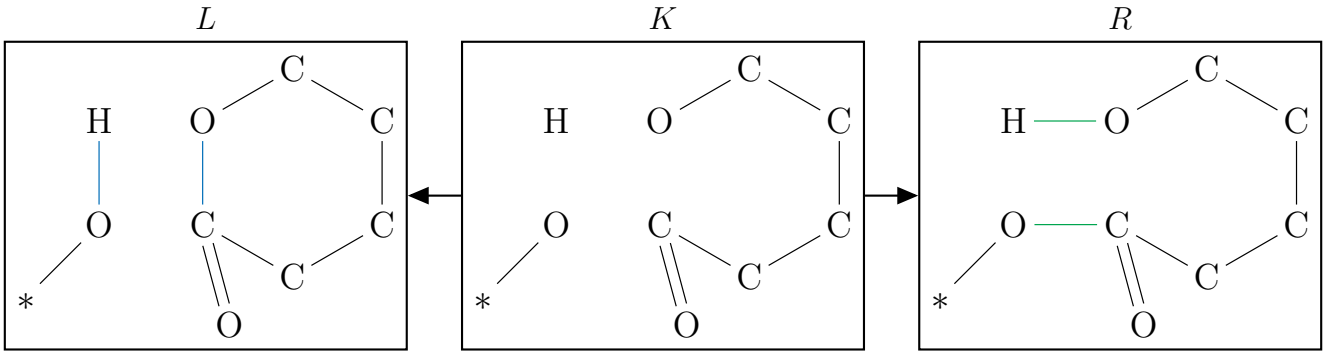
Files: out/796_r_162_11300100_{L, K, R}



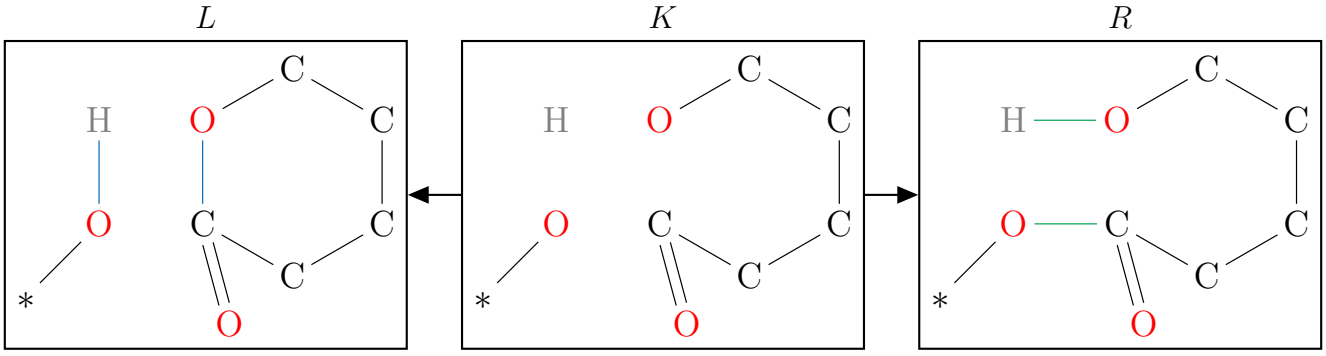
File: out/797_r_162_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

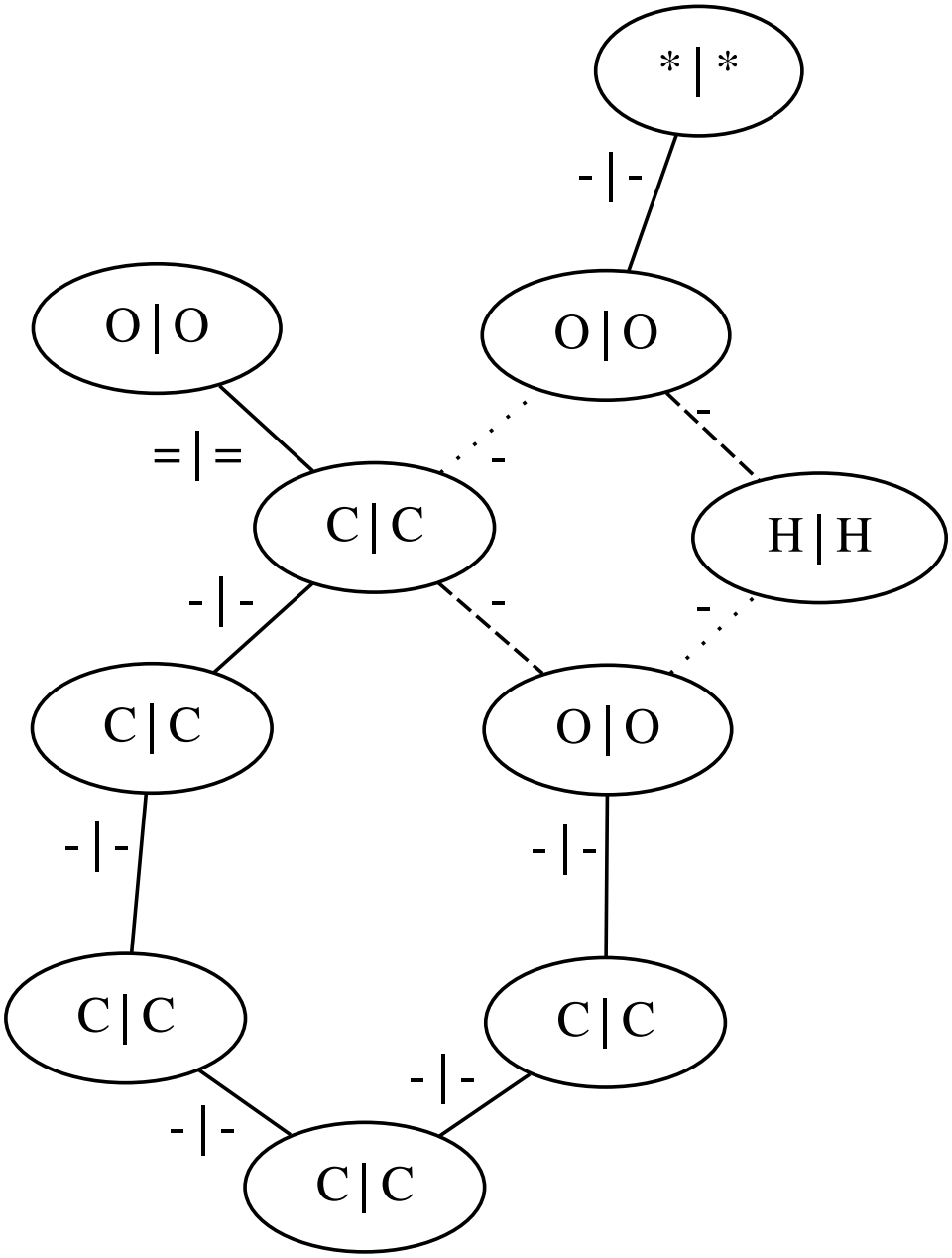
0.0.161 Ring Closure 6 membered, inverse O, O



Files: out/800_r_163_10300000_{L, K, R}



Files: out/801_r_163_11300100_{L, K, R}

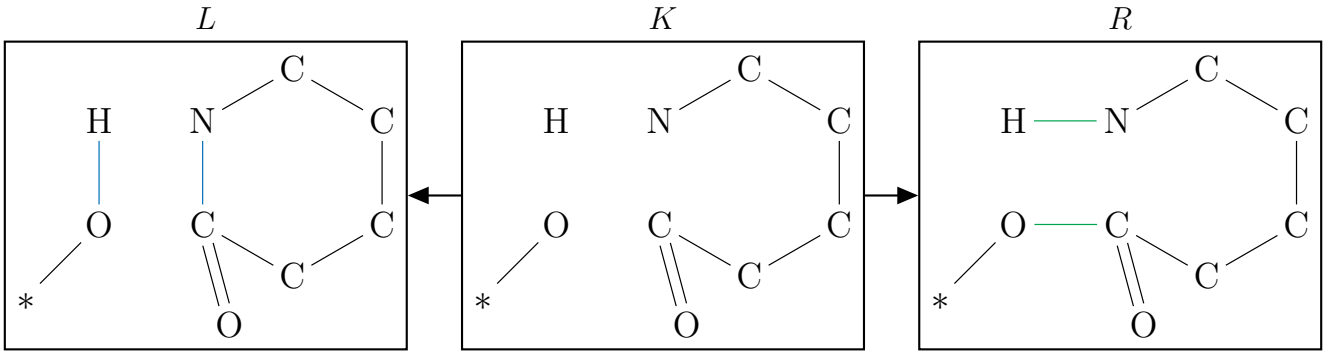


File: out/802_r_163_combined

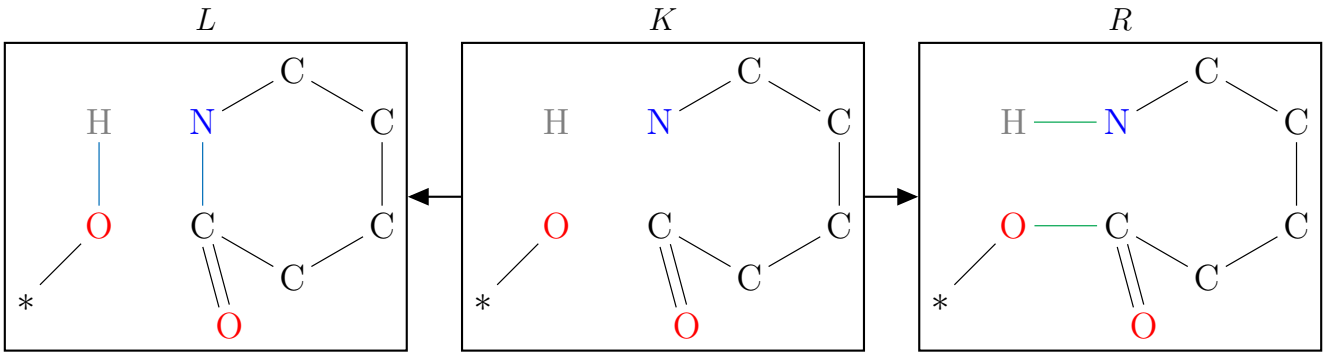
$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 1$$

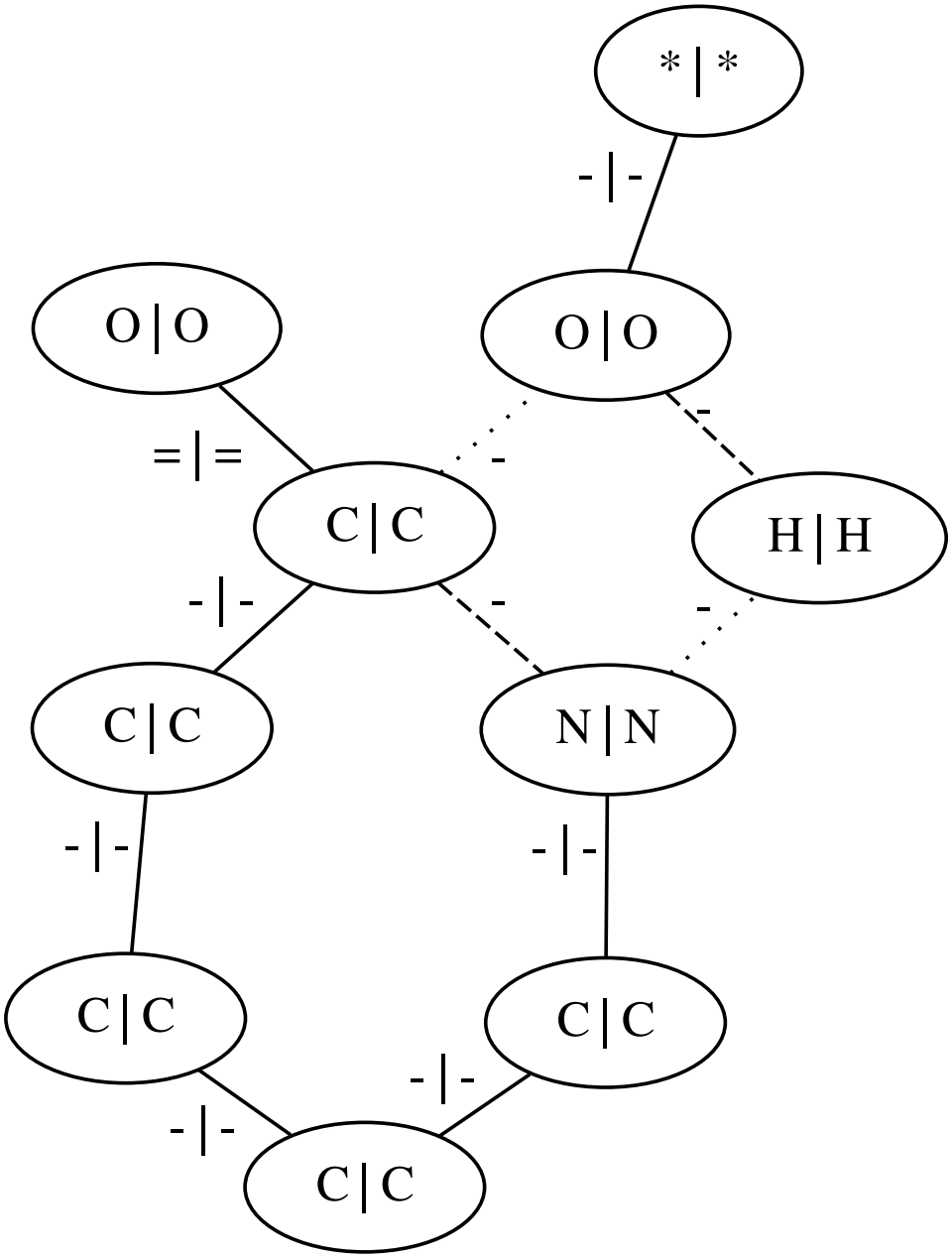
0.0.162 Ring Closure 6 membered, inverse O, N



Files: out/805_r_164_10300000_{L, K, R}



Files: out/806_r_164_11300100_{L, K, R}

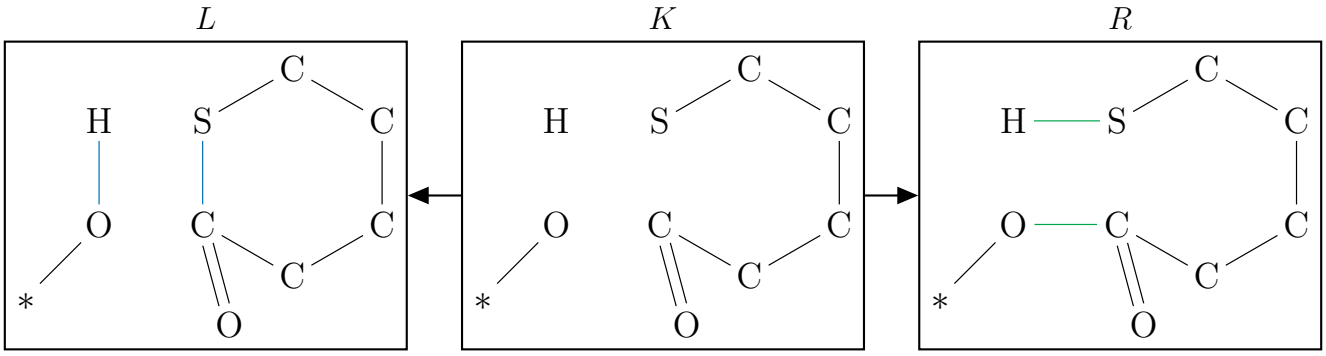


File: out/807_r_164_combined

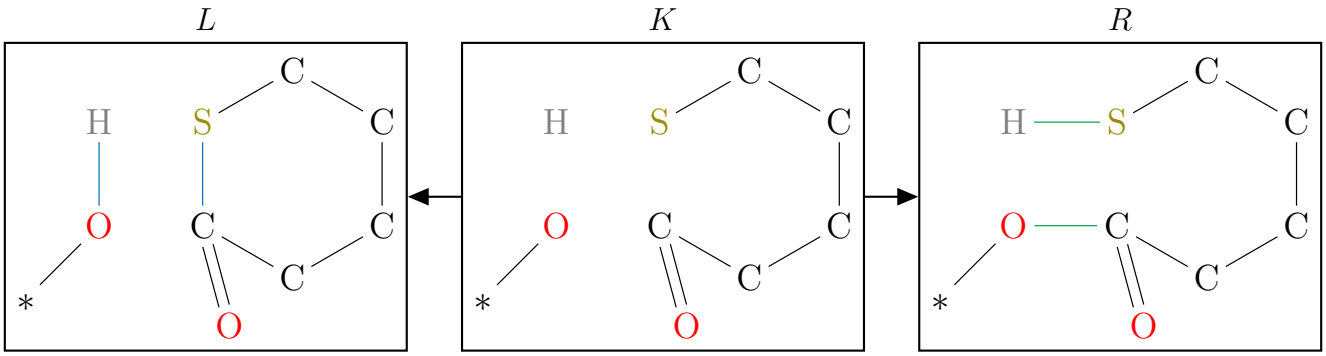
$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 1$$

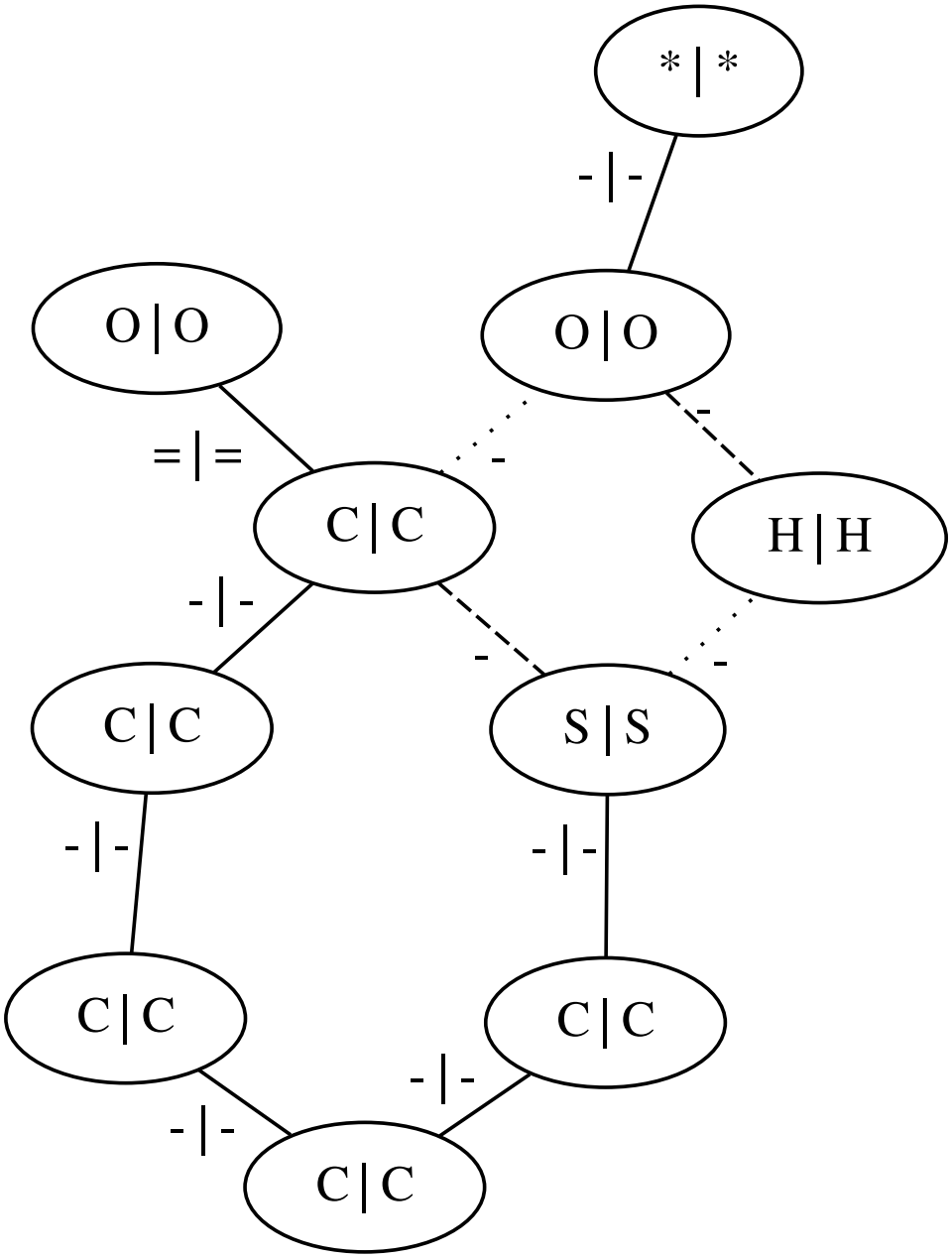
0.0.163 Ring Closure 6 membered, inverse O, S



Files: out/810_r_165_10300000_{L, K, R}



Files: out/811_r_165_11300100_{L, K, R}

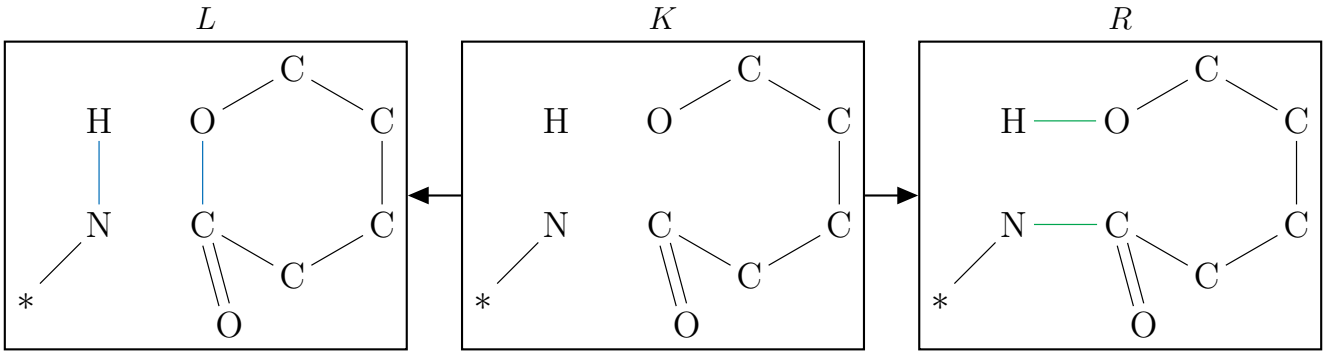


File: out/812_r_165_combined

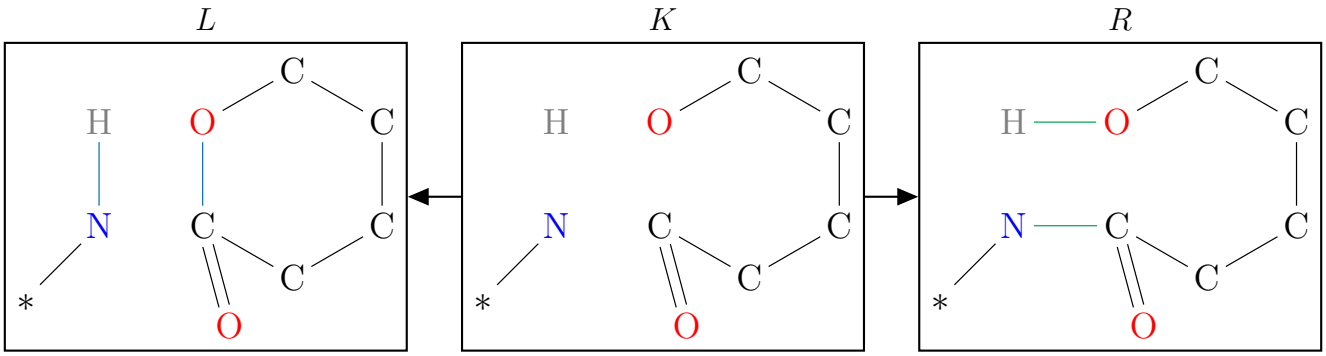
$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 1
\end{aligned}
$$

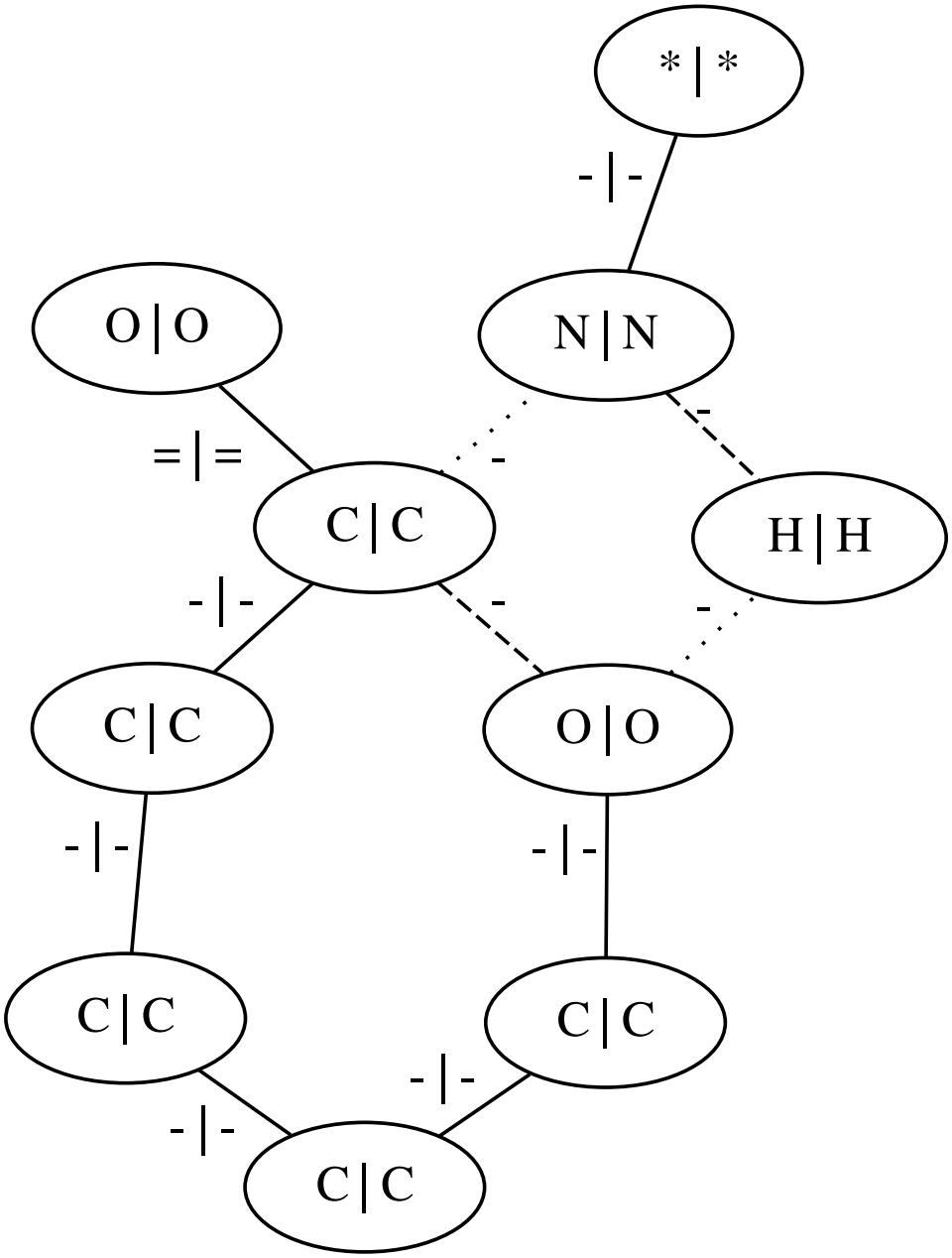
0.0.164 Ring Closure 6 membered, inverse N, O



Files: out/815_r_166_10300000_{L, K, R}



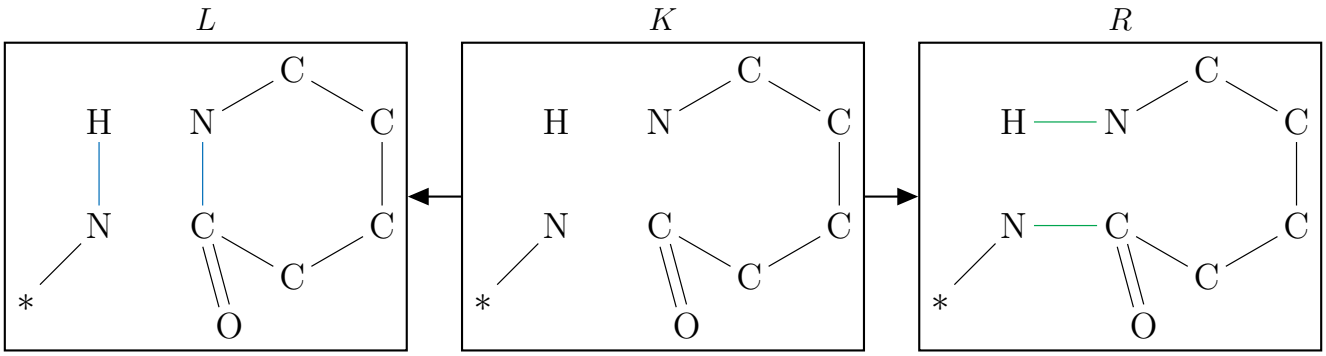
Files: out/816_r_166_11300100_{L, K, R}



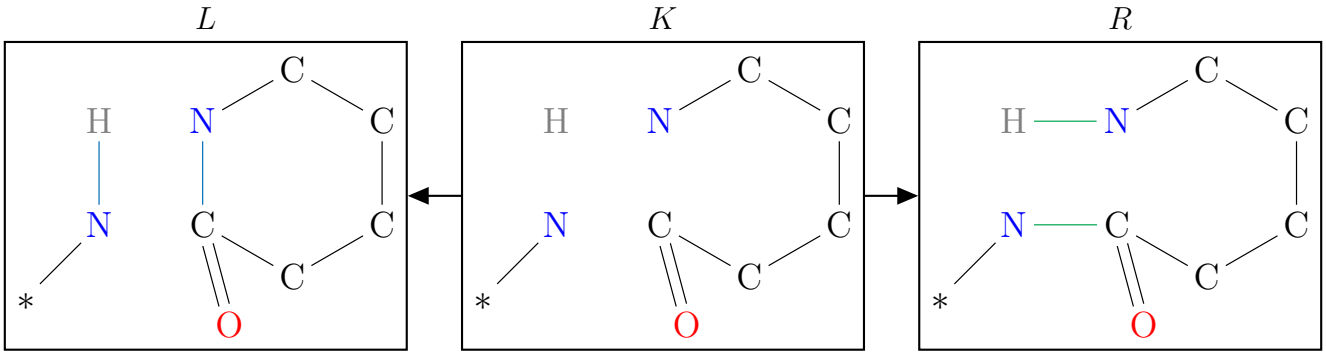
File: out/817_r_166_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(9) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

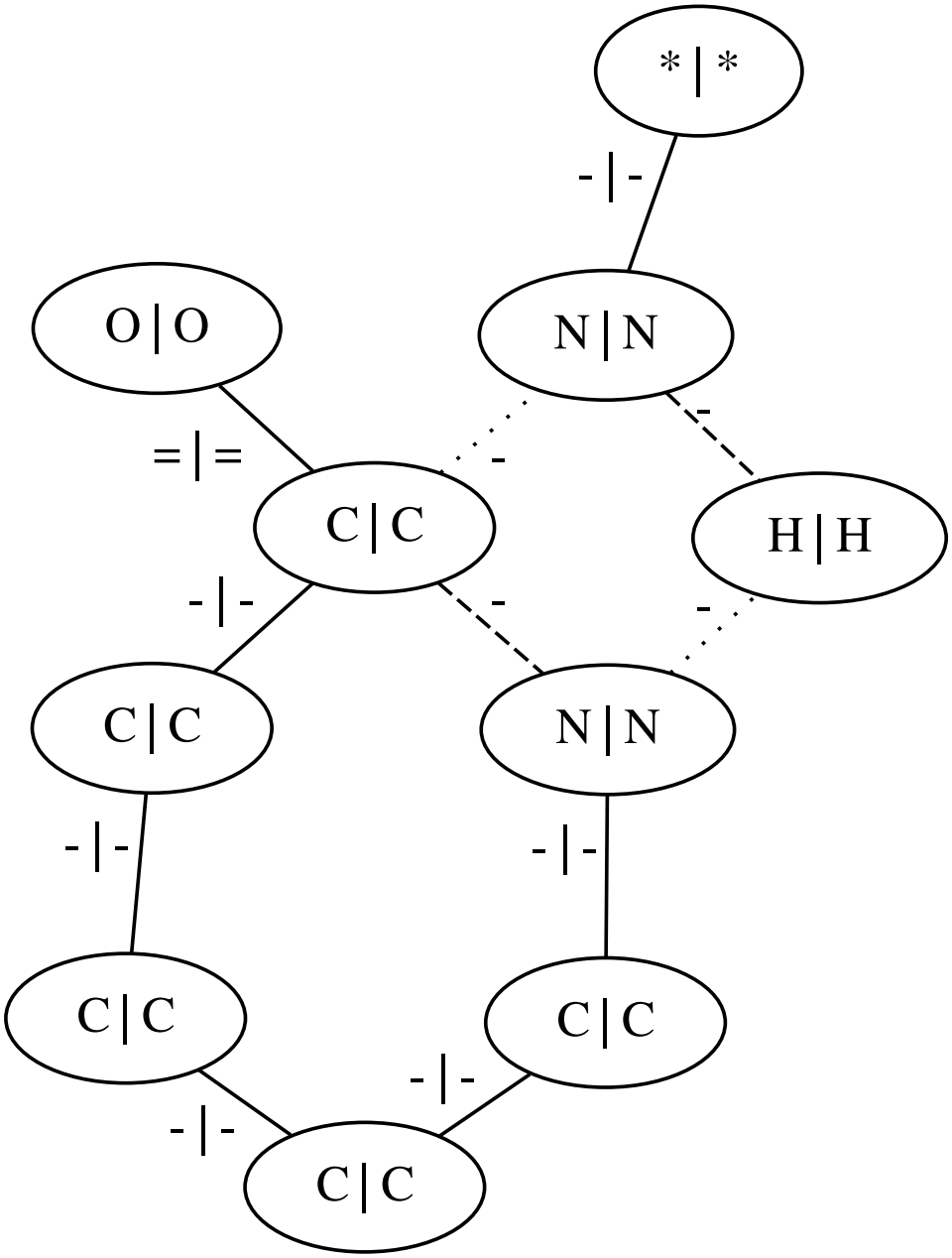
0.0.165 Ring Closure 6 membered, inverse N, N



Files: out/820_r_167_10300000_{L, K, R}



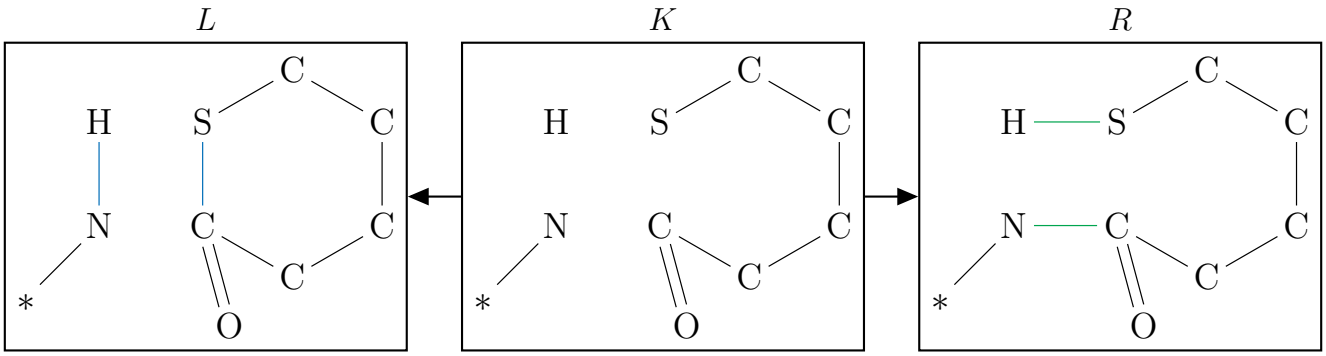
Files: out/821_r_167_11300100_{L, K, R}



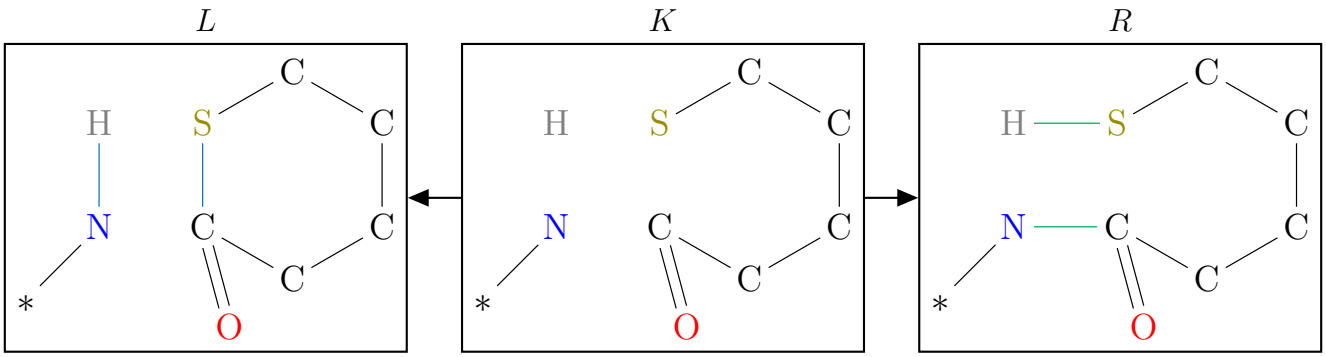
File: out/822_r_167_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

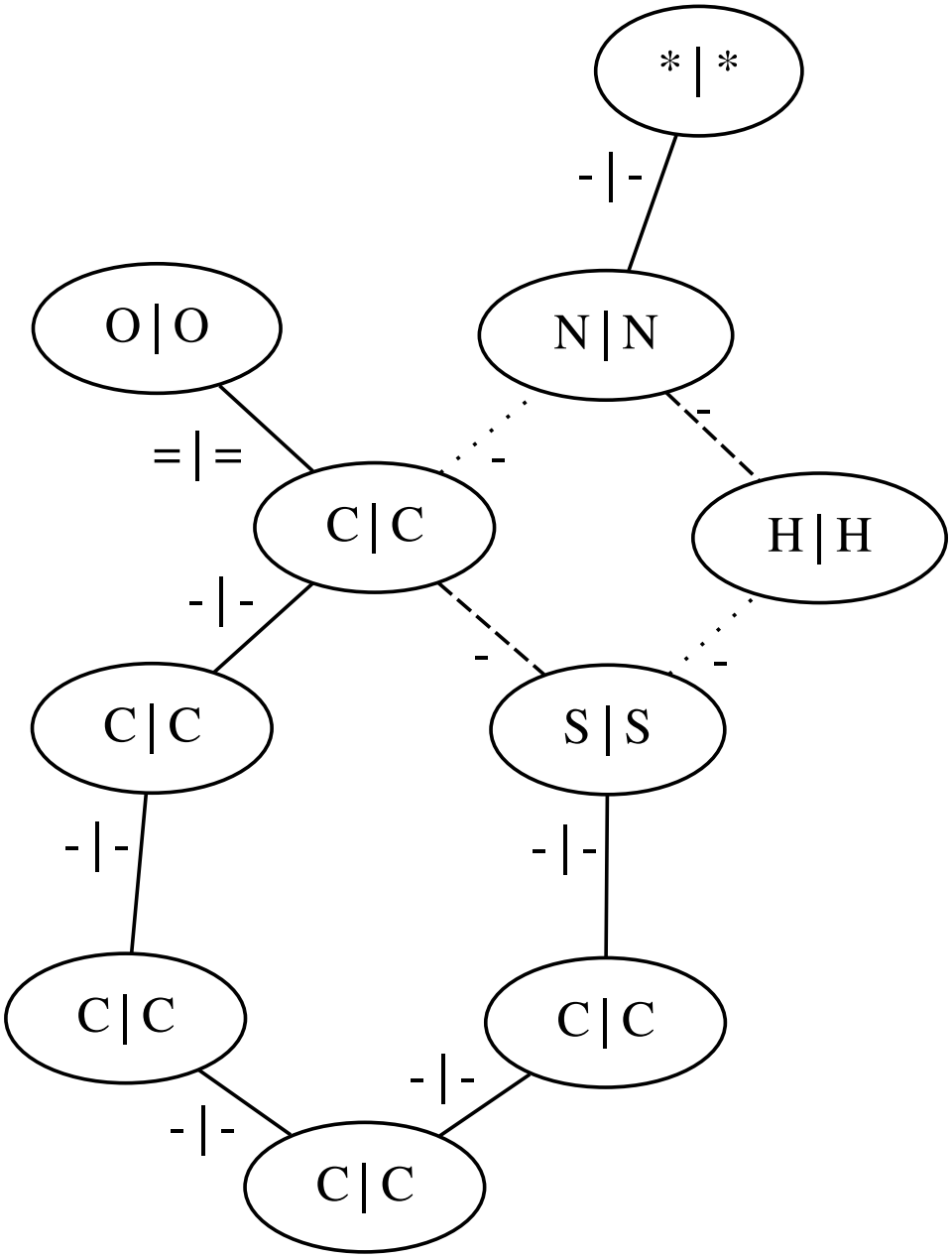
0.0.166 Ring Closure 6 membered, inverse N, S



Files: out/825_r_168_10300000_{L, K, R}



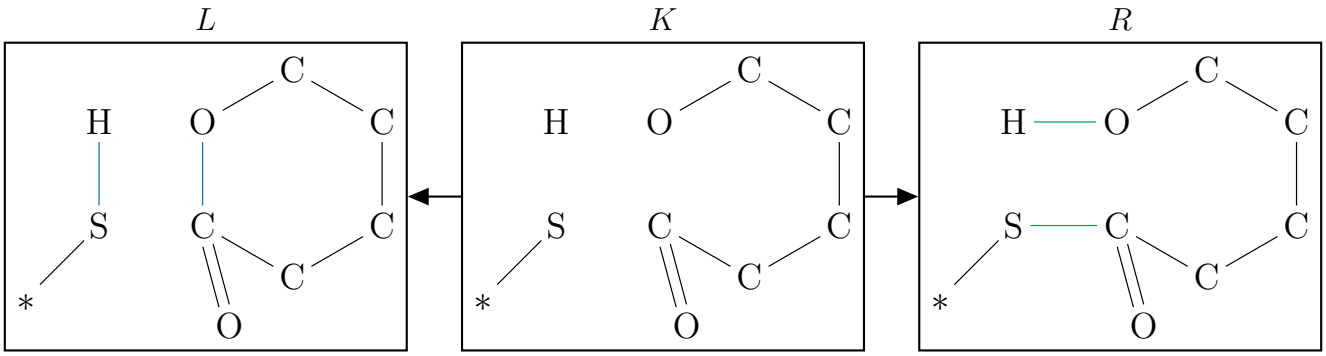
Files: out/826_r_168_11300100_{L, K, R}



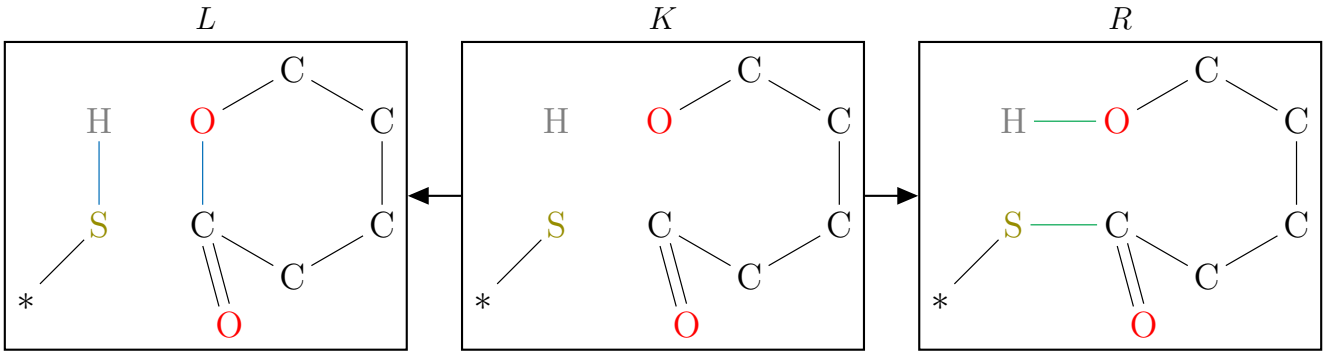
File: out/827_r_168_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

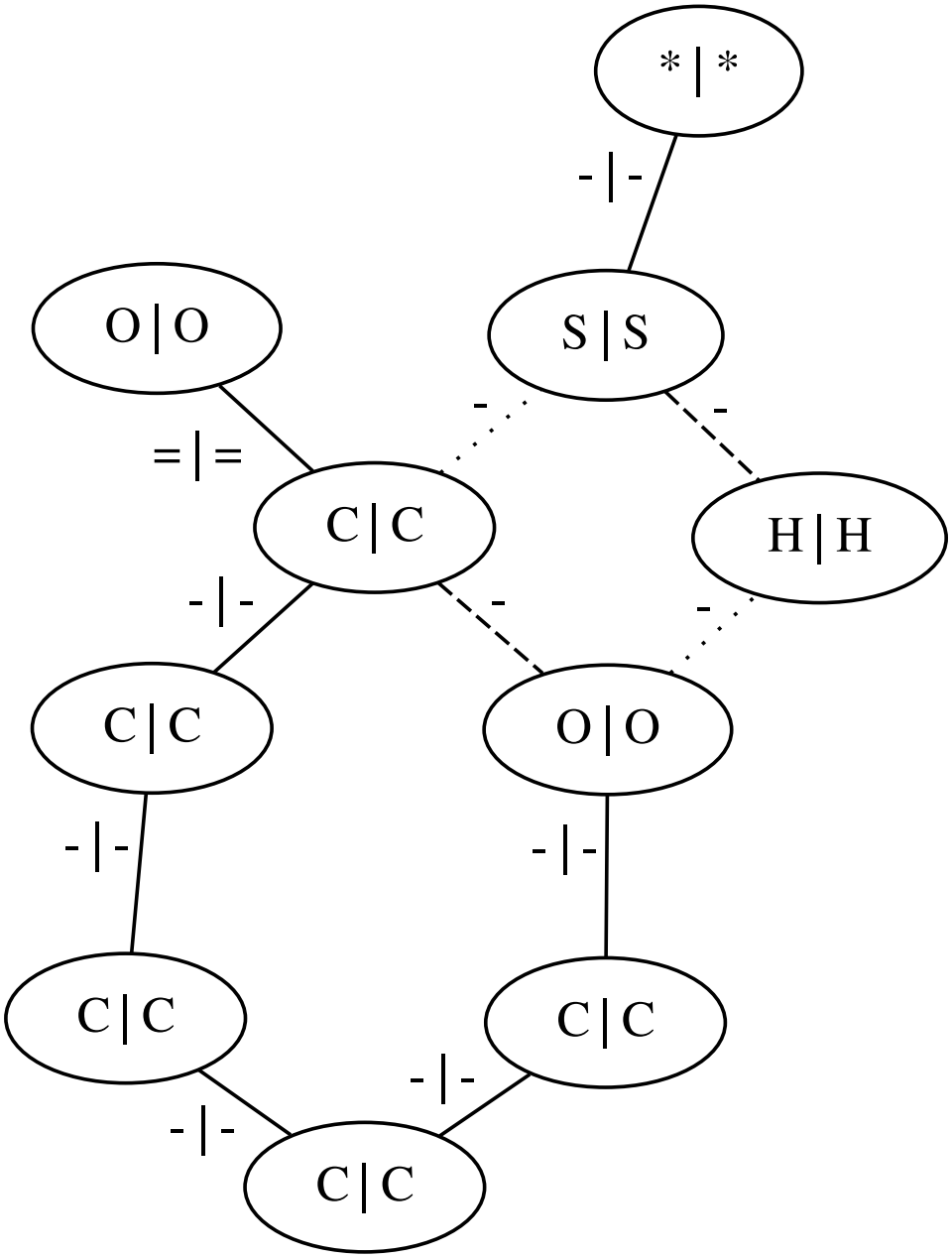
0.0.167 Ring Closure 6 membered, inverse S, O



Files: out/830_r_169_10300000_{L, K, R}



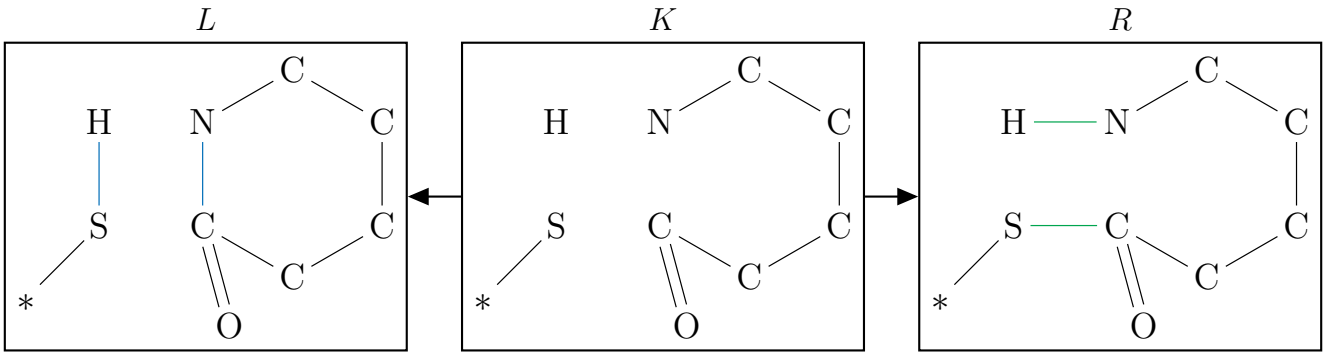
Files: out/831_r_169_11300100_{L, K, R}



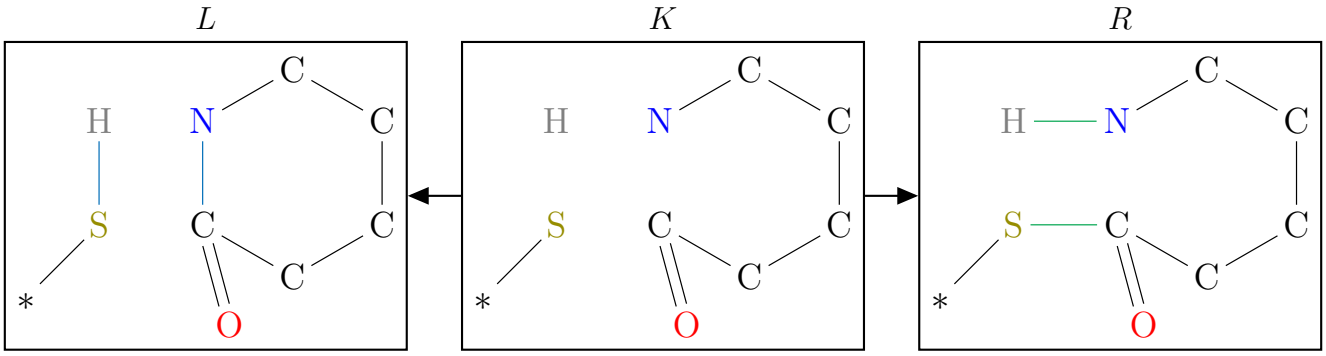
File: out/832_r_169_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

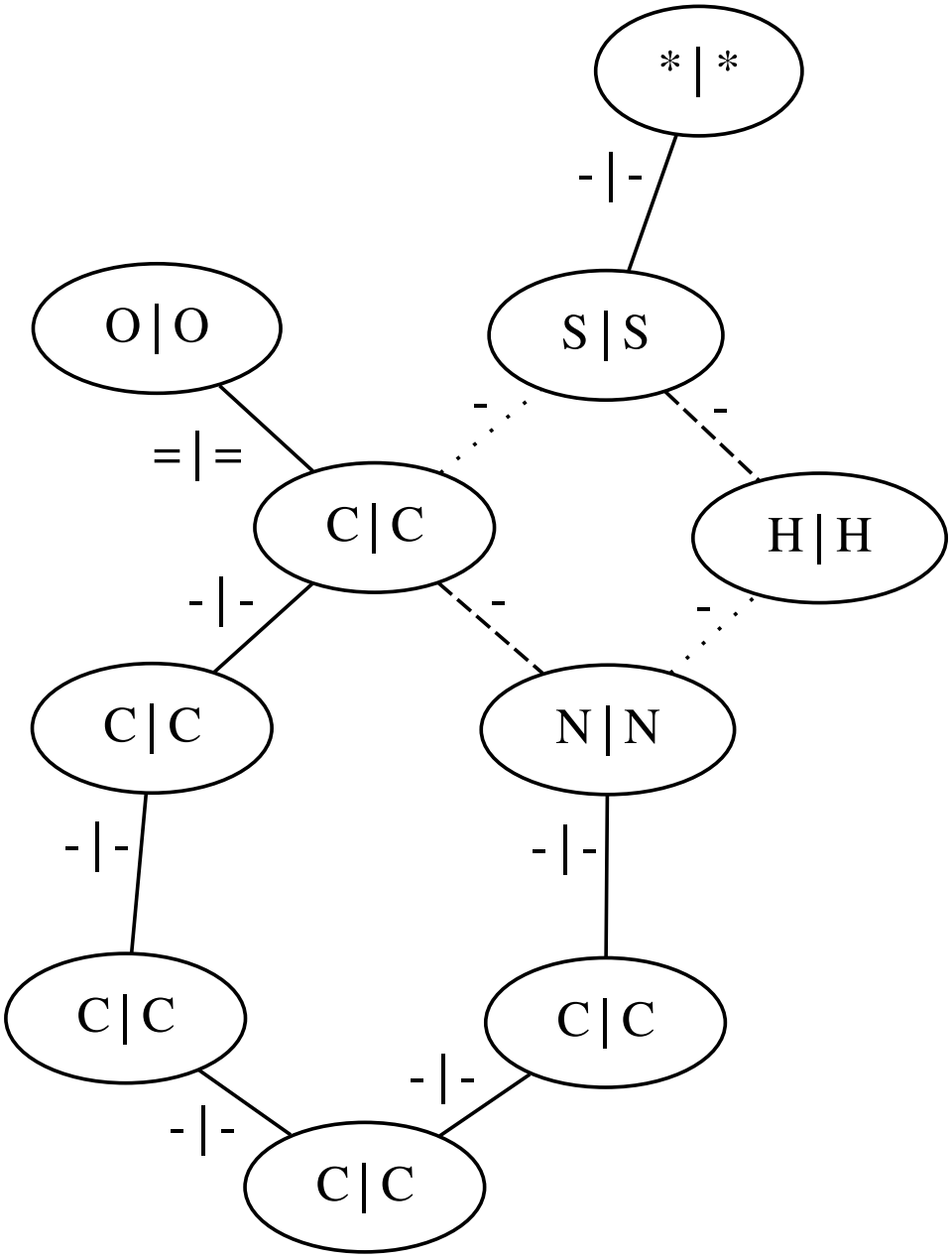
0.0.168 Ring Closure 6 membered, inverse S, N



Files: out/835_r_170_10300000_{L, K, R}



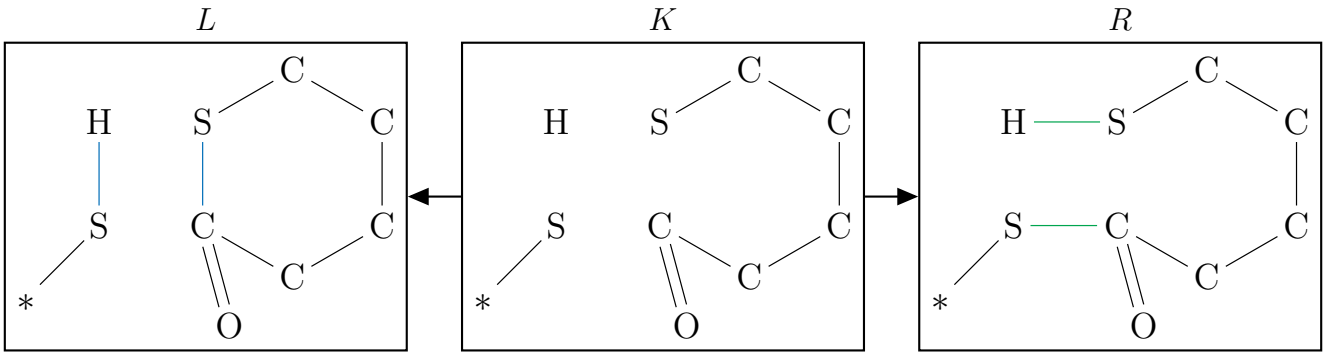
Files: out/836_r_170_11300100_{L, K, R}



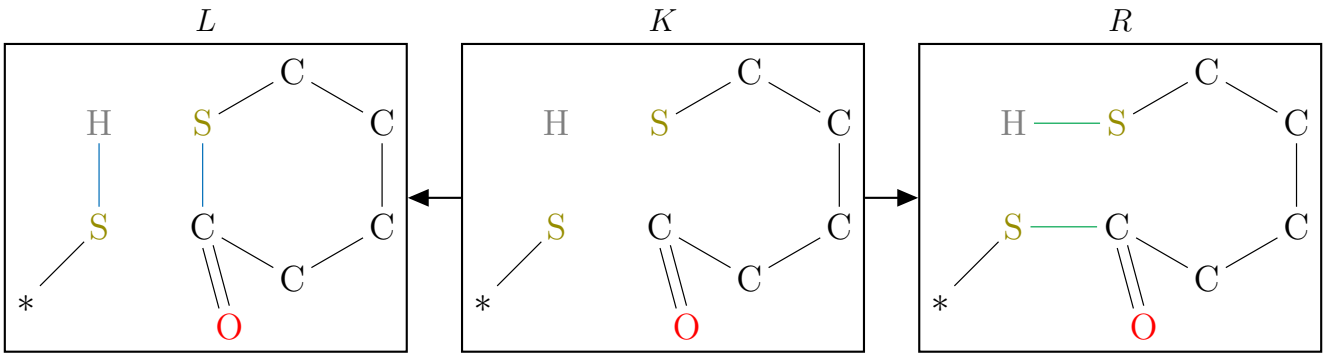
File: out/837_r_170_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

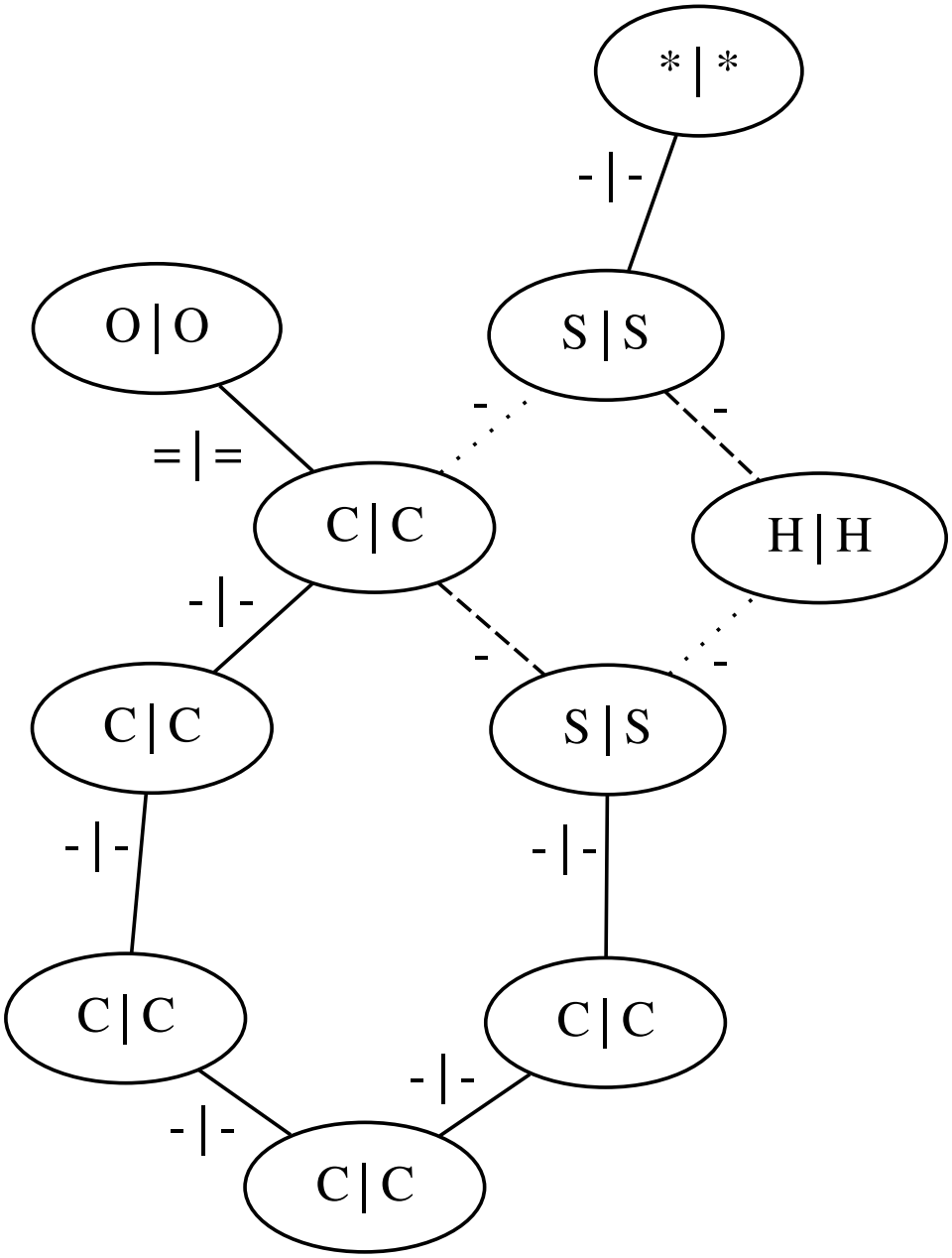
0.0.169 Ring Closure 6 membered, inverse S, S



Files: out/840_r_171_10300000_{L, K, R}



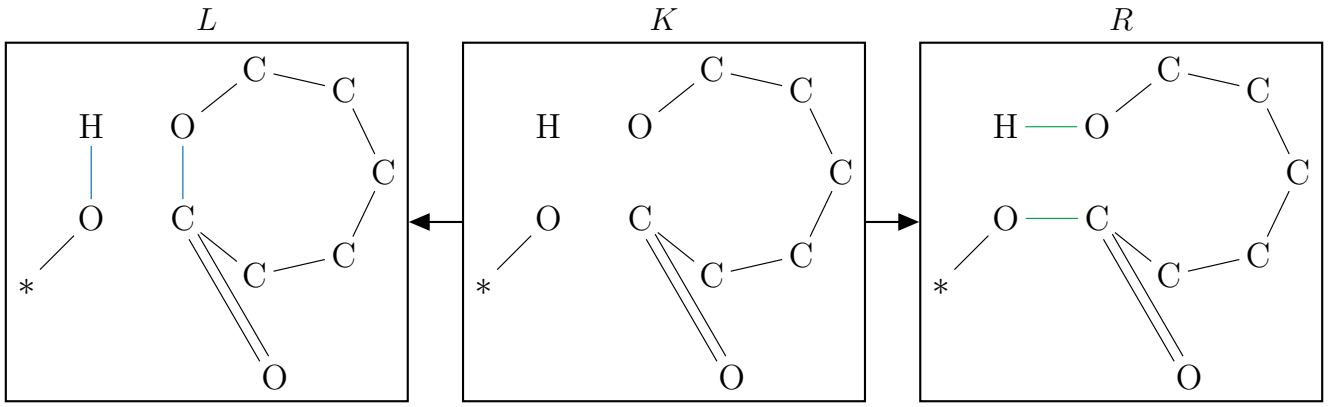
Files: out/841_r_171_11300100_{L, K, R}



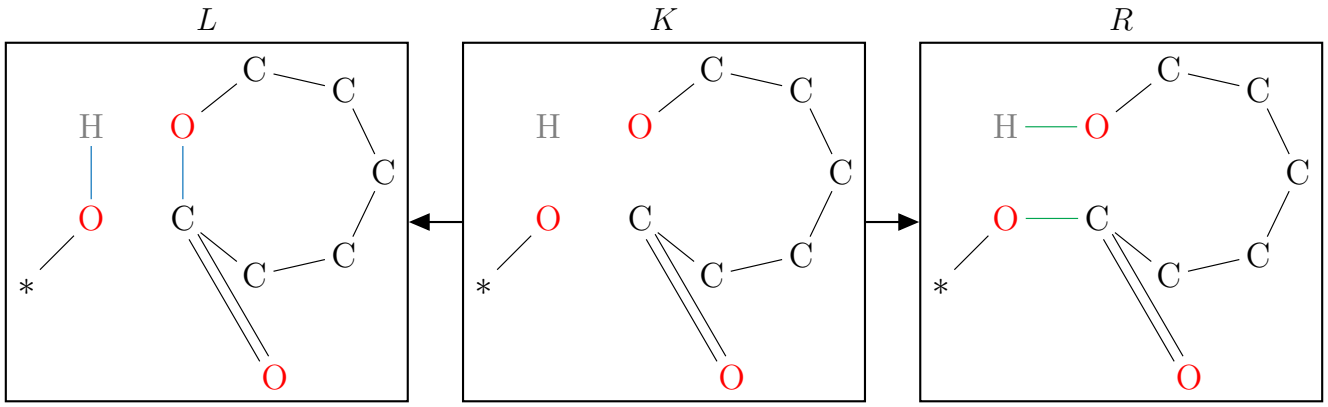
File: out/842_r_171_combined

$$|\{e \in \text{outEdges}(9) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

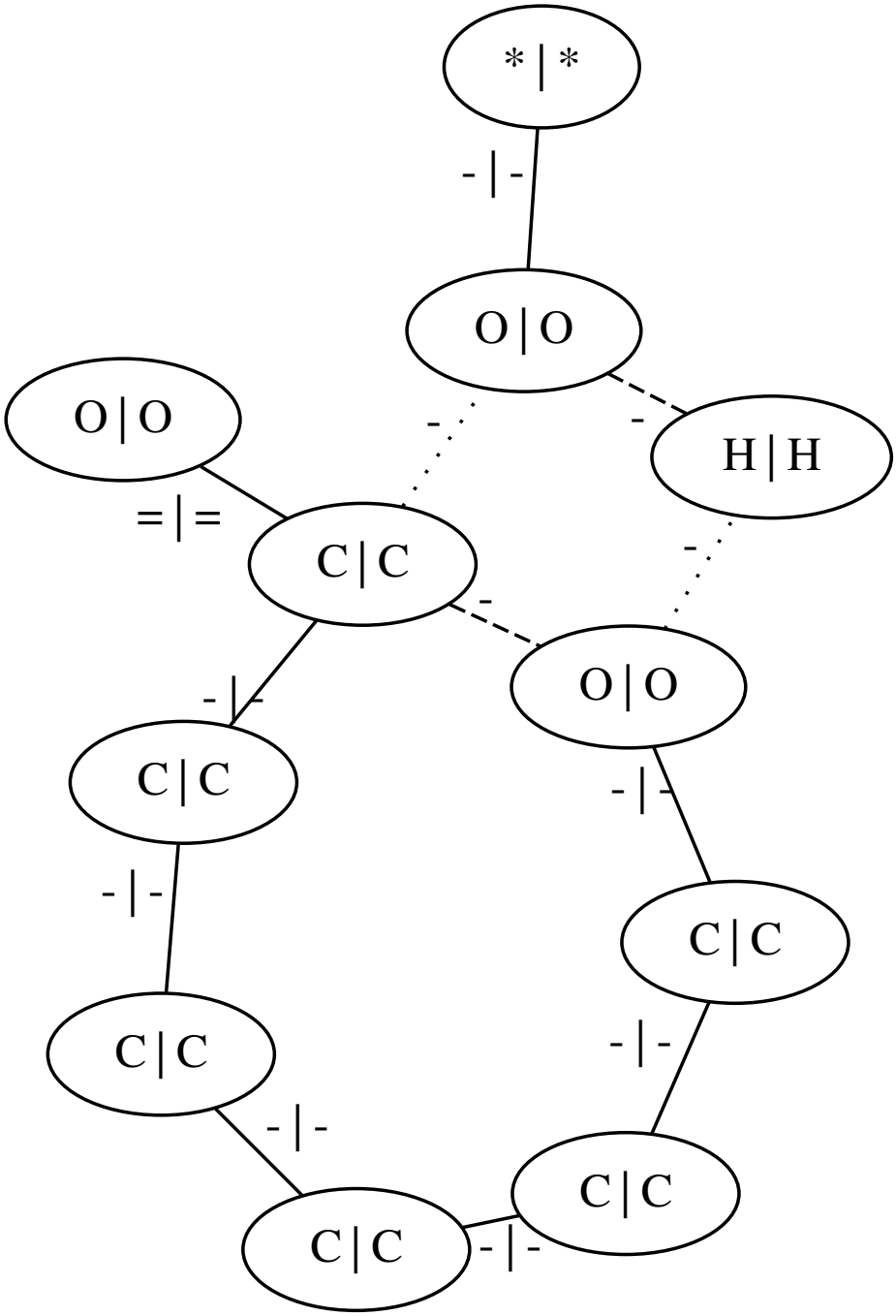
0.0.170 Ring Closure 7 membered, inverse O, O



Files: out/845_r_172_10300000_{L, K, R}



Files: out/846_r_172_11300100_{L, K, R}

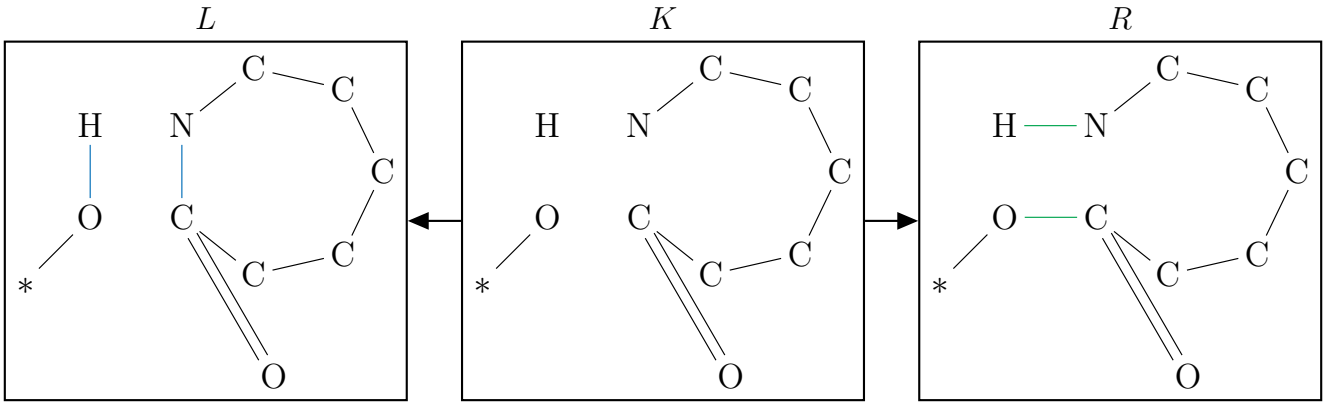


File: out/847_r_172_combined

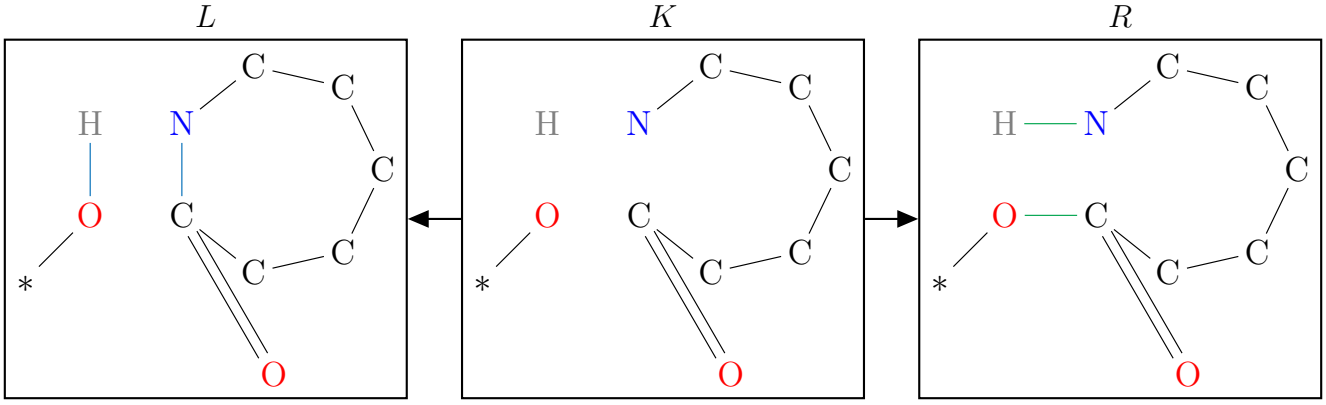
$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 1$$

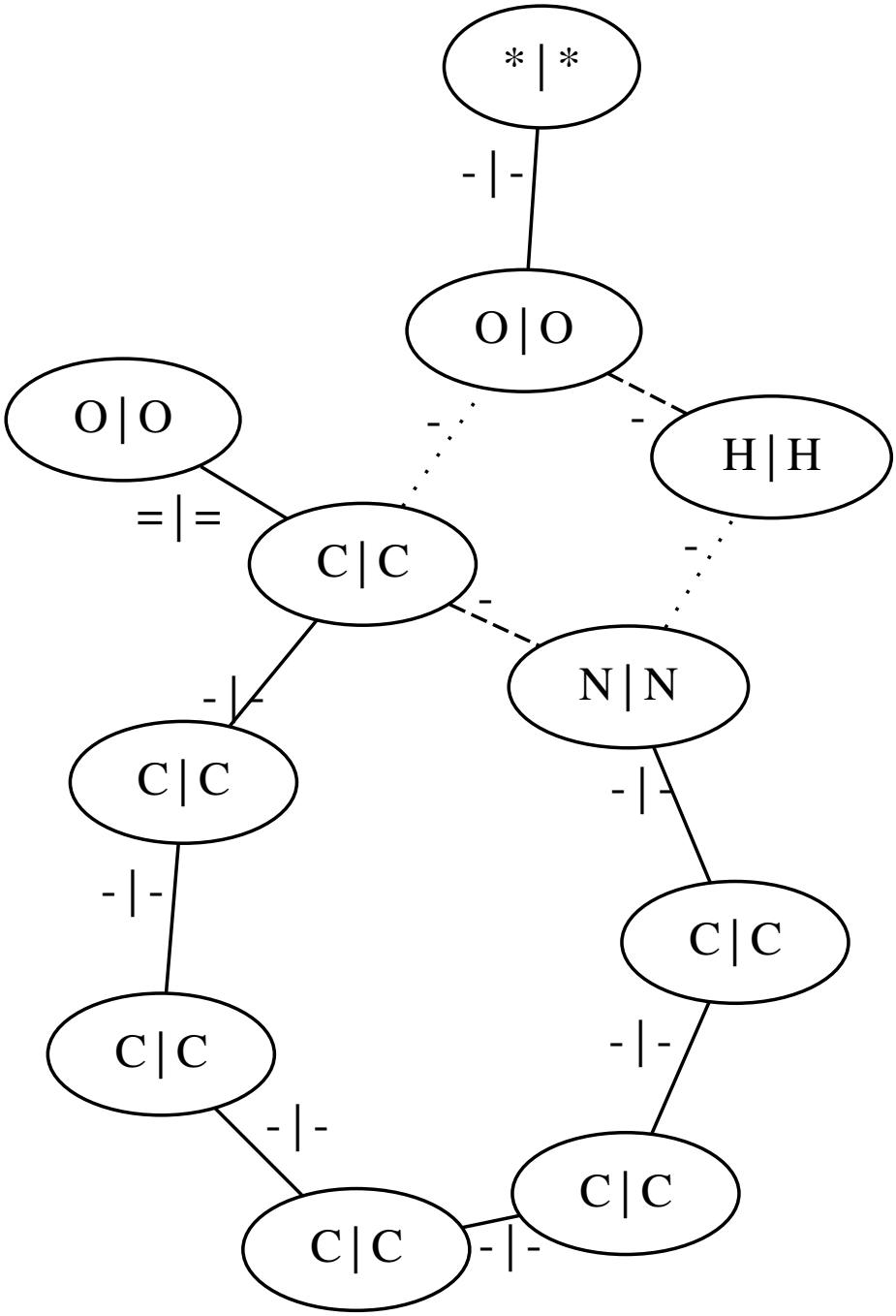
0.0.171 Ring Closure 7 membered, inverse O, N



Files: out/850_r_173_10300000_{L, K, R}



Files: out/851_r_173_11300100_{L, K, R}

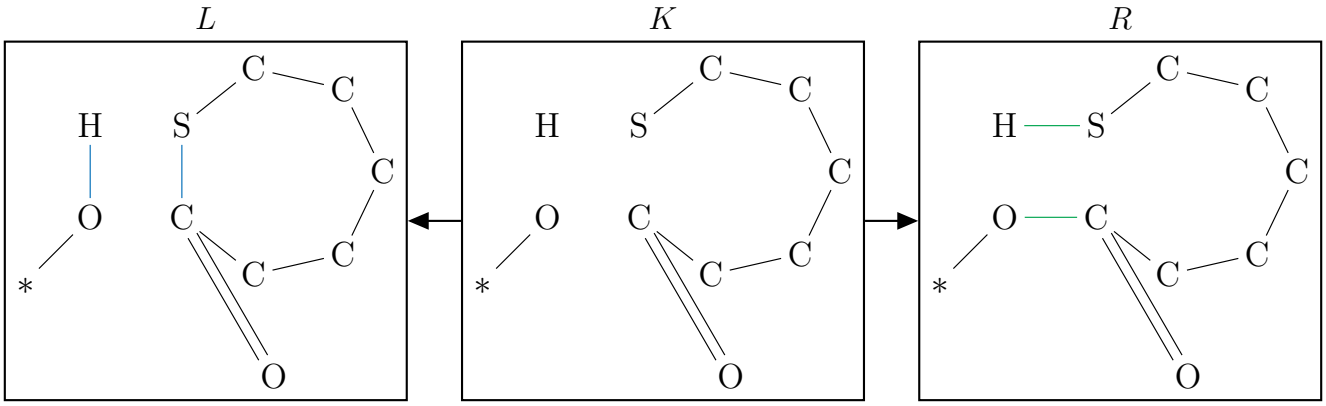


File: out/852_r_173_combined

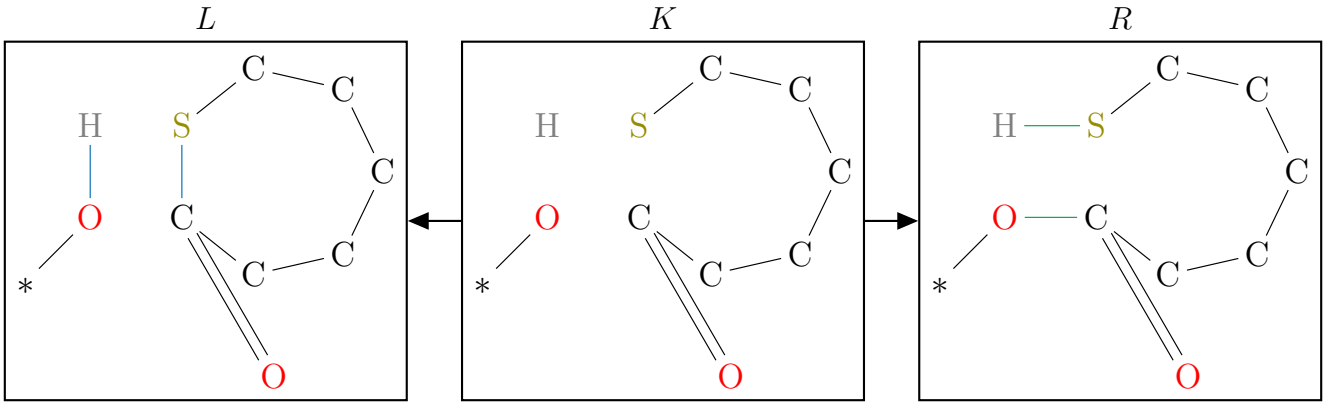
$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`C'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 1
\end{aligned}
$$

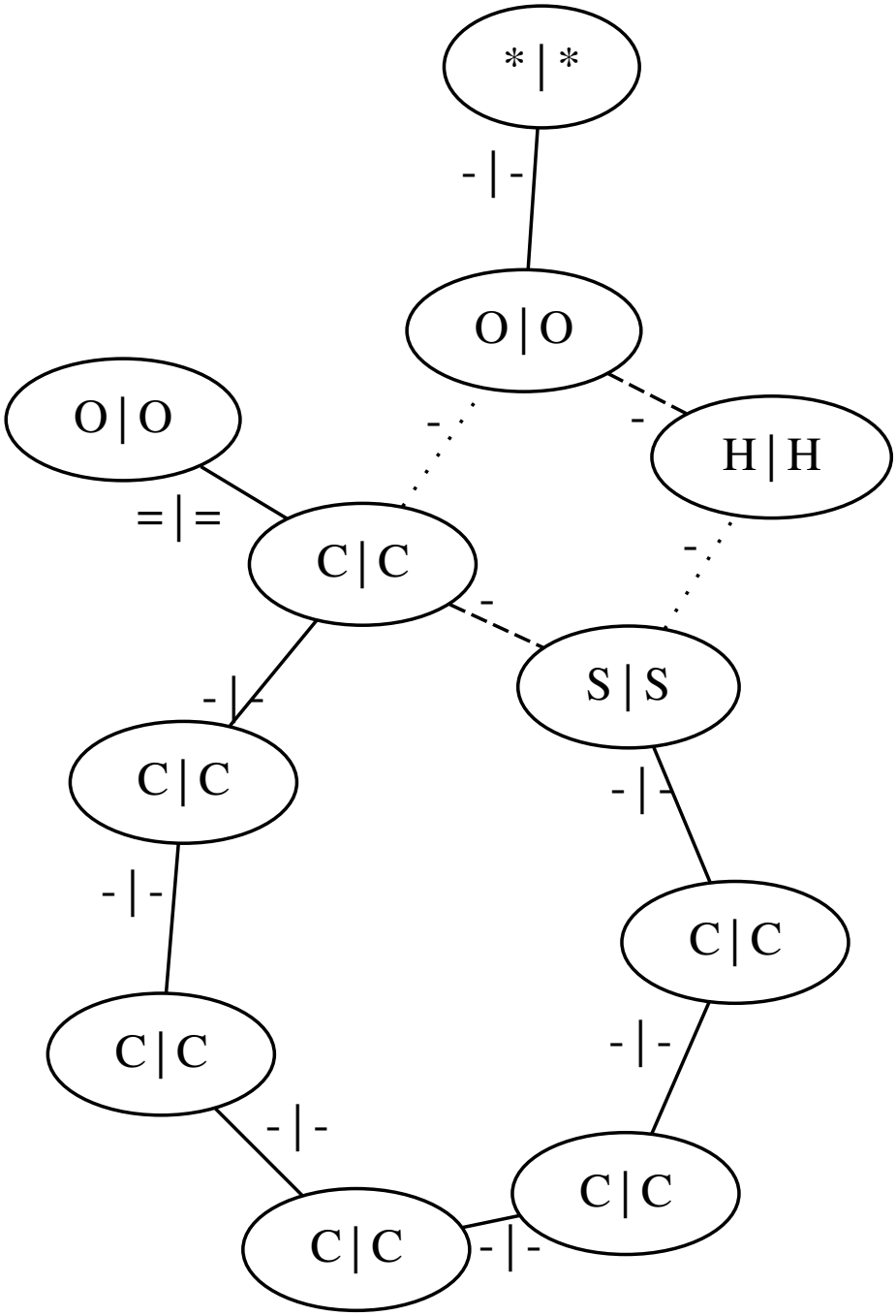
0.0.172 Ring Closure 7 membered, inverse O, S



Files: out/855_r_174_10300000_{L, K, R}



Files: out/856_r_174_11300100_{L, K, R}

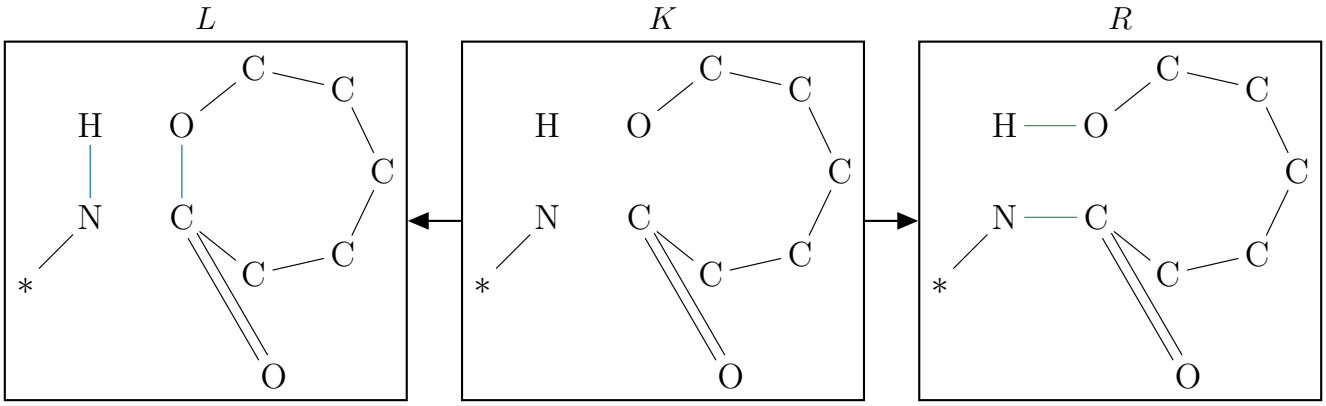


File: out/857_r_174_combined

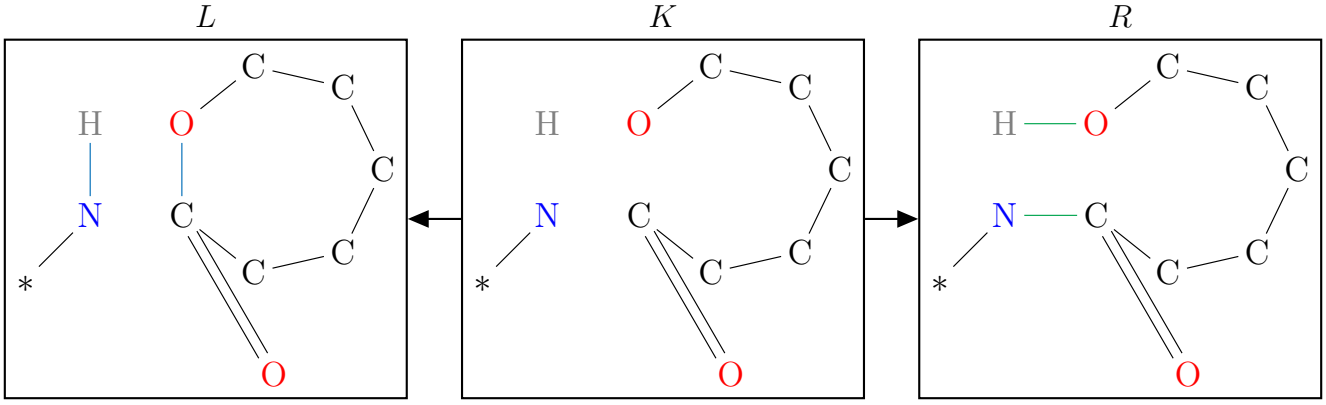
$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

$$|\{e \in \text{outEdges}(2) \mid \text{label}(\text{target}(e)) \in \{\text{`C'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 1$$

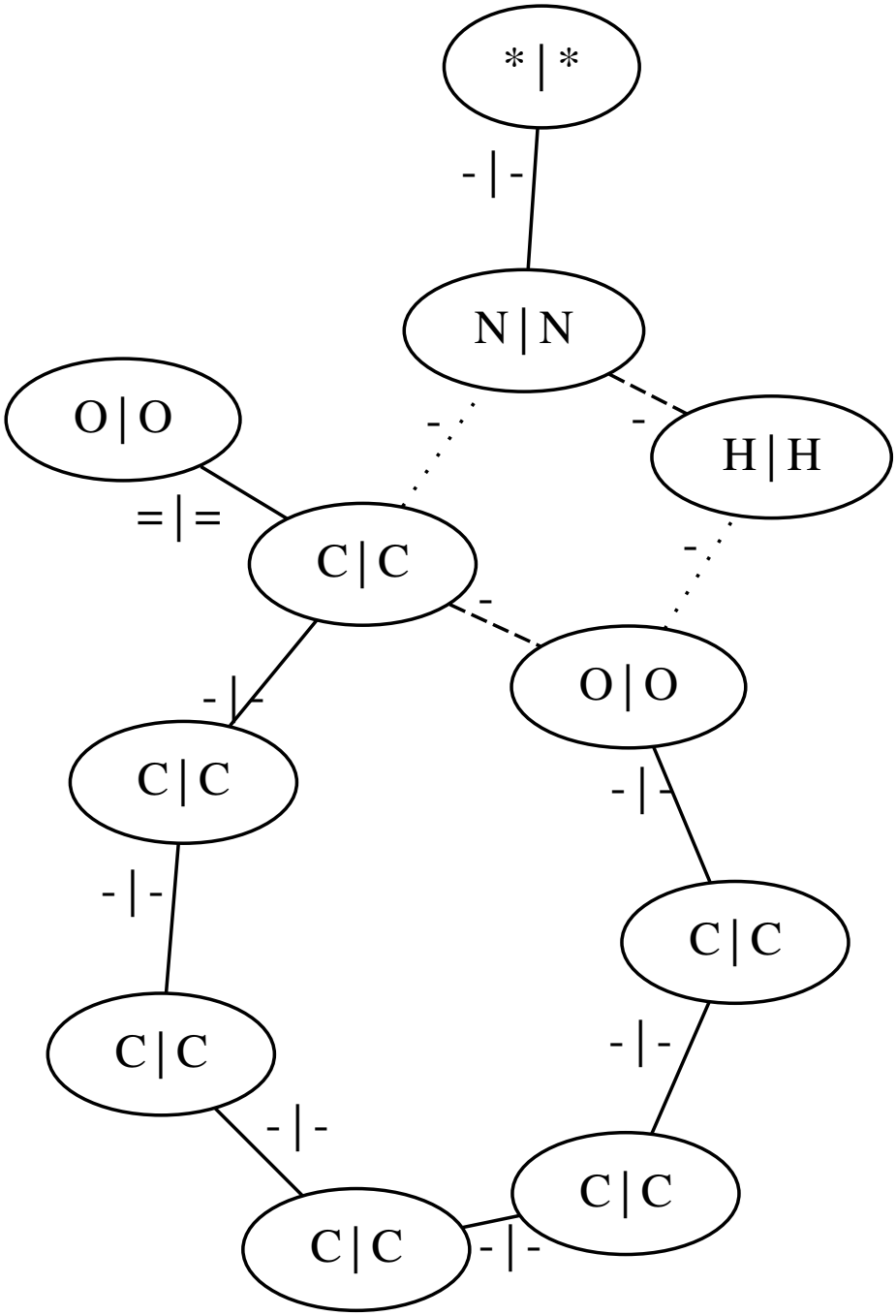
0.0.173 Ring Closure 7 membered, inverse N, O



Files: out/860_r_175_10300000_{L, K, R}



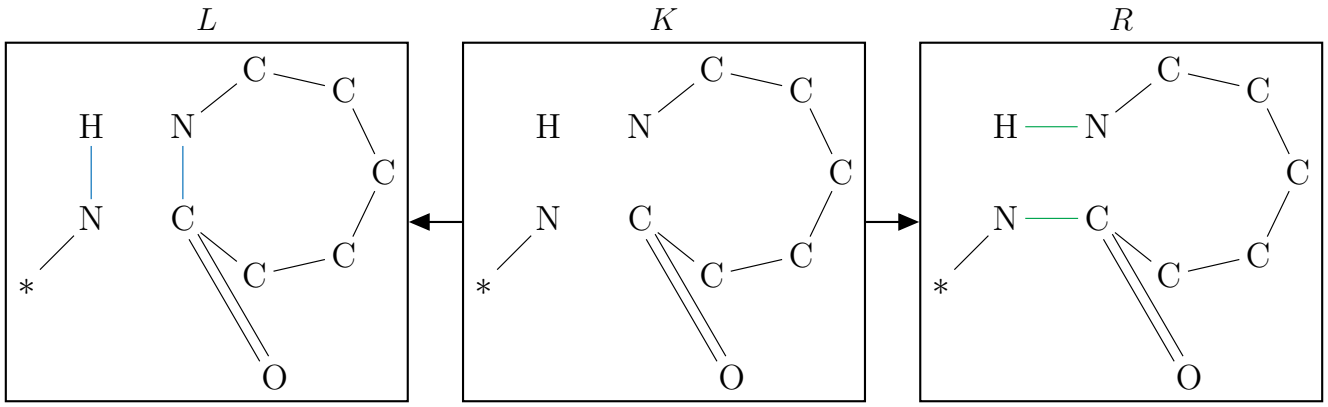
Files: out/861_r_175_11300100_{L, K, R}



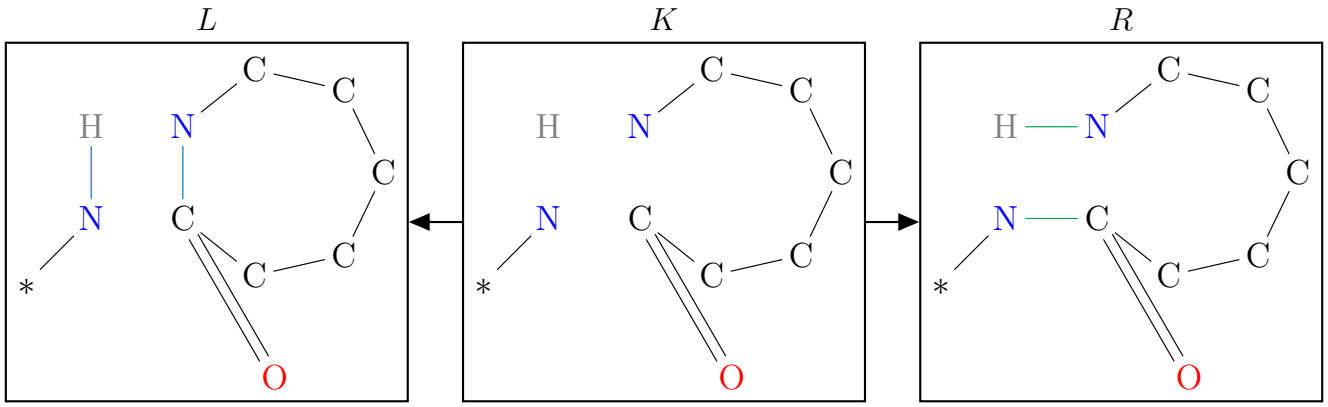
File: out/862_r_175_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

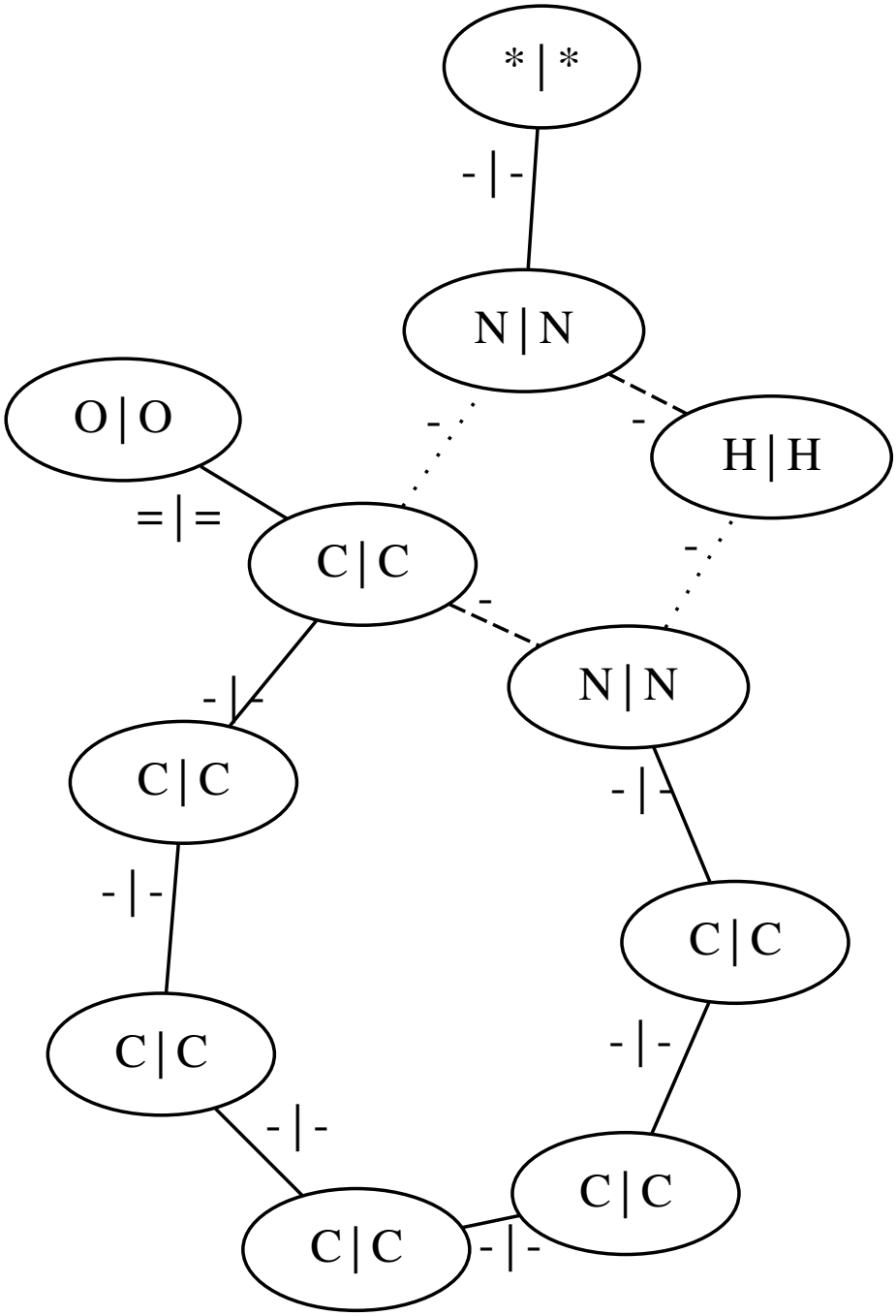
0.0.174 Ring Closure 7 membered, inverse N, N



Files: out/865_r_176_10300000_{L, K, R}



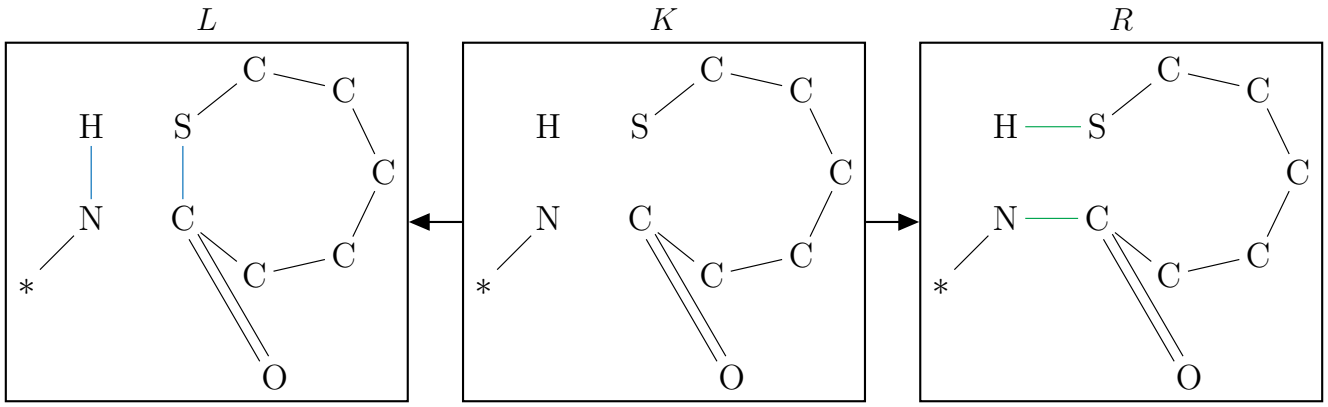
Files: out/866_r_176_11300100_{L, K, R}



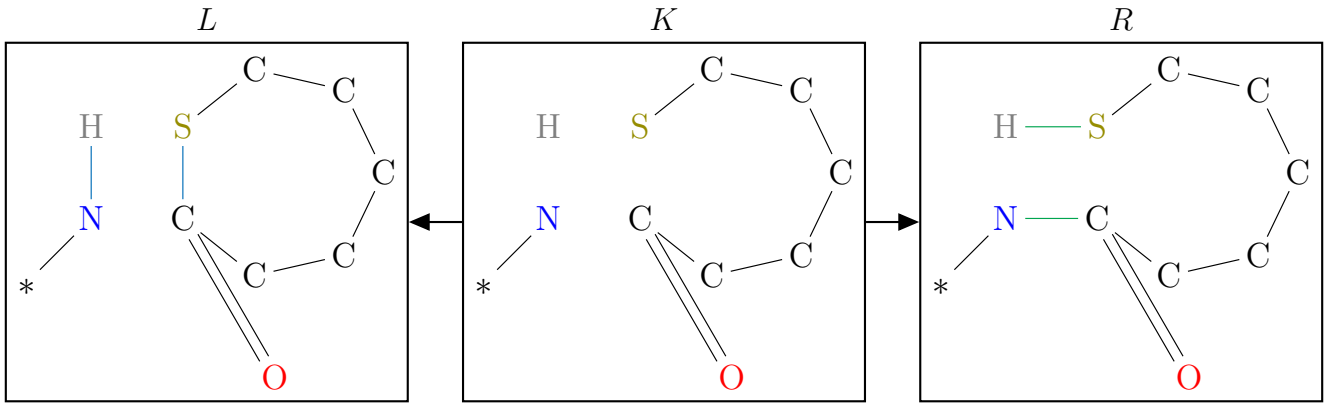
File: out/867_r_176_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

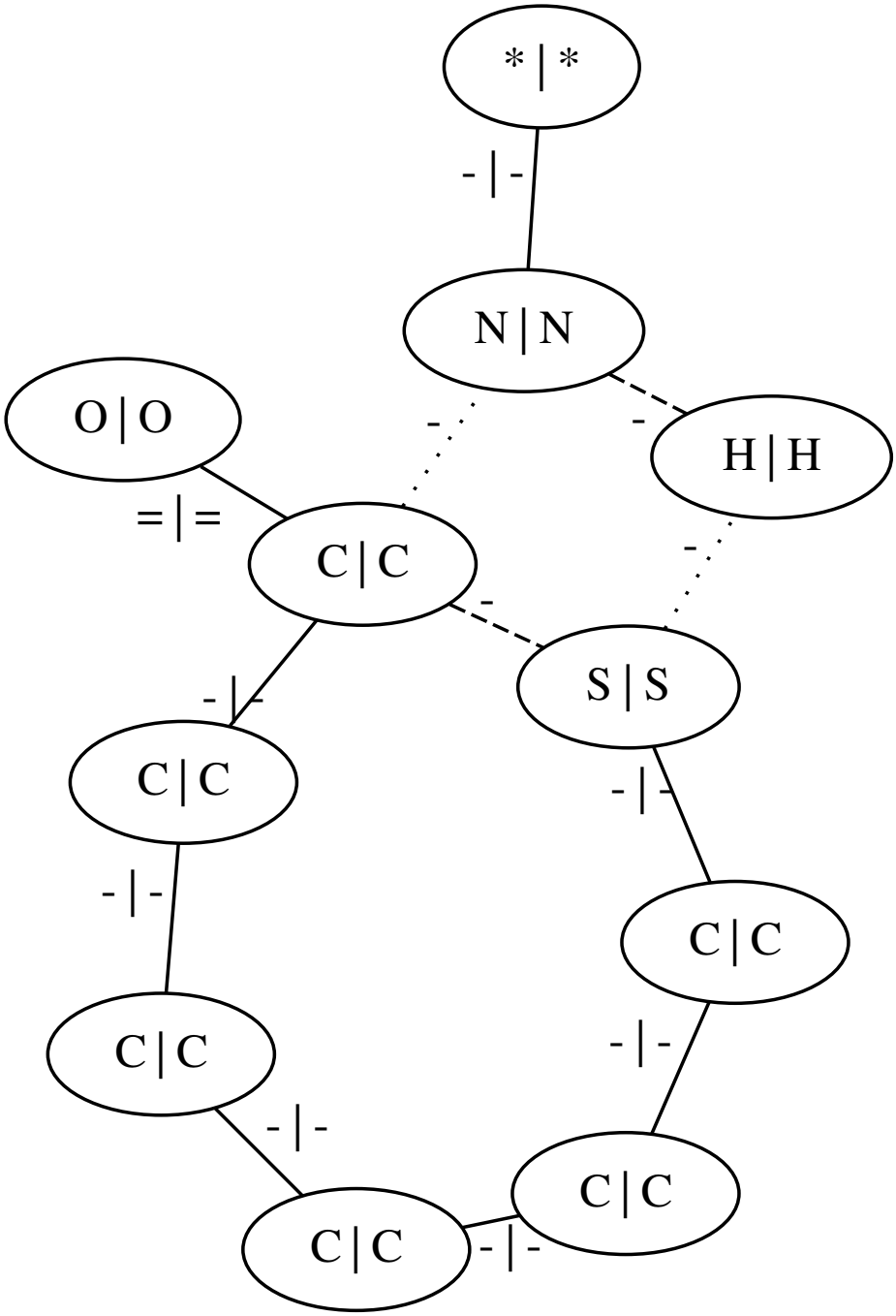
0.0.175 Ring Closure 7 membered, inverse N, S



Files: out/870_r_177_10300000_{L, K, R}



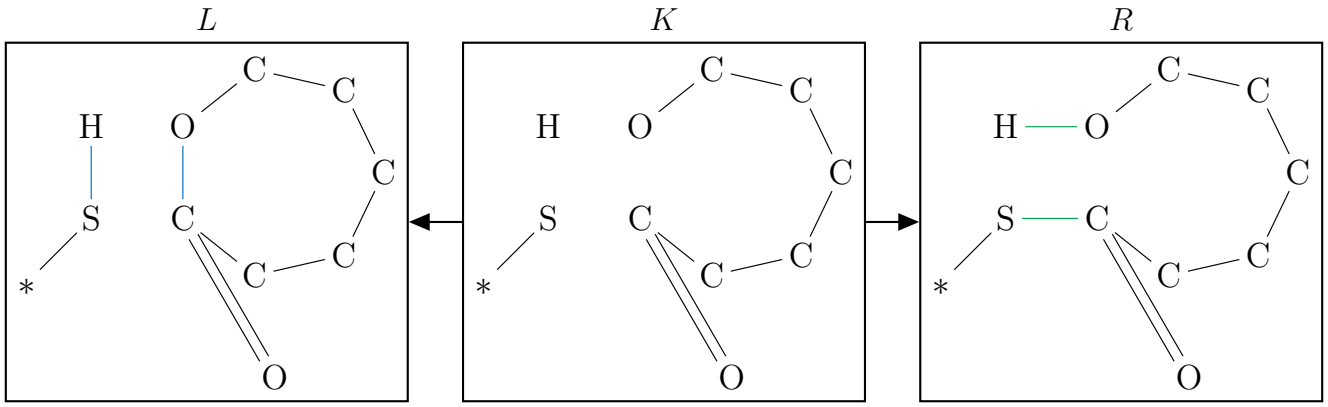
Files: out/871_r_177_11300100_{L, K, R}



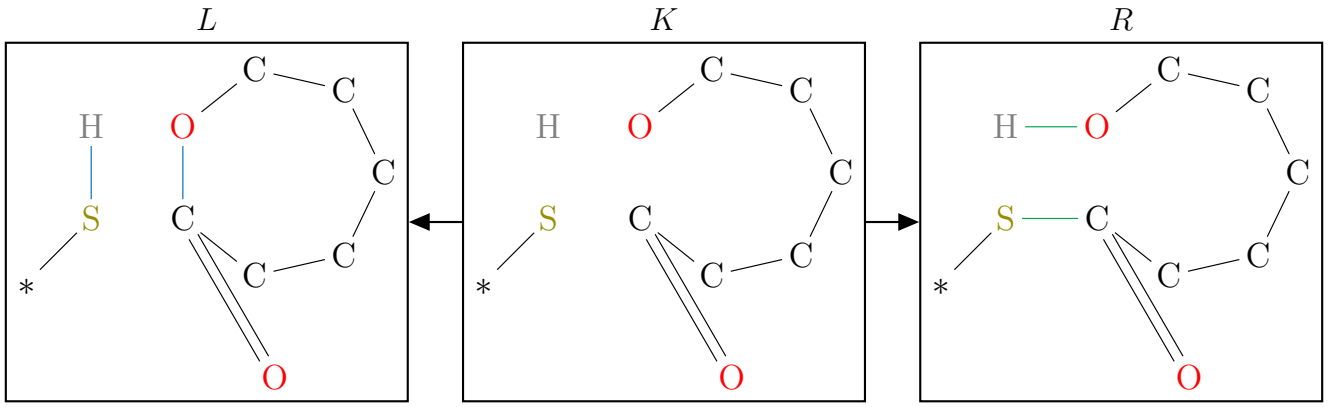
File: out/872_r_177_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`S'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

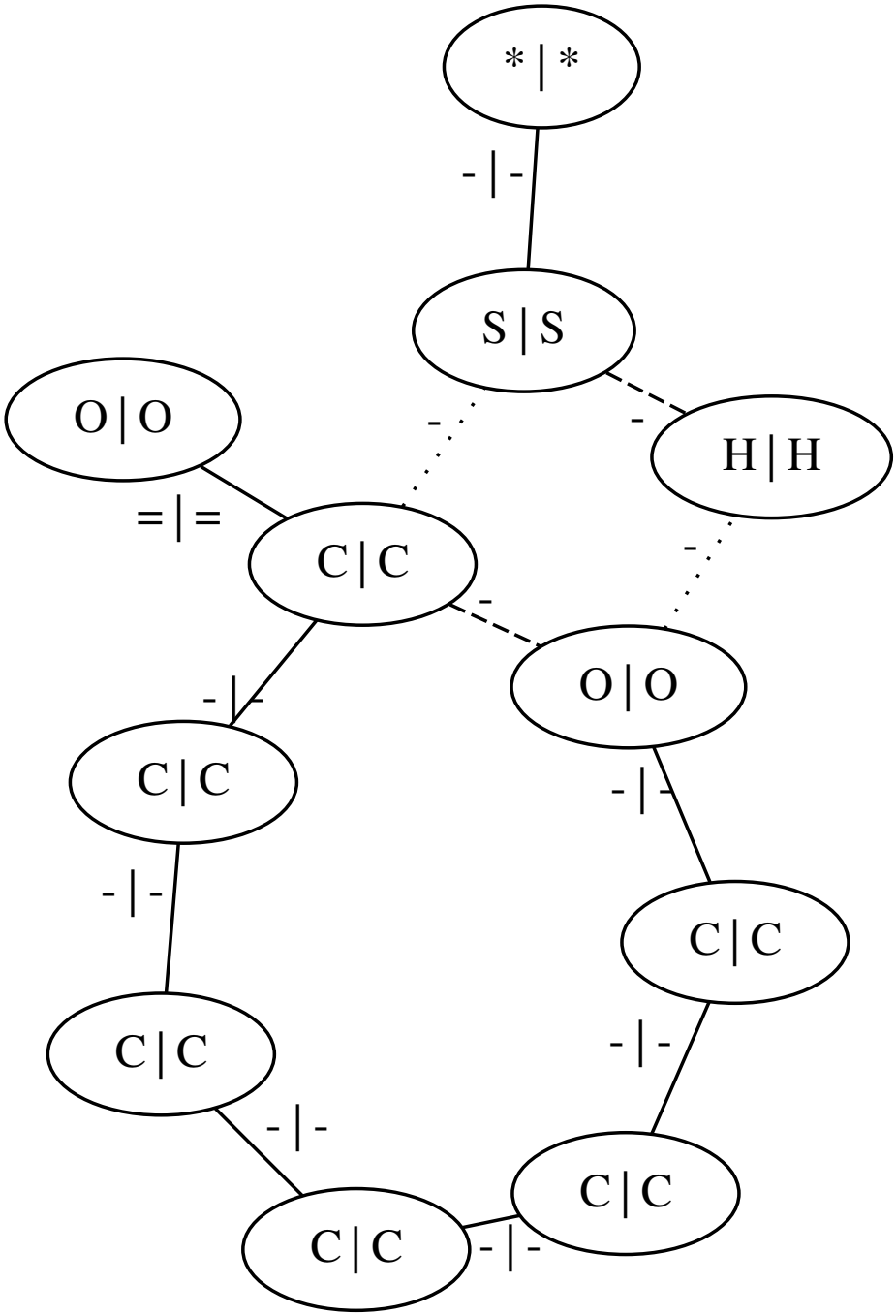
0.0.176 Ring Closure 7 membered, inverse S, O



Files: out/875_r_178_10300000_{L, K, R}



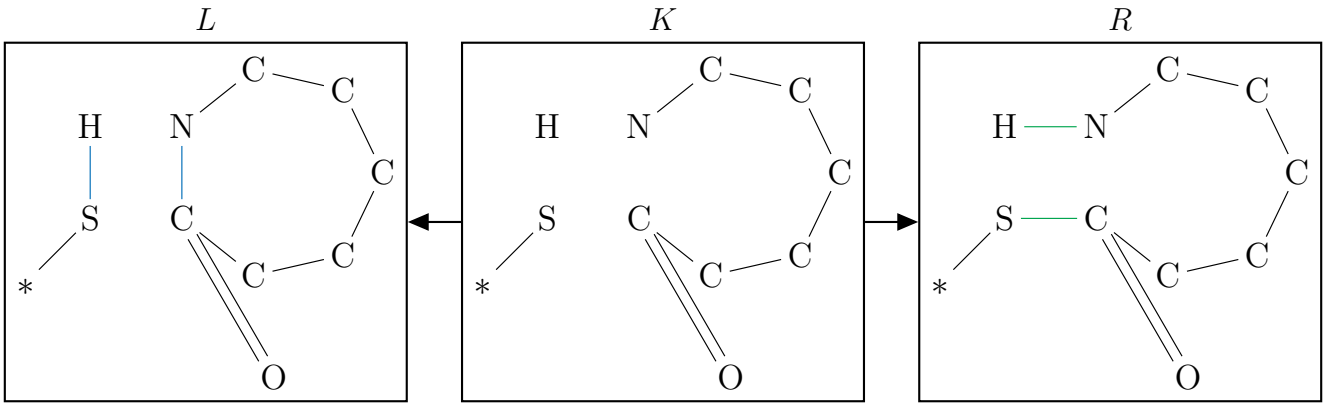
Files: out/876_r_178_11300100_{L, K, R}



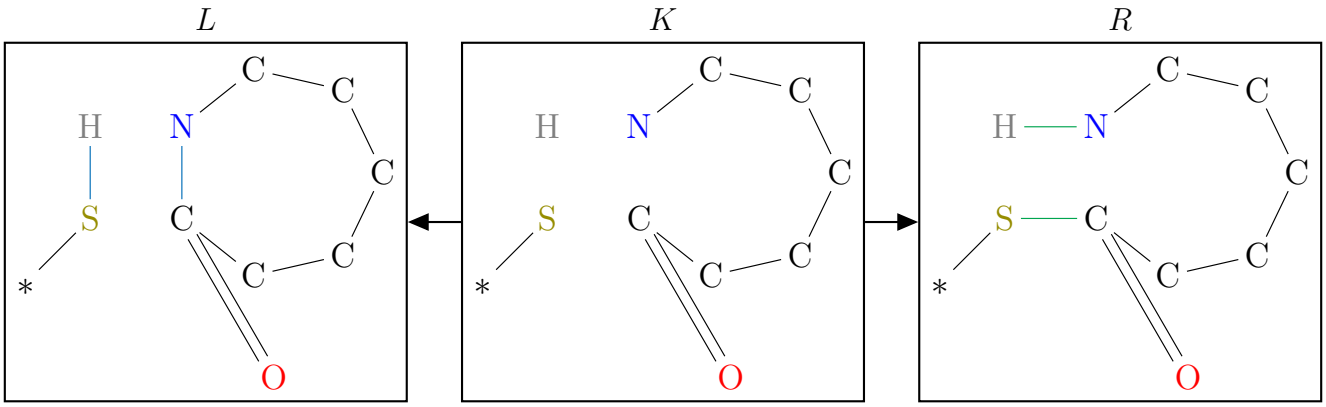
File: out/877_r_178_combined

$$|\{e \in \text{outEdges}(10) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| \leq 1$$

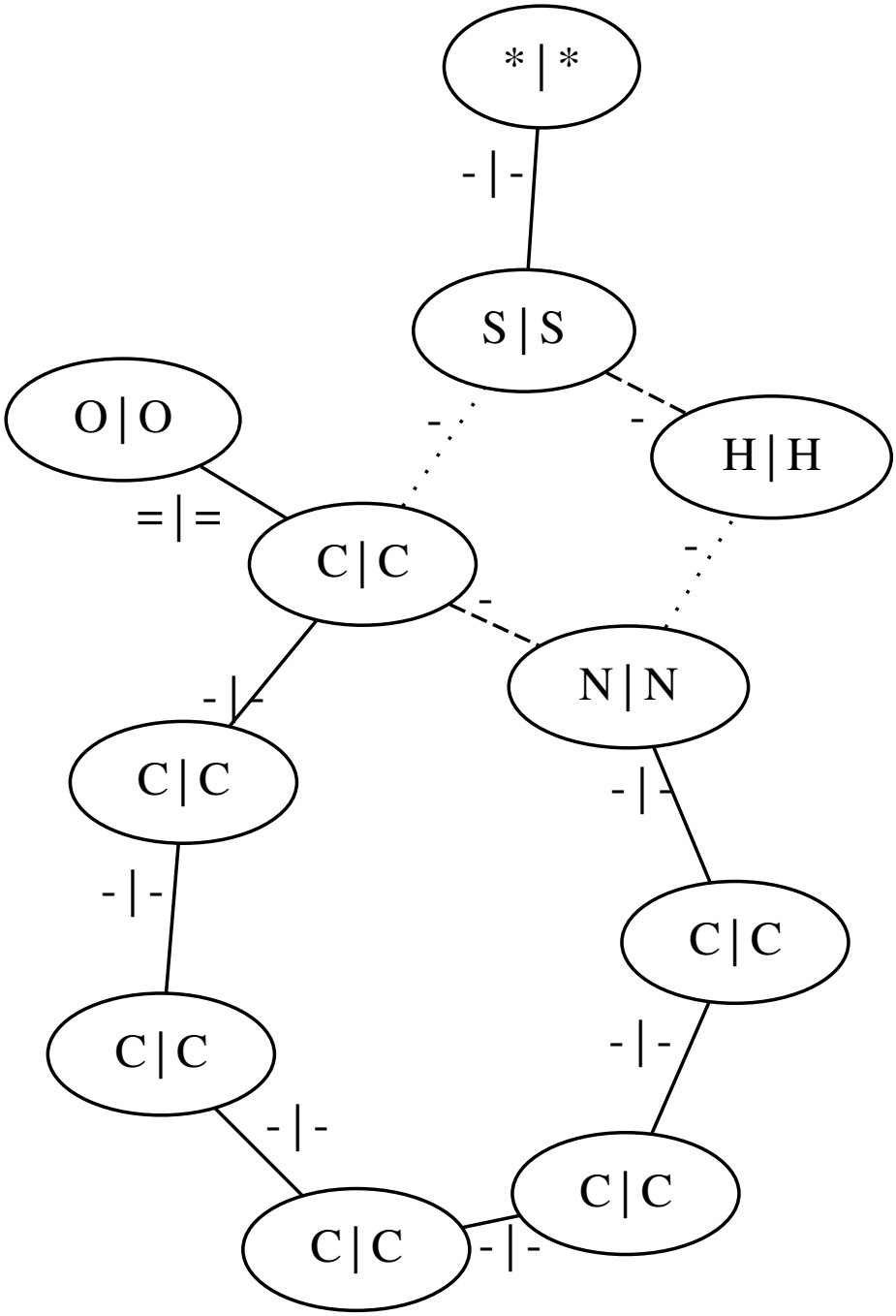
0.0.177 Ring Closure 7 membered, inverse S, N



Files: out/880_r_179_10300000_{L, K, R}



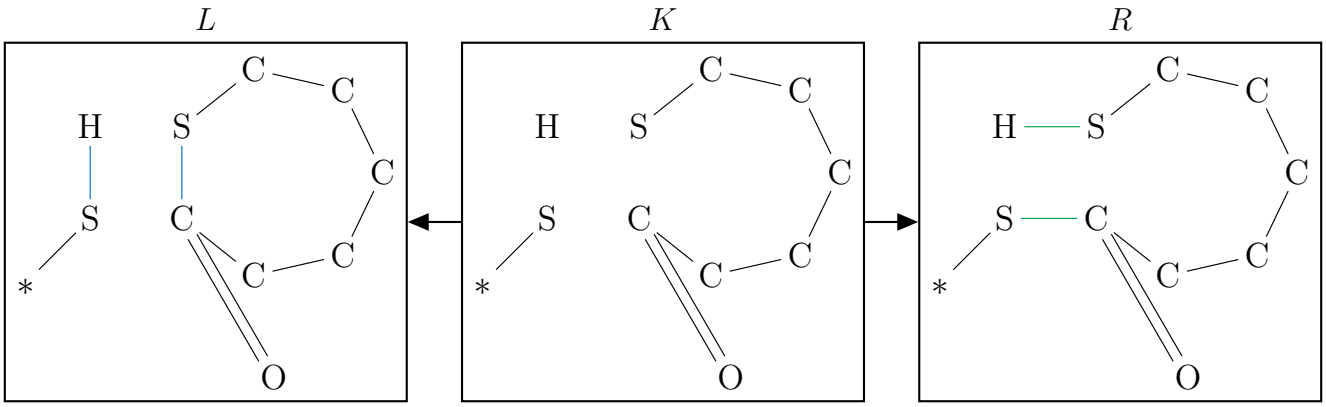
Files: out/881_r_179_11300100_{L, K, R}



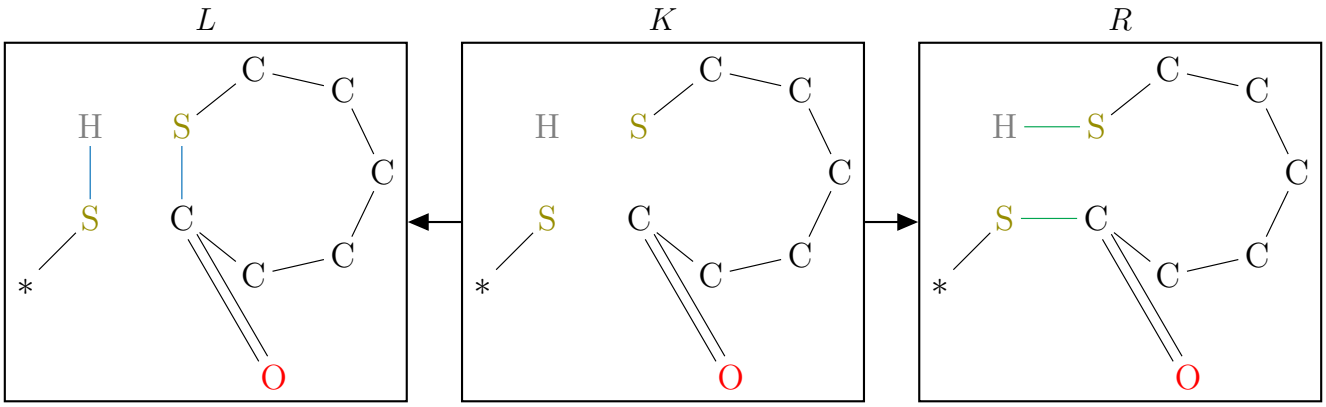
File: out/882_r_179_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

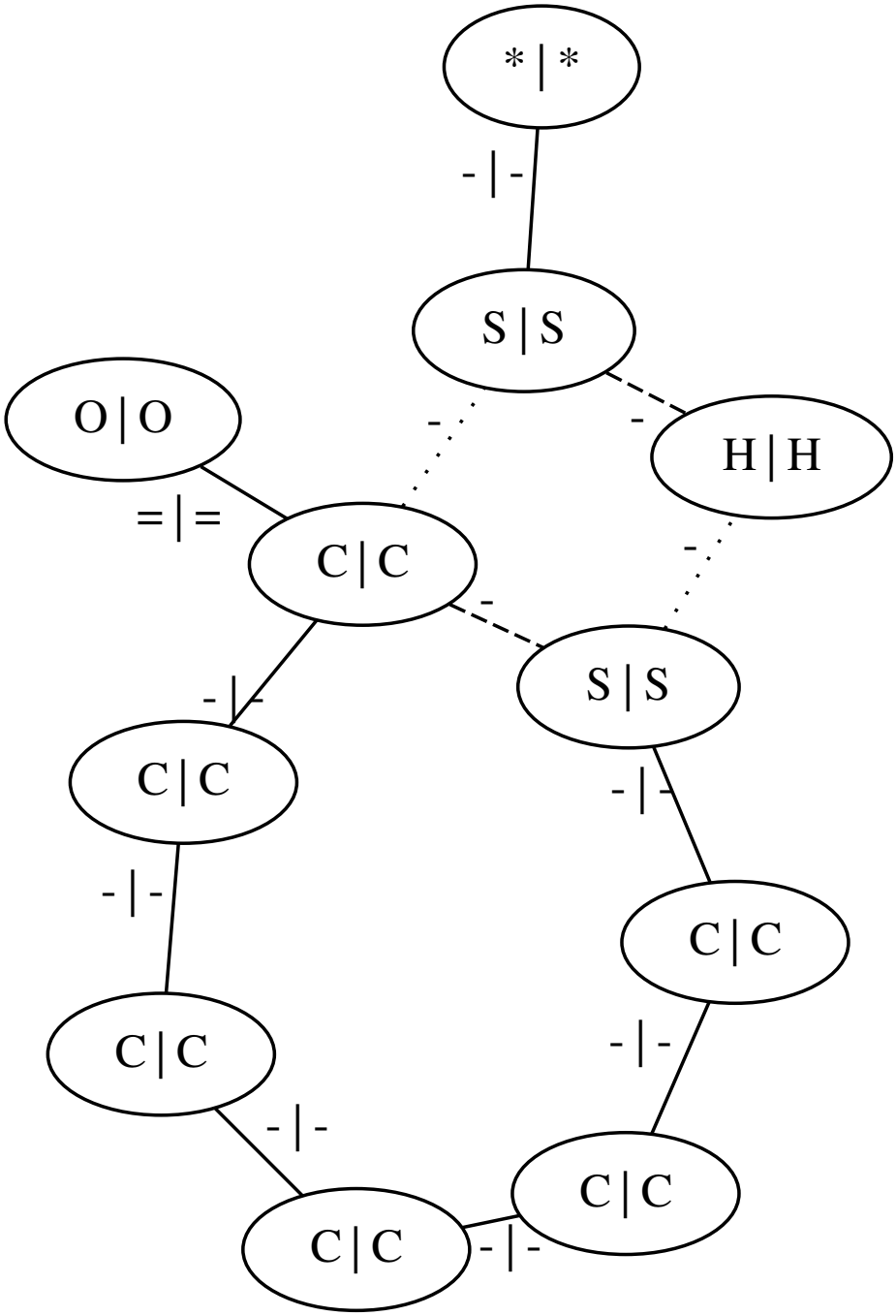
0.0.178 Ring Closure 7 membered, inverse S, S



Files: out/885_r_180_10300000_{L, K, R}



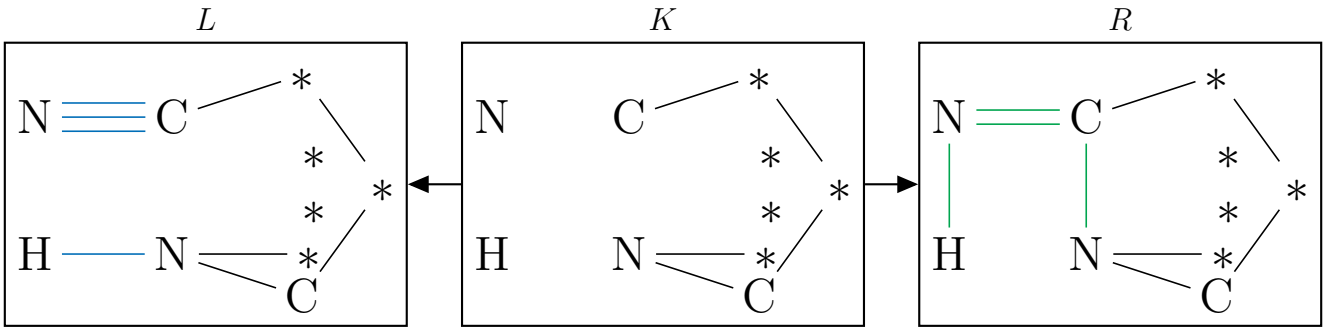
Files: out/886_r_180_11300100_{L, K, R}



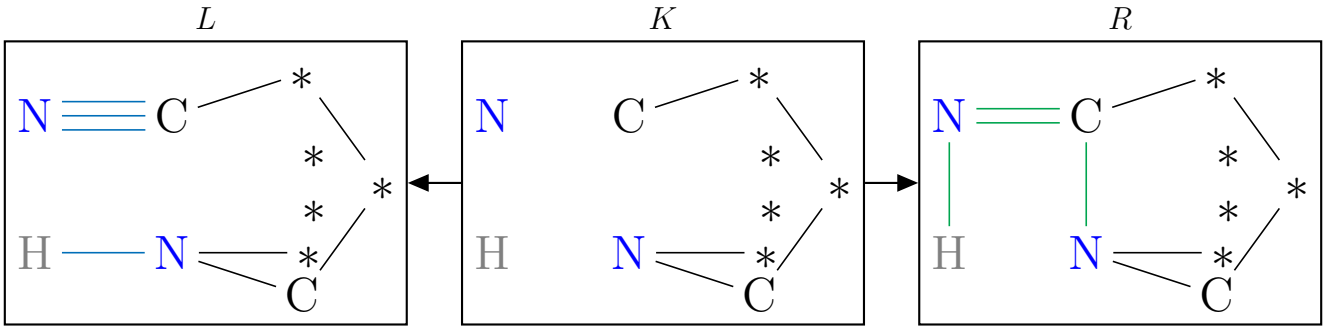
File: out/887_r_180_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(10) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| \leq 1
\end{aligned}
$$

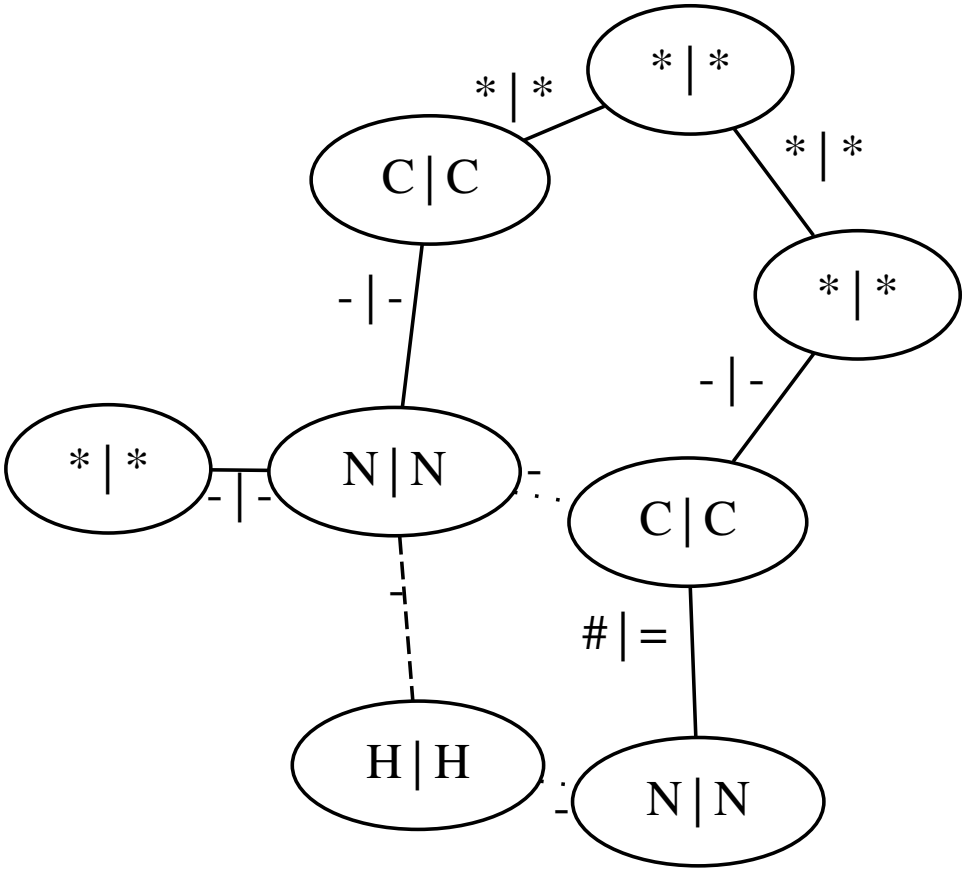
0.0.179 Amine Nitrile Ring Closure 5



Files: out/890_r_181_10300000_{L, K, R}



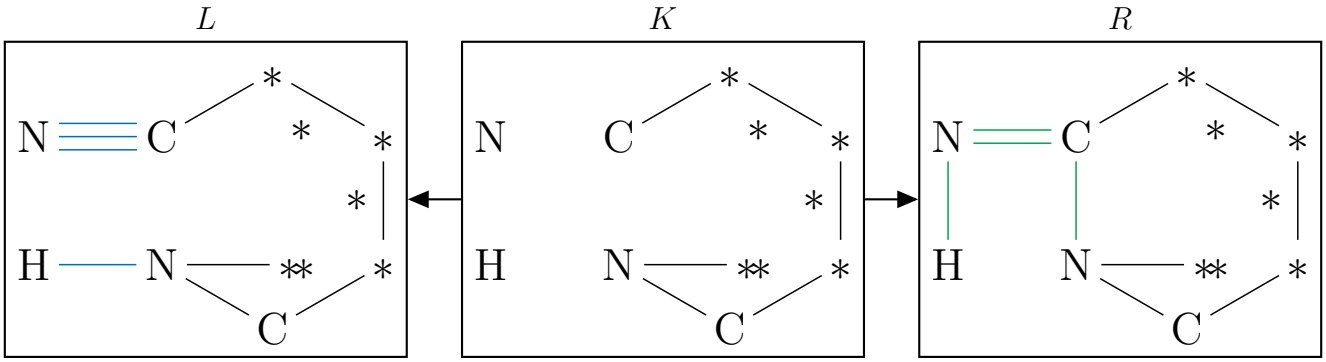
Files: out/891_r_181_11300100_{L, K, R}



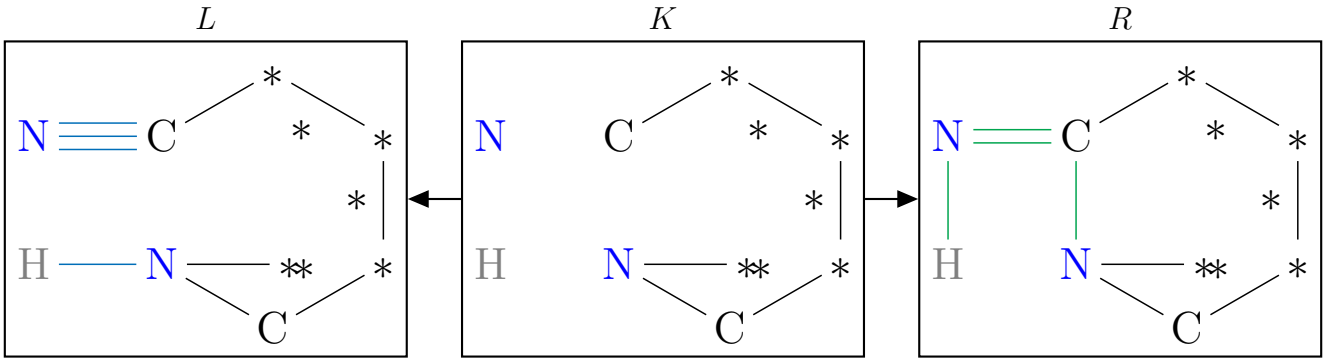
File: out/892_r_181_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

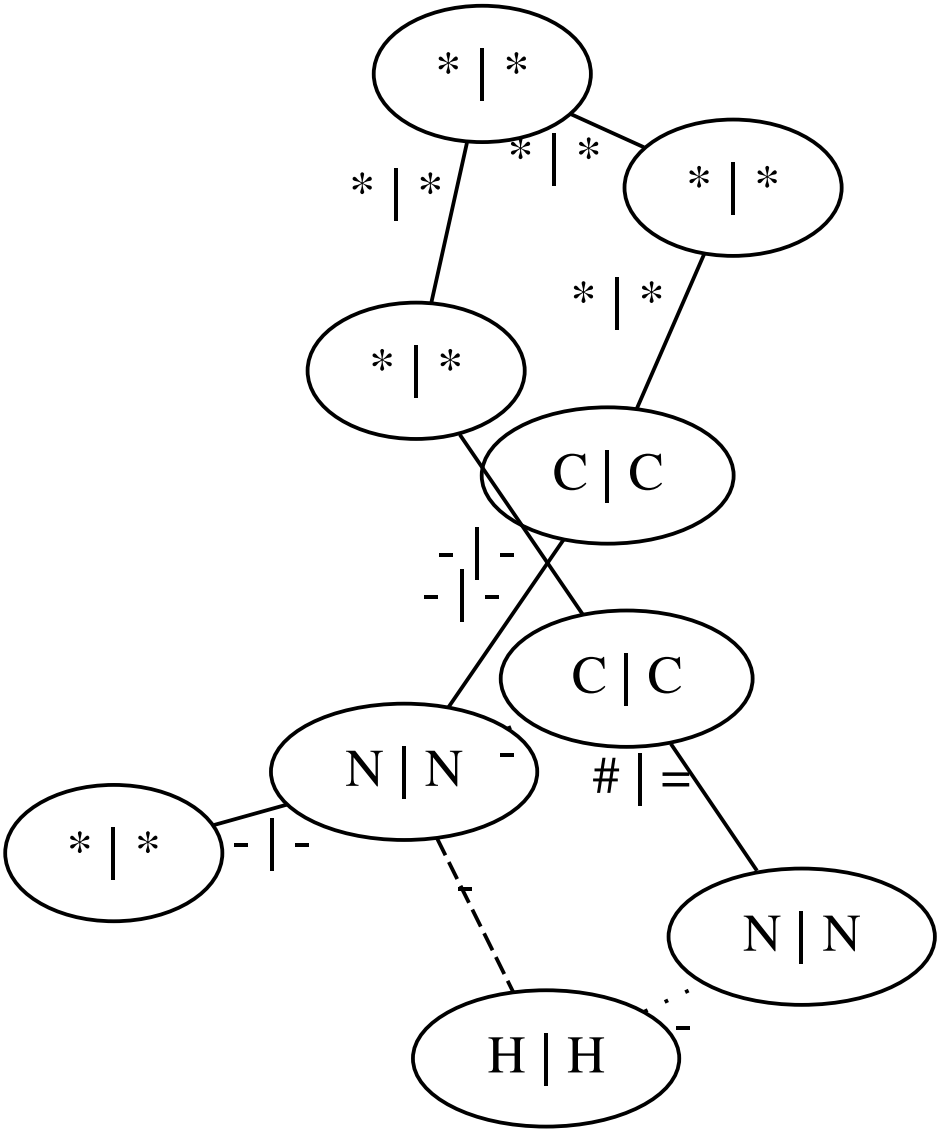
0.0.180 Amine Nitrile Ring Closure 6



Files: out/895_r_182_10300000_{L, K, R}



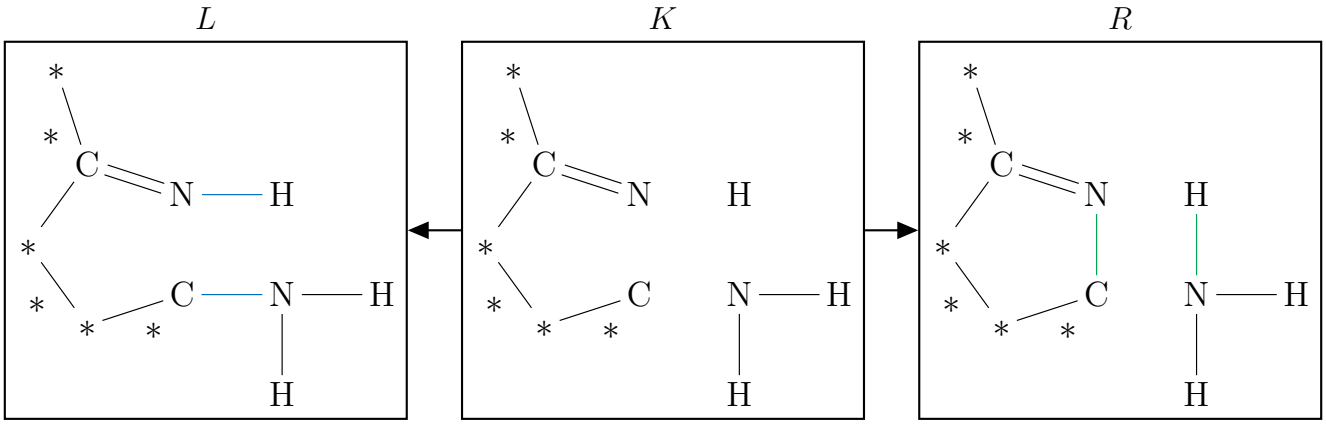
Files: out/896_r_182_11300100_{L, K, R}



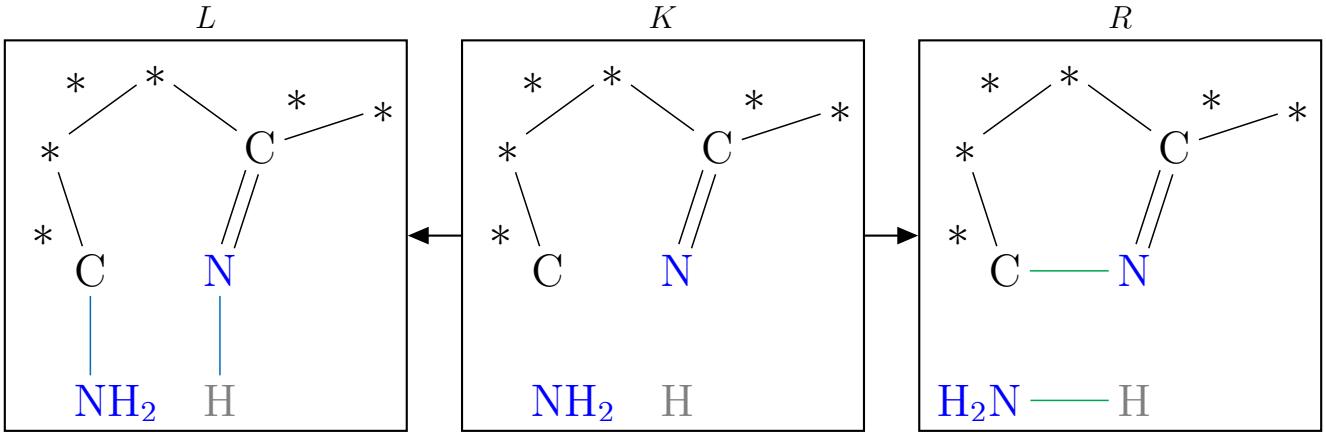
File: out/897_r_182_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}, \text{`-'}\} \\
&\}| = 1
\end{aligned}
$$

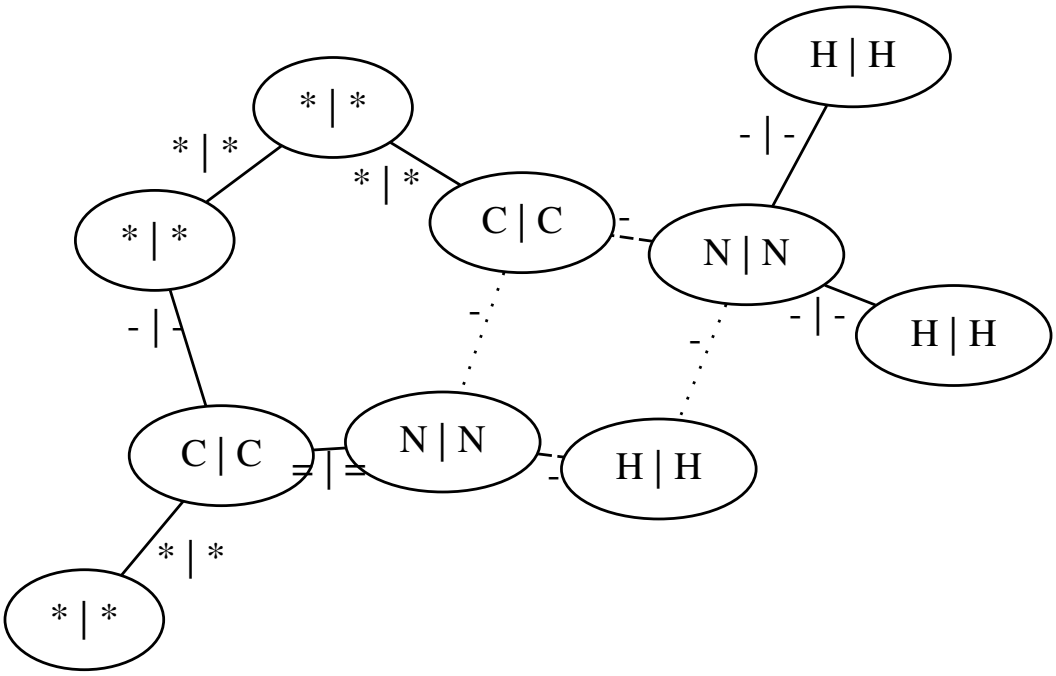
0.0.181 Amine Imine Ring Closure 5



Files: out/900_r_183_10300000_{L, K, R}

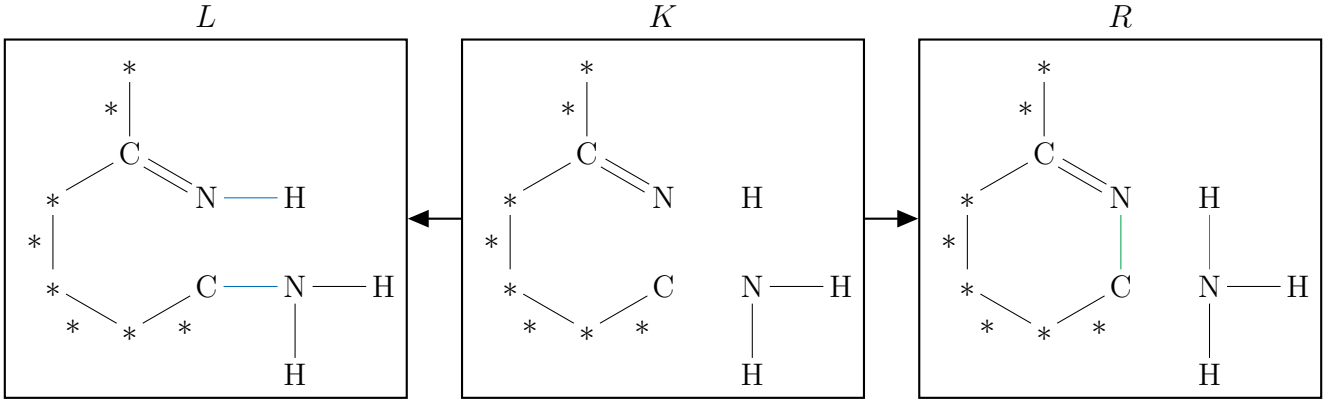


Files: out/901_r_183_11300100_{L, K, R}

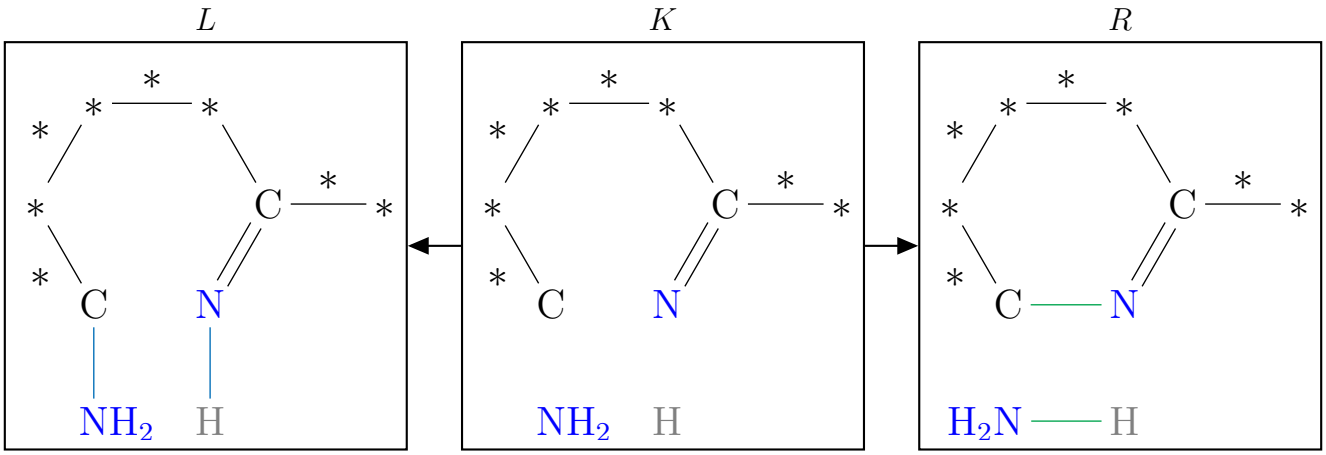


File: out/902_r_183_combined

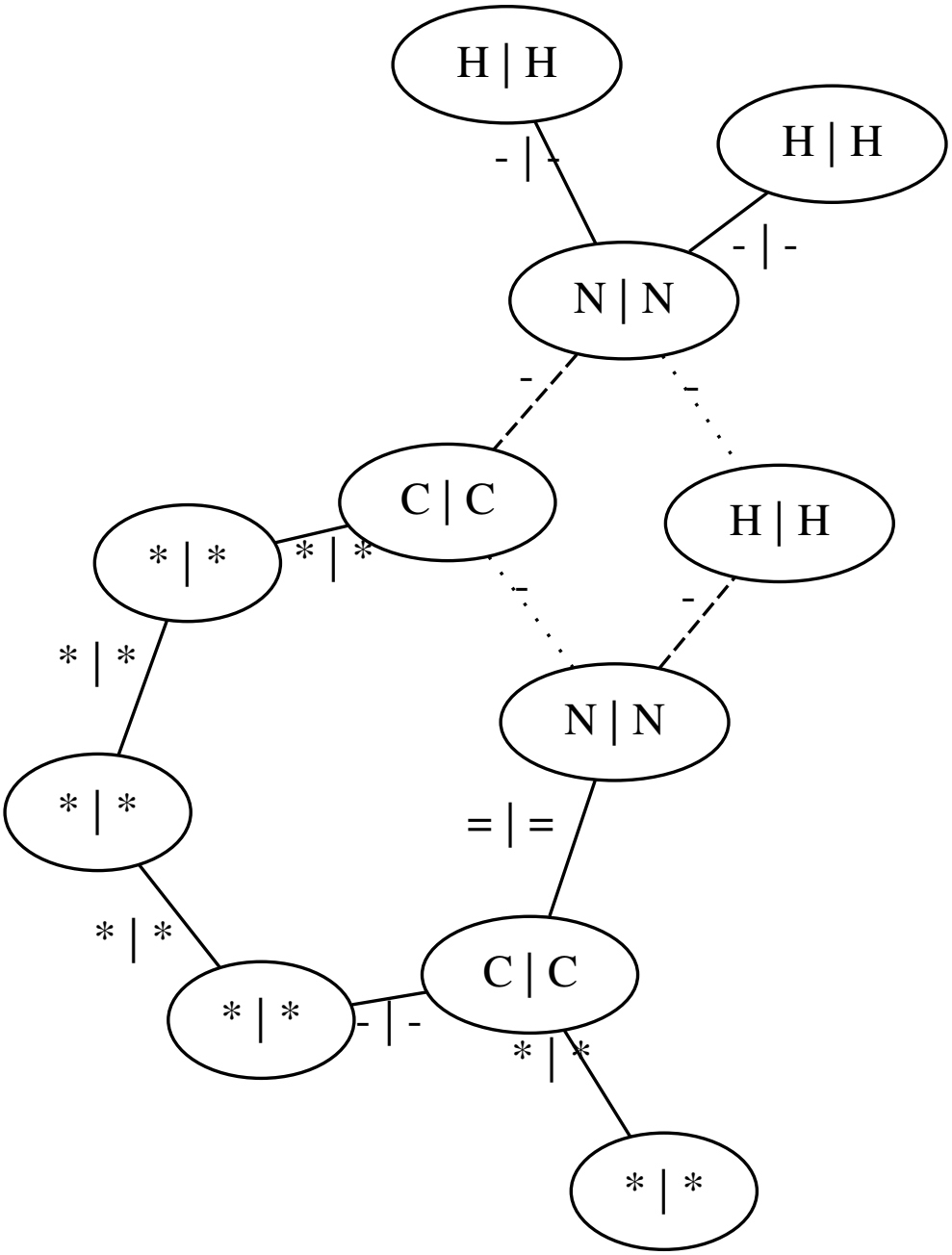
0.0.182 Amine Imine Ring Closure 6



Files: out/905_r_184_10300000_{L, K, R}

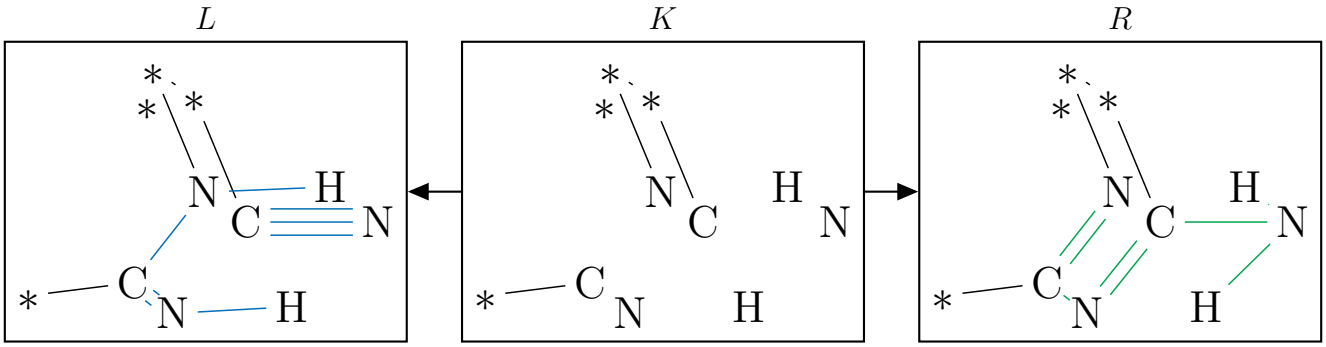


Files: out/906_r_184_11300100_{L, K, R}

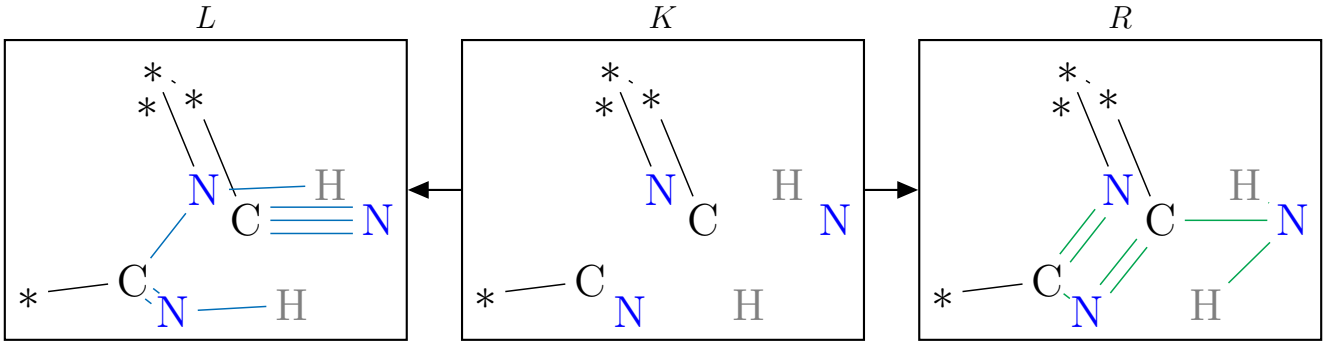


File: out/907_r_184_combined

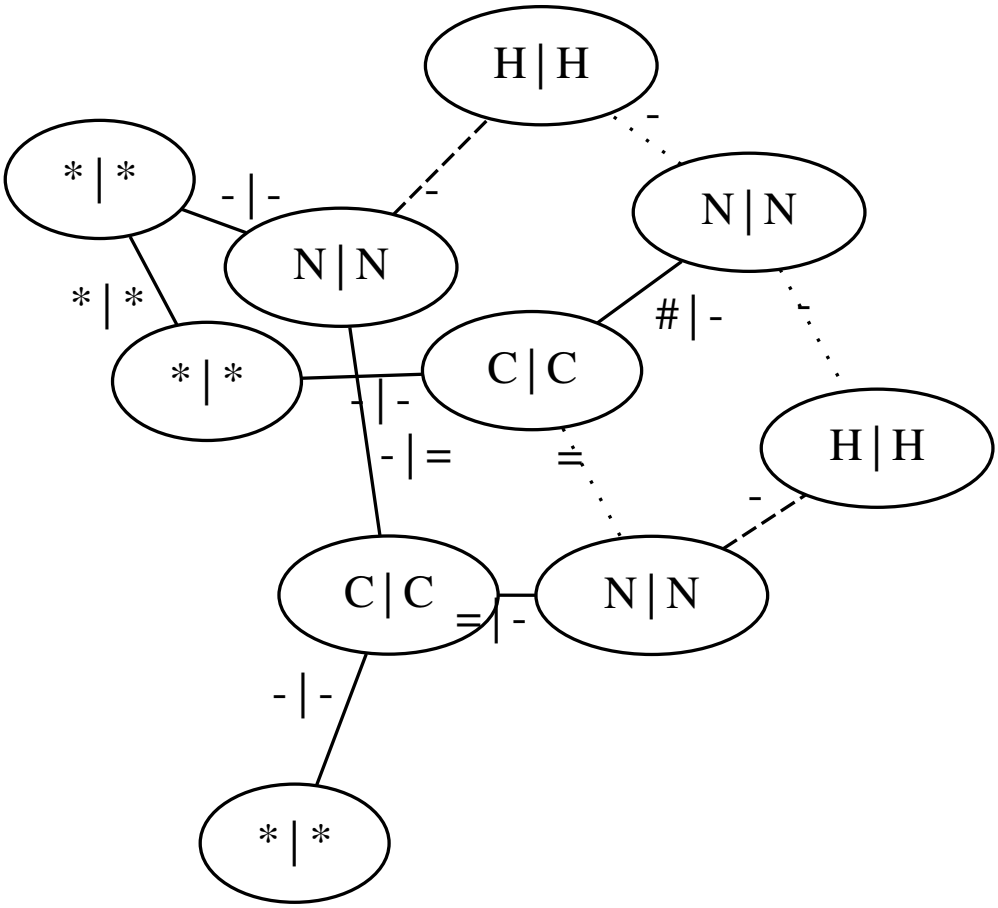
0.0.183 Amidine Nitrile Ring Closure 6



Files: out/910_r_185_10300000_{L, K, R}

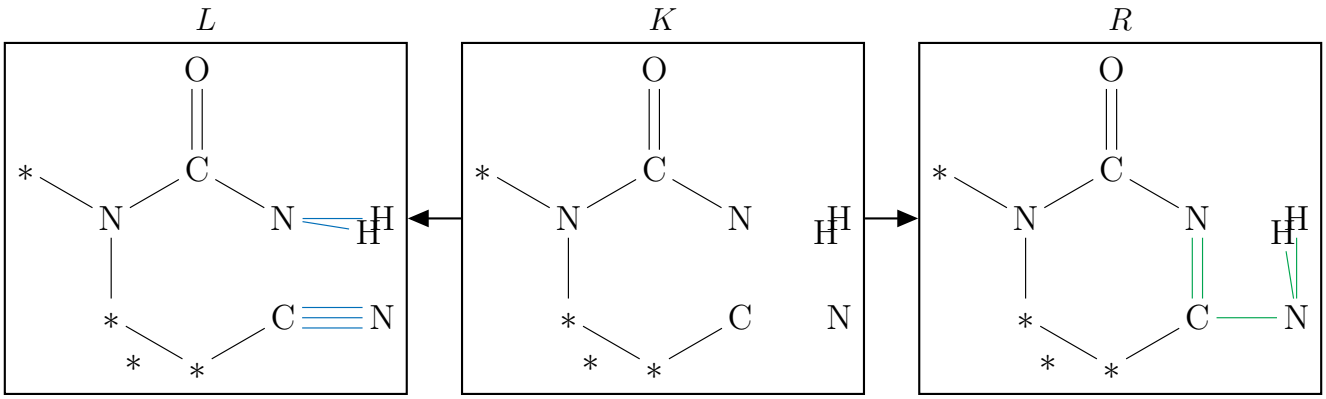


Files: out/911_r_185_11300100_{L, K, R}

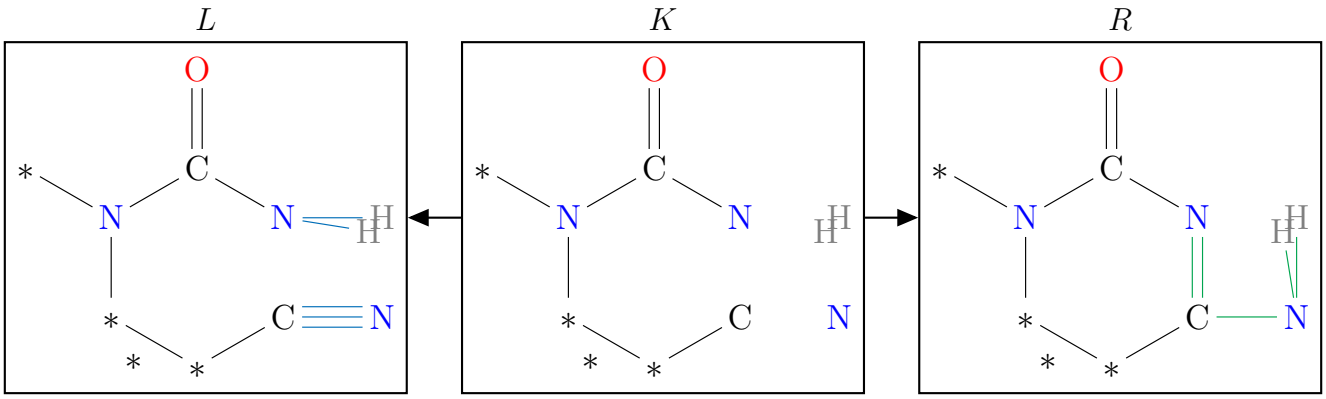


File: out/912_r_185_combined

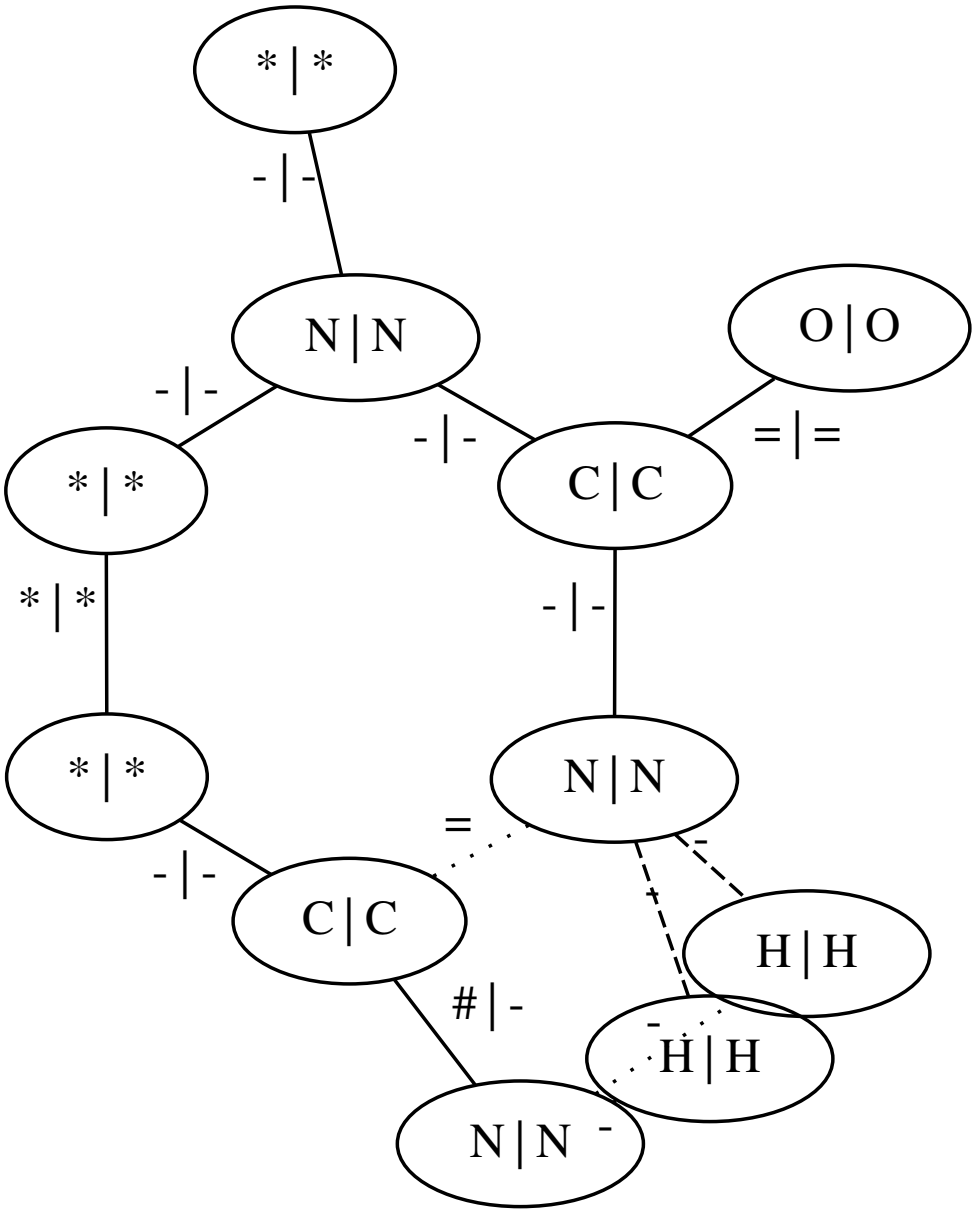
0.0.184 Amide Nitrile Ring Closure 6



Files: out/915_r_186_10300000_{L, K, R}

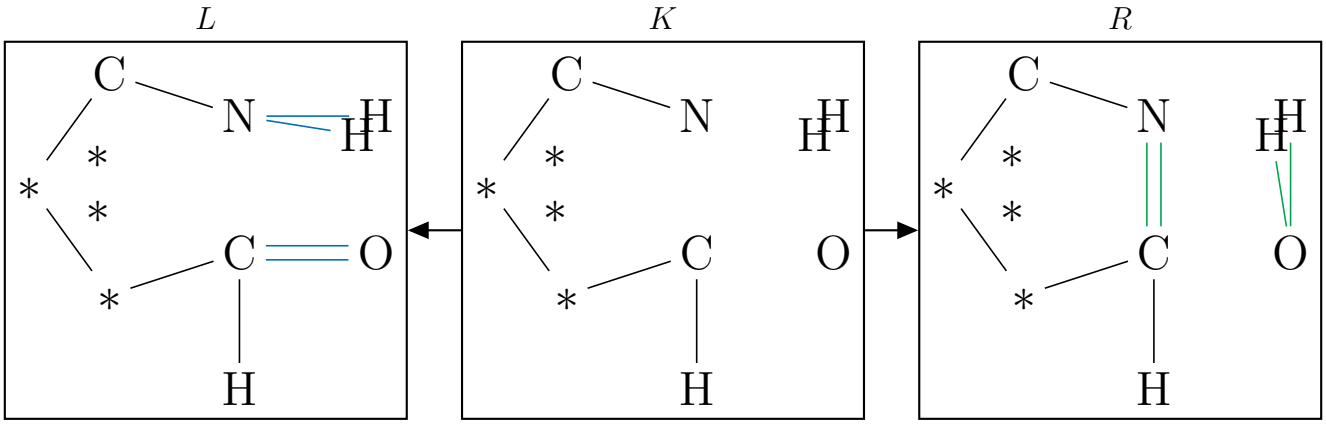


Files: out/916_r_186_11300100_{L, K, R}

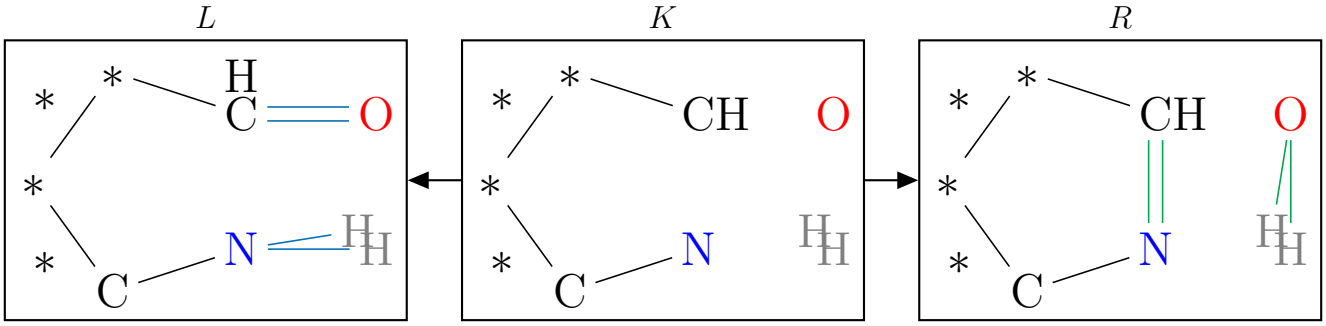


File: out/917_r_186_combined

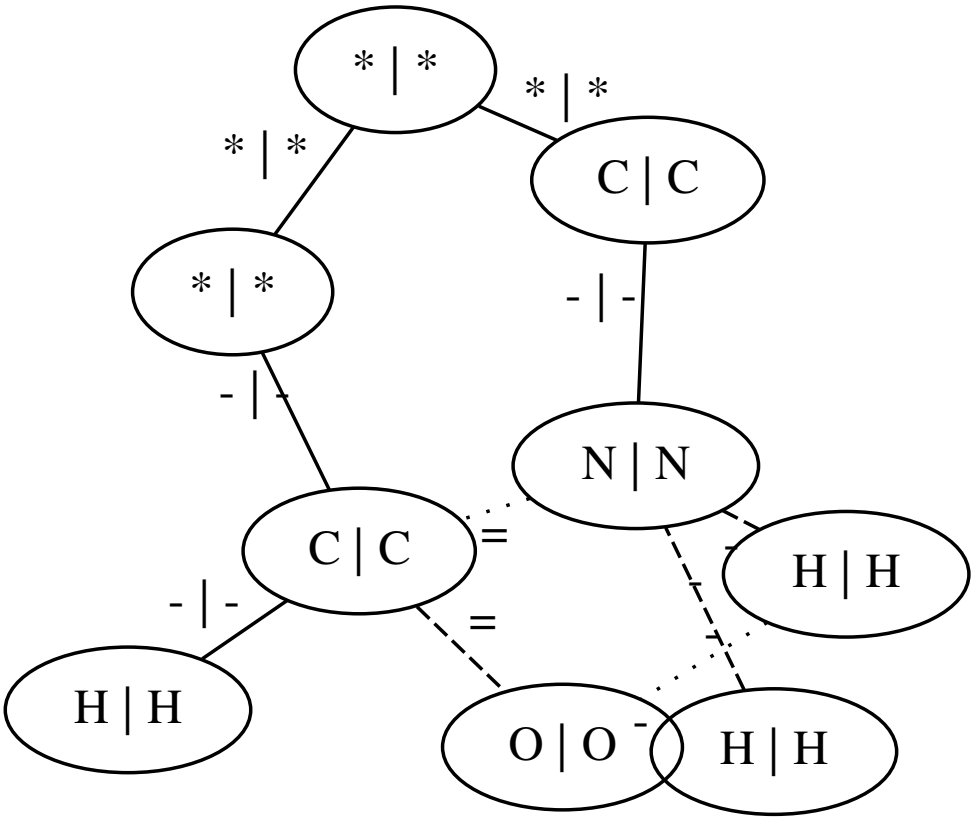
0.0.185 Amine Carbonyl Ring Closure, H, 5



Files: out/920_r_187_10300000_{L, K, R}

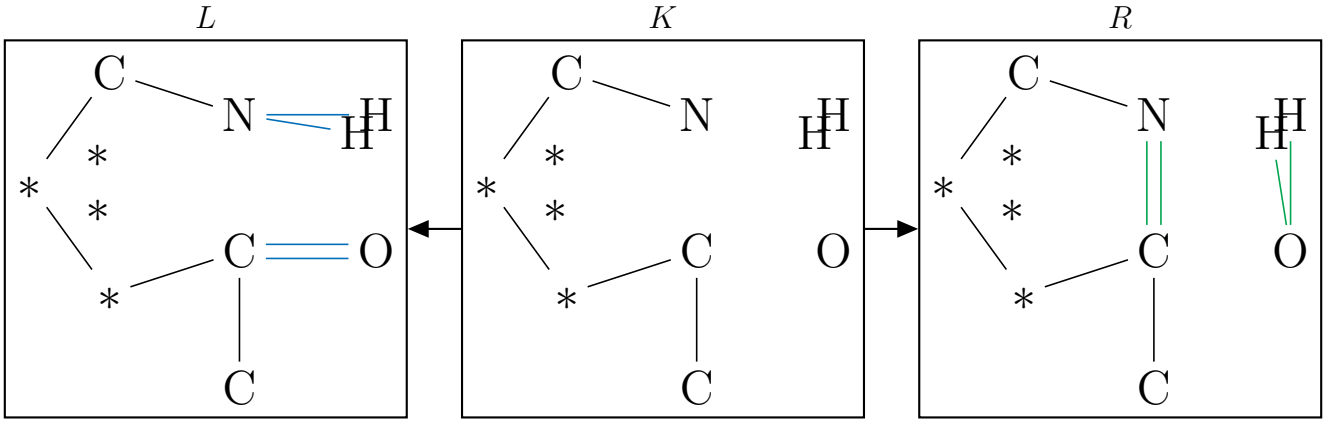


Files: out/921_r_187_11300100_{L, K, R}

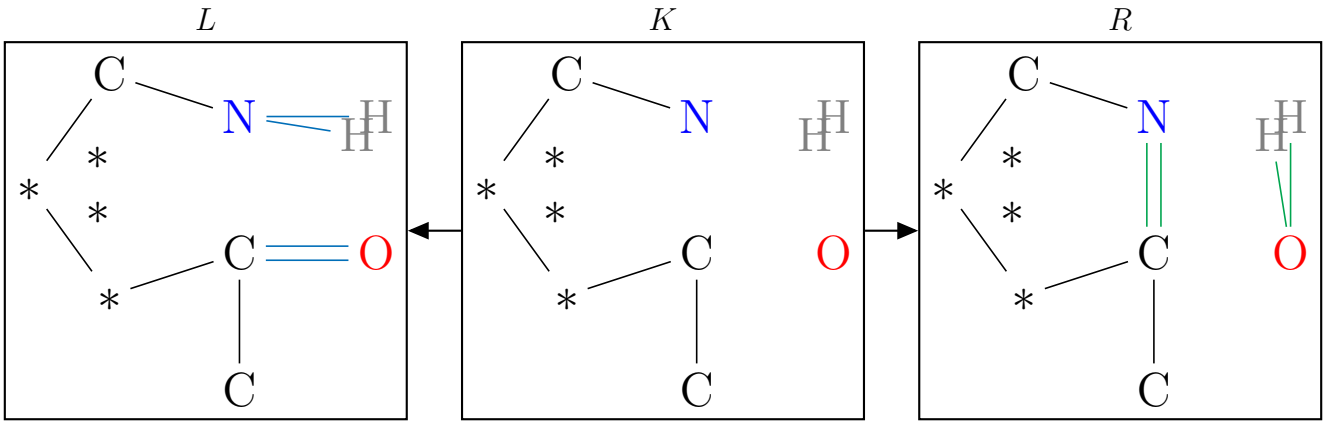


File: out/922_r_187_combined

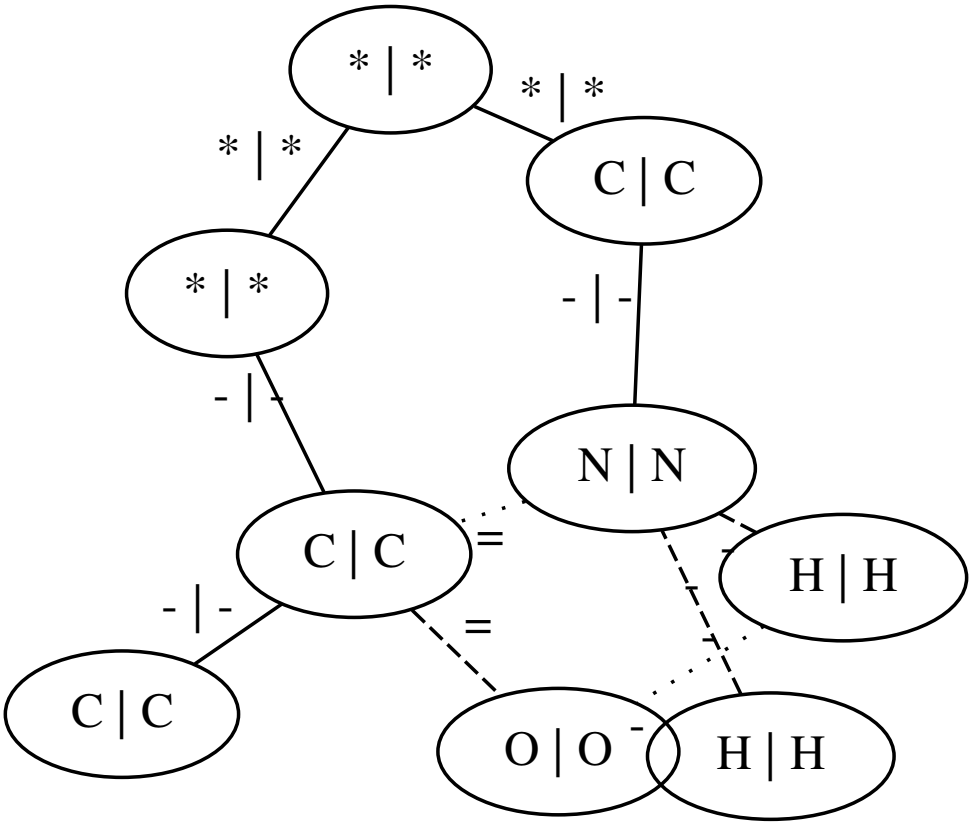
0.0.186 Amine Carbonyl Ring Closure, C, 5



Files: out/925_r_188_10300000_{L, K, R}

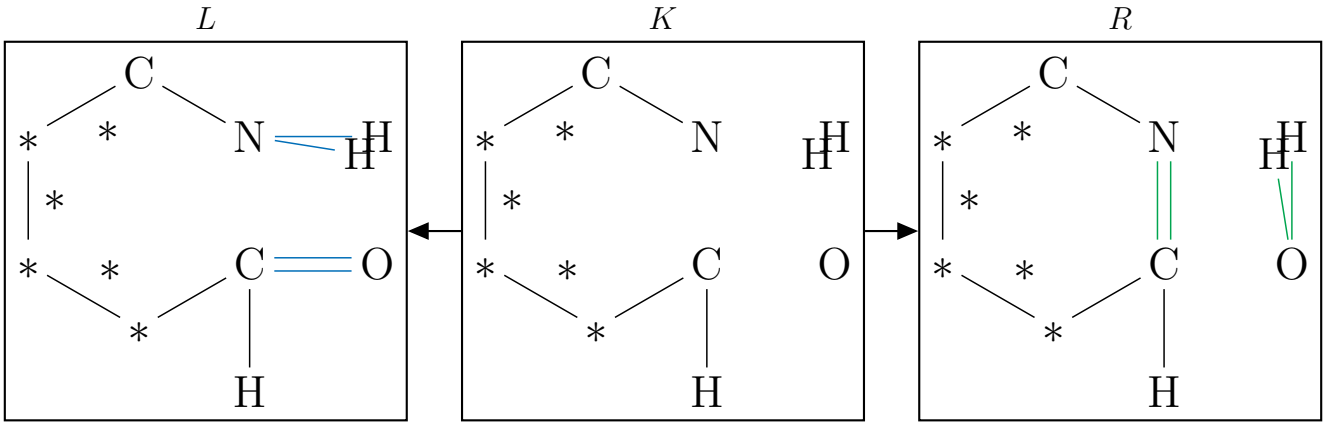


Files: out/926_r_188_11300100_{L, K, R}

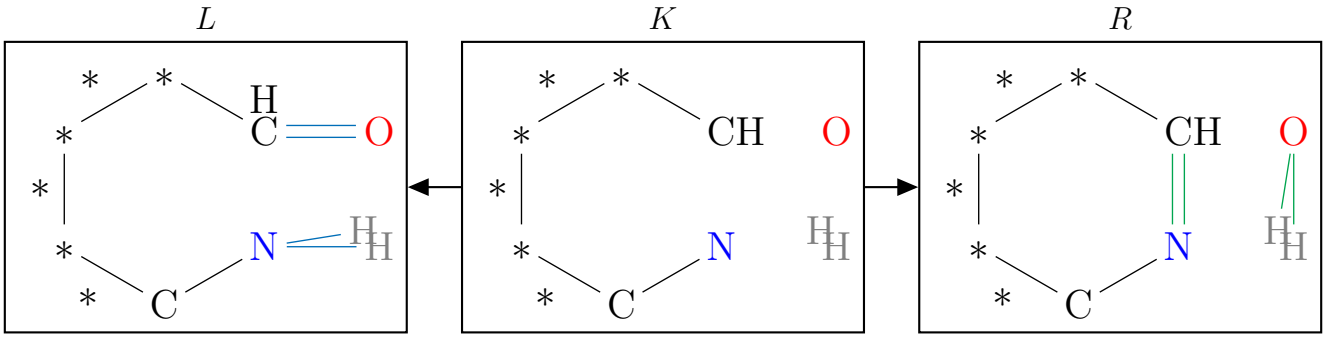


File: out/927_r_188_combined

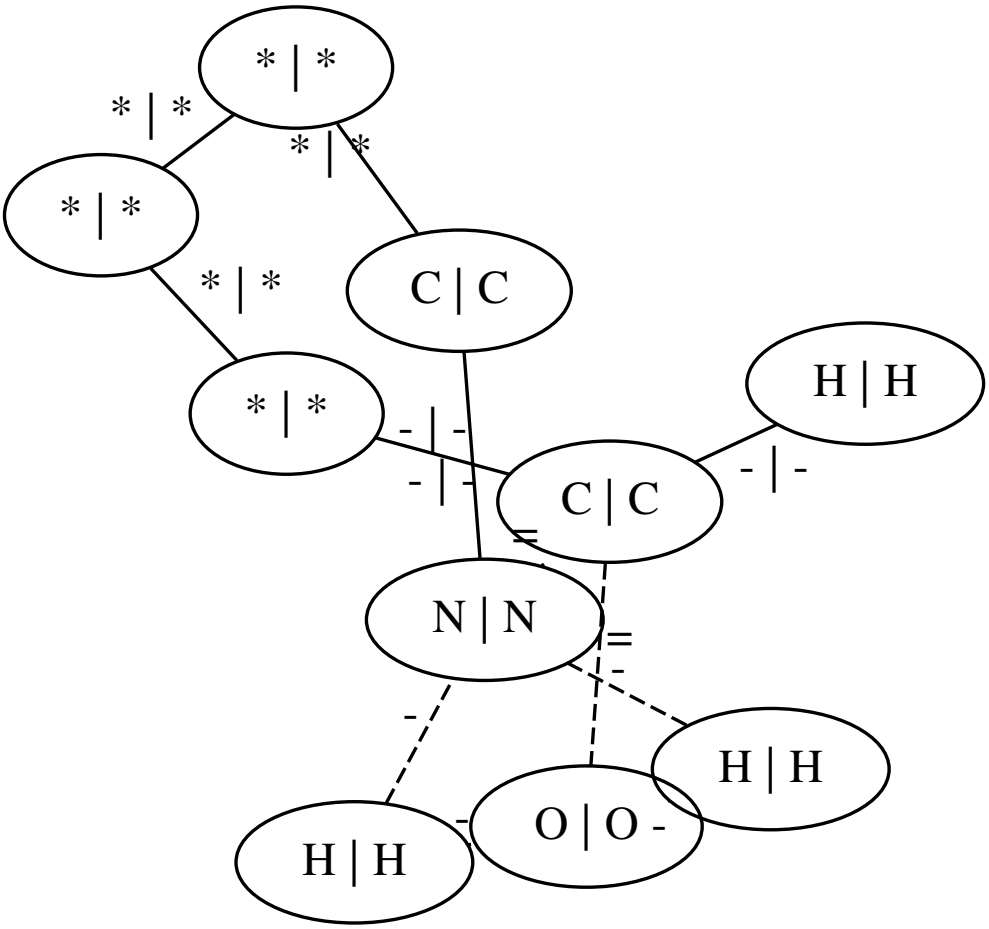
0.0.187 Amine Carbonyl Ring Closure, H, 6



Files: out/930_r_189_10300000_{L, K, R}

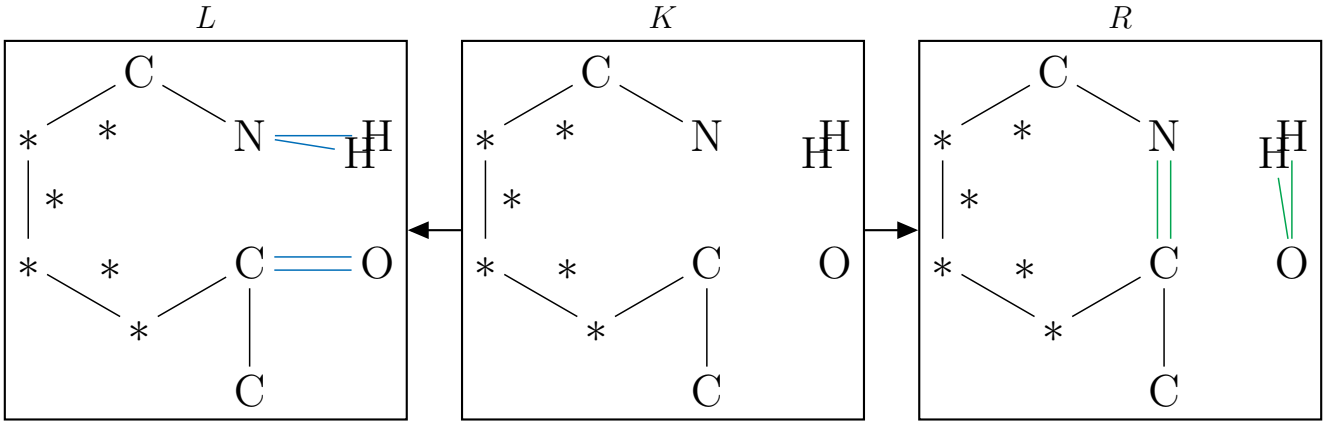


Files: out/931_r_189_11300100_{L, K, R}

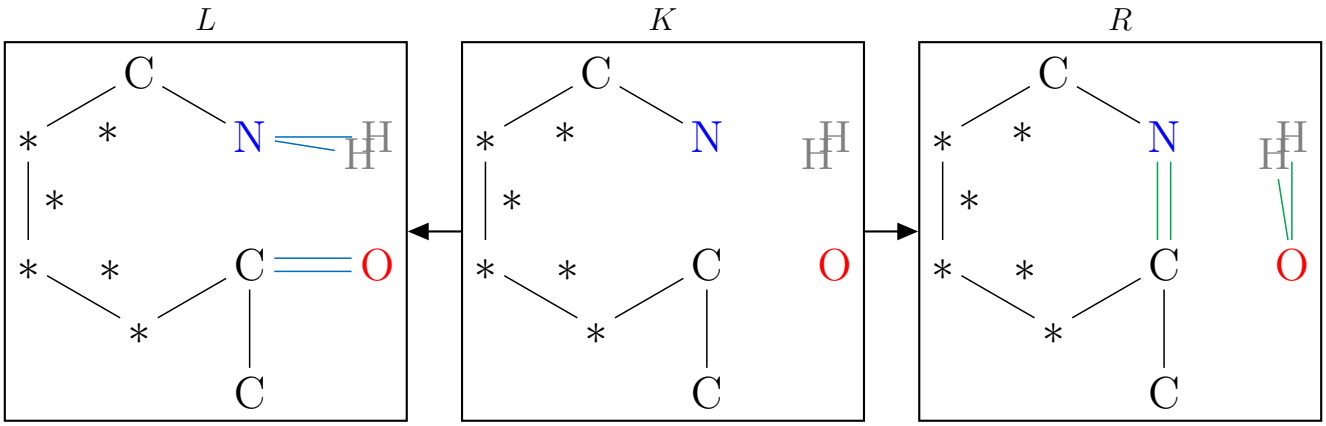


File: out/932_r_189_combined

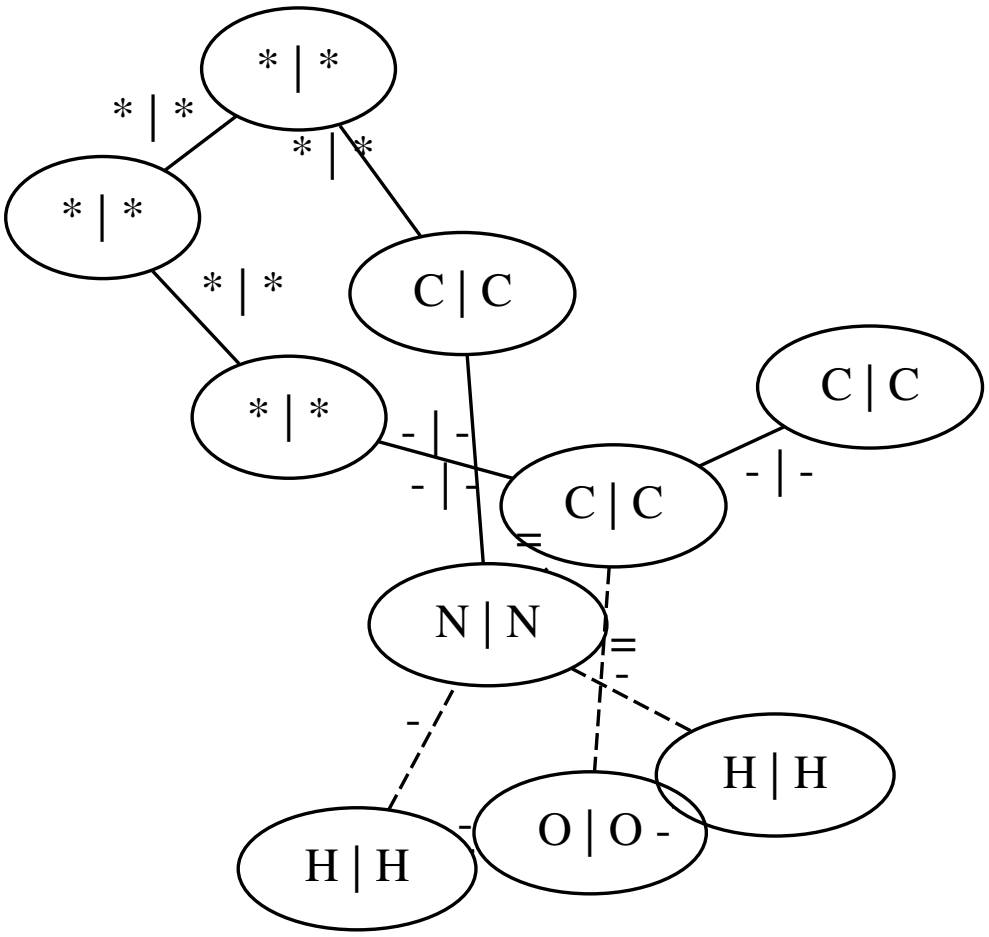
0.0.188 Amine Carbonyl Ring Closure, C, 6



Files: out/935_r_190_10300000_{L, K, R}

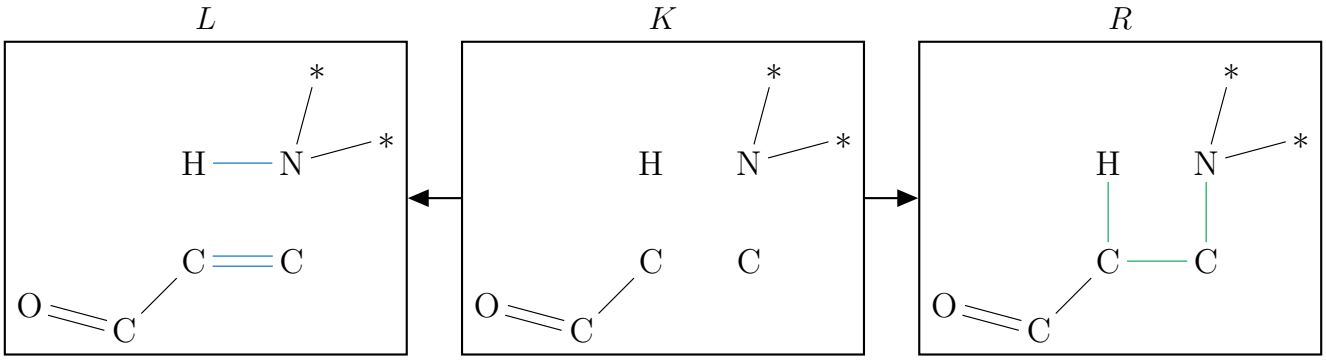


Files: out/936_r_190_11300100_{L, K, R}

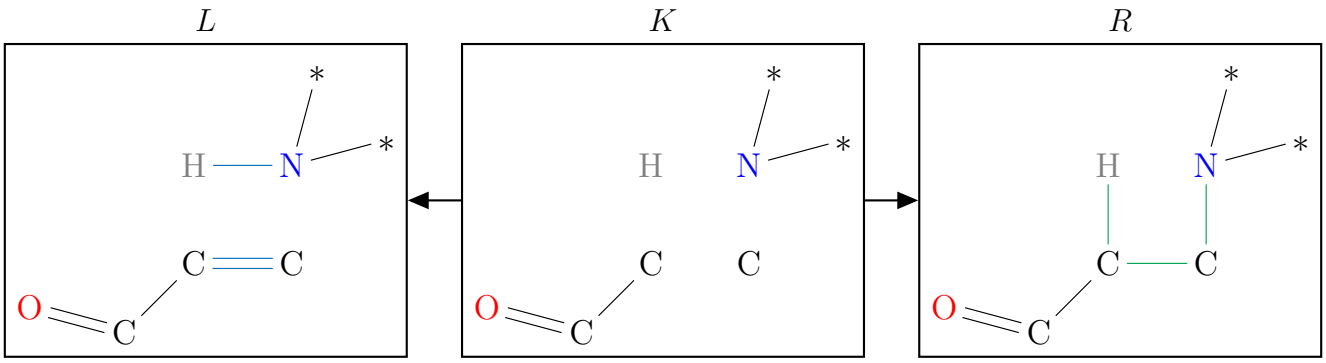


File: out/937_r_190_combined

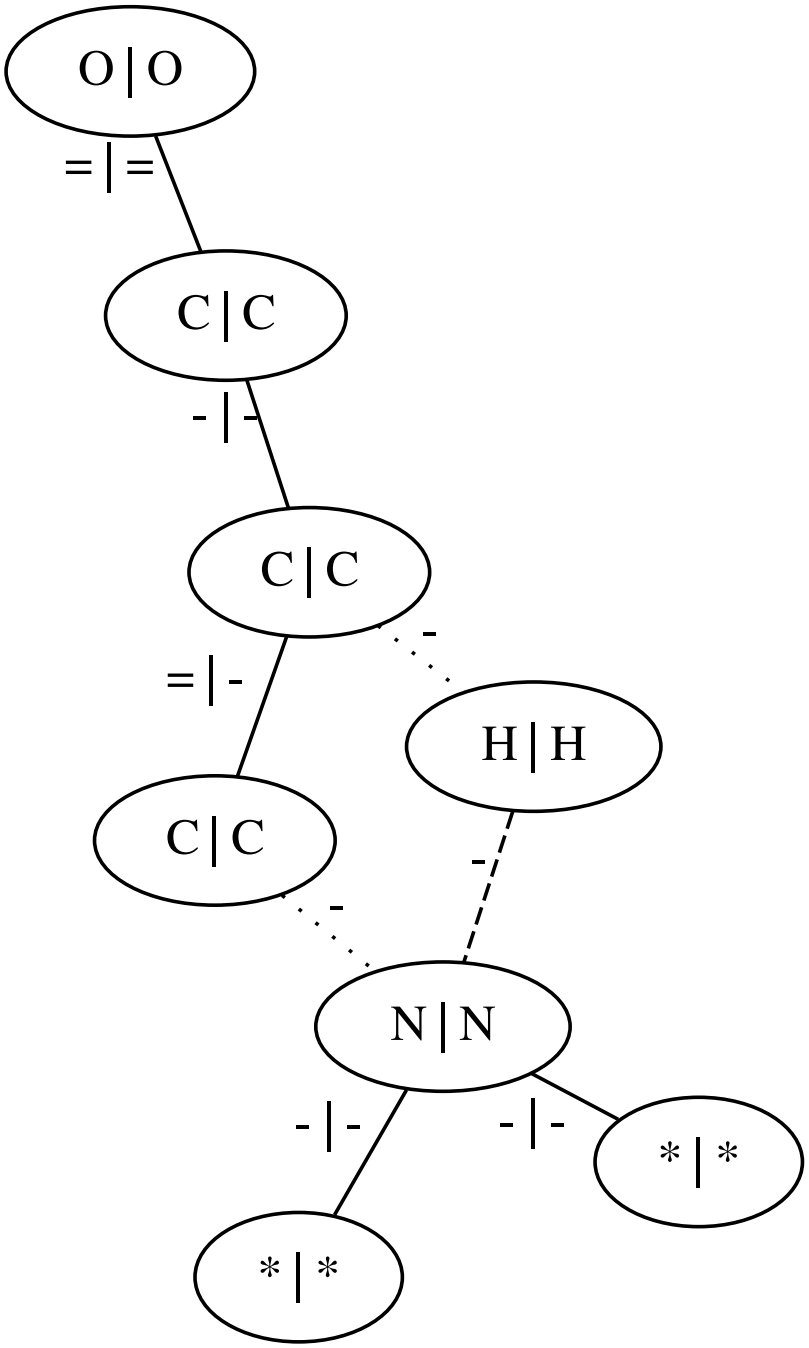
0.0.189 Michael Addition 0,0,



Files: out/940_r_191_10300000_{L, K, R}



Files: out/941_r_191_11300100_{L, K, R}



File: out/942_r_191_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

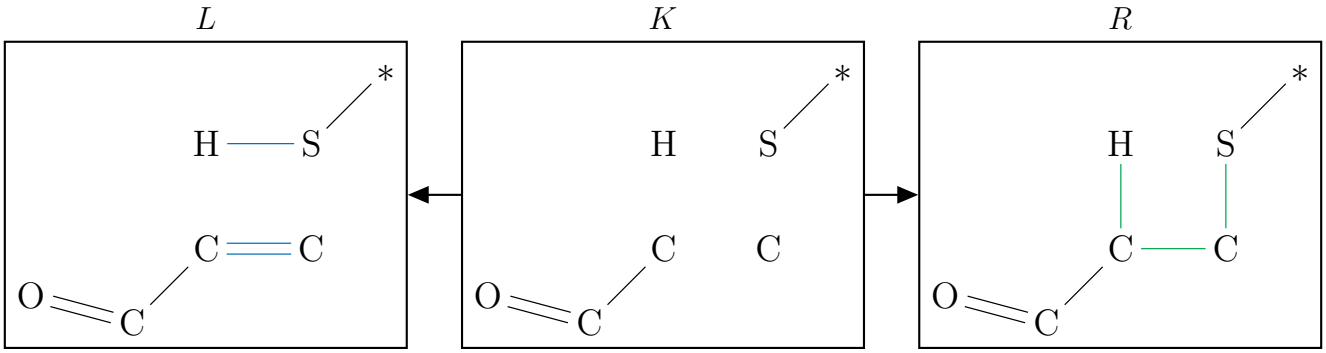
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

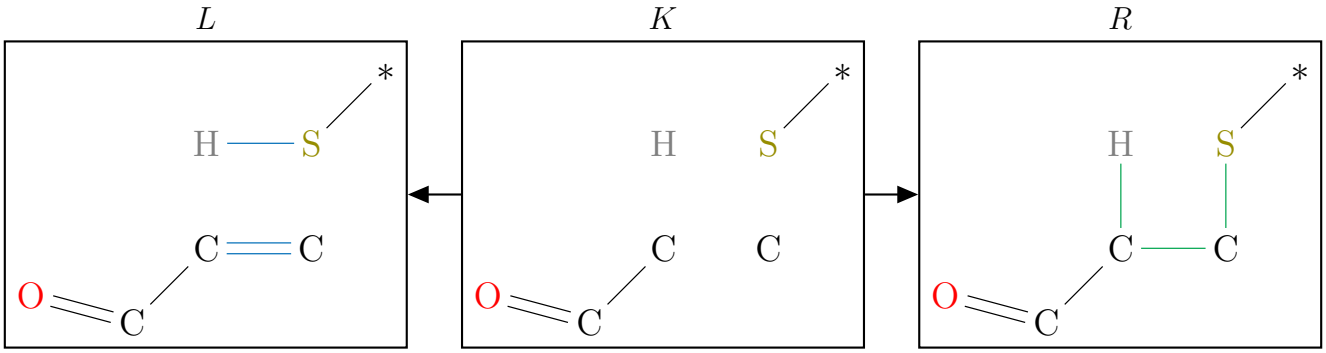
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

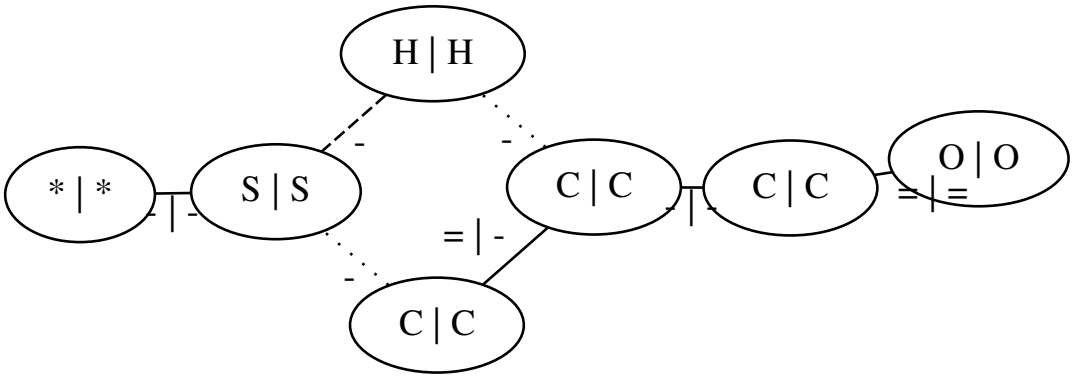
0.0.190 Michael Addition 0,1,



Files: out/945_r_192_10300000_{L, K, R}



Files: out/946_r_192_11300100_{L, K, R}



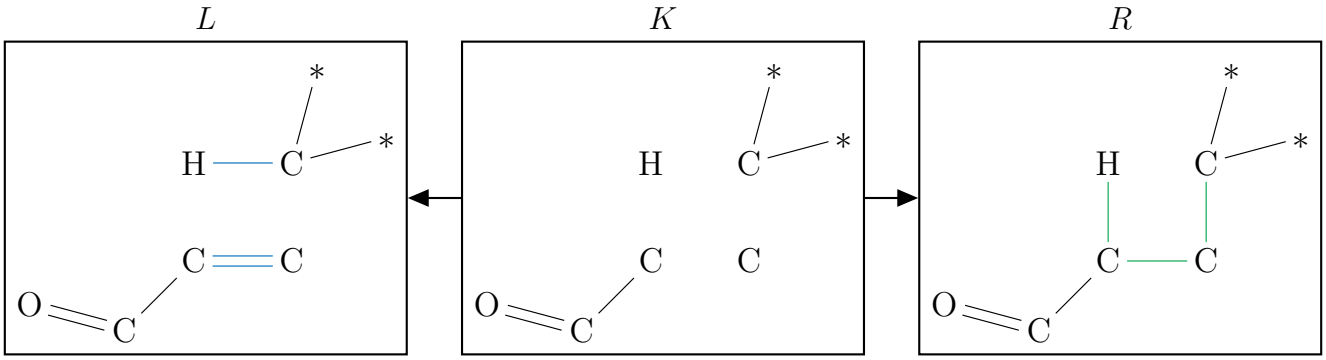
File: out/947_r_192_combined

$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

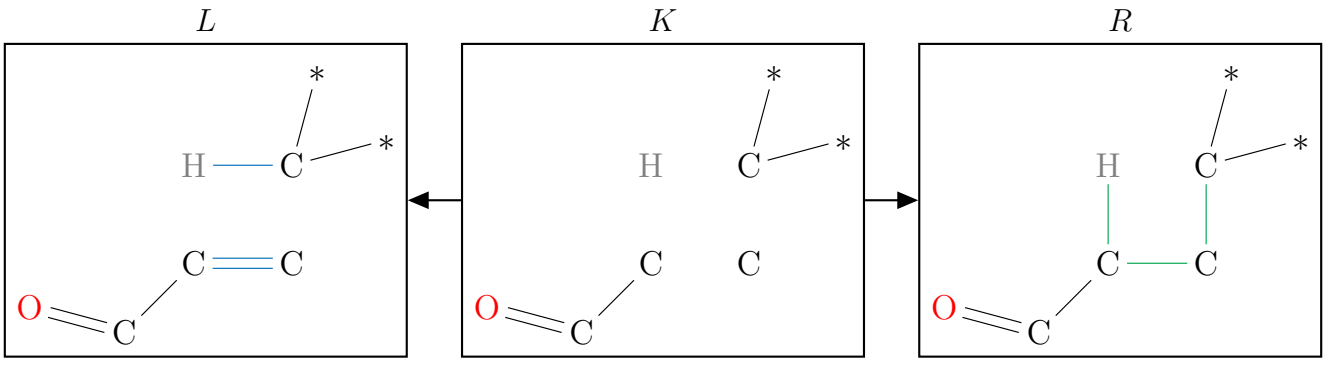
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

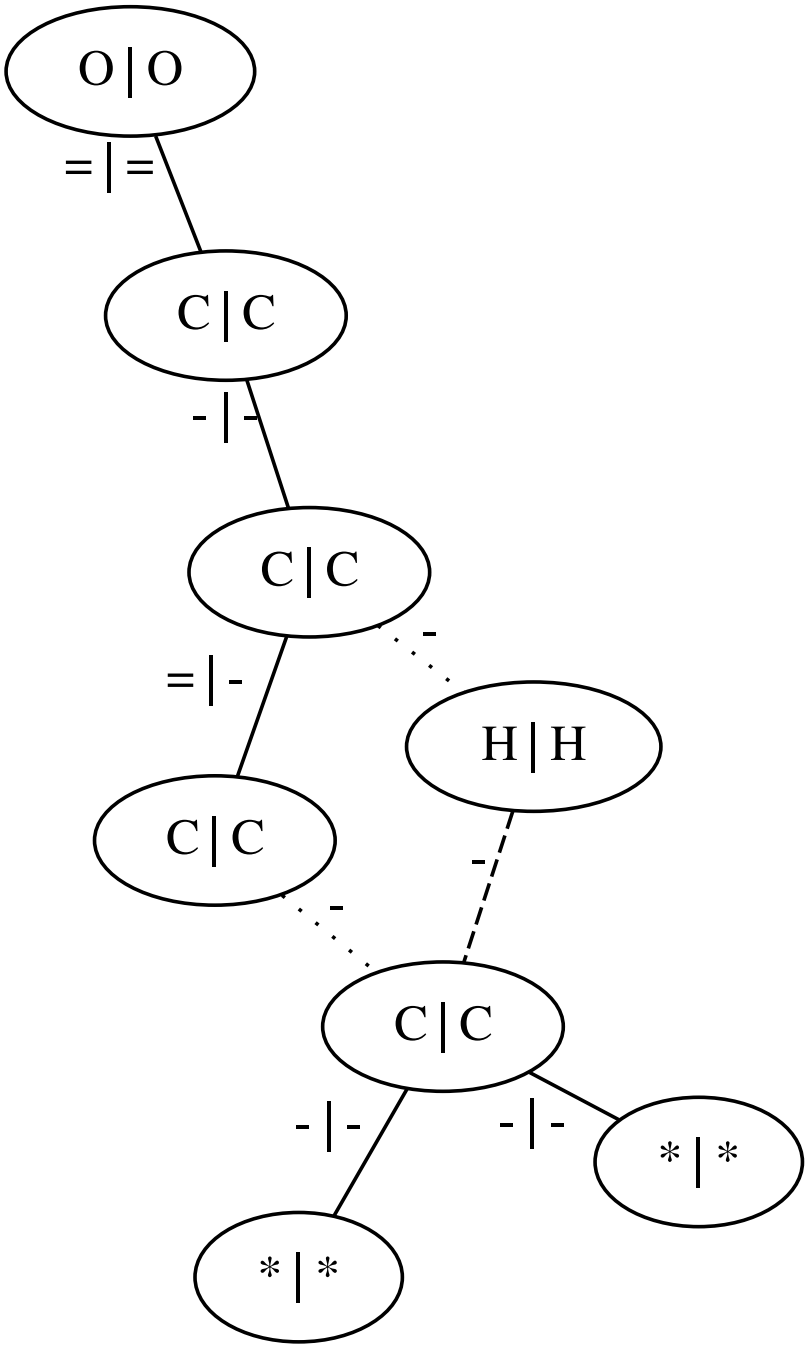
0.0.191 Michael Addition 0,2,



Files: out/950_r_193_10300000_{L, K, R}



Files: out/951_r_193_11300100_{L, K, R}



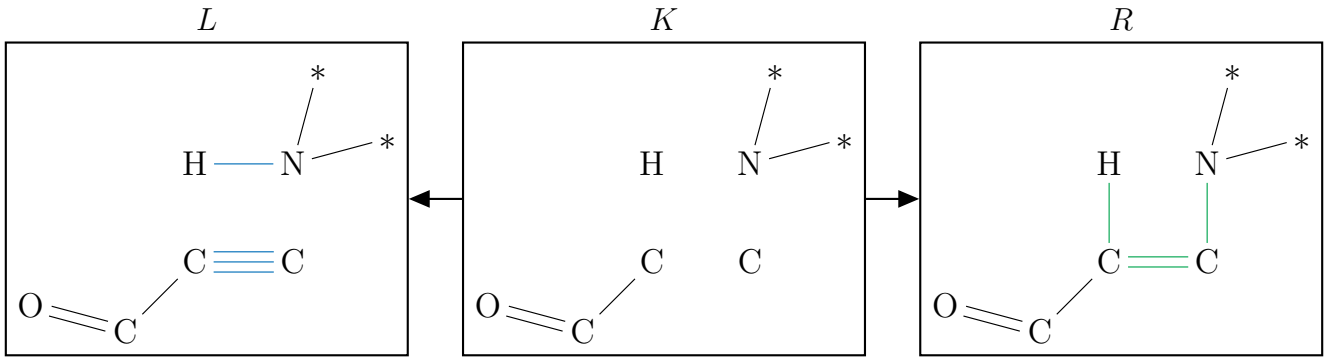
File: out/952_r_193_combined

$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

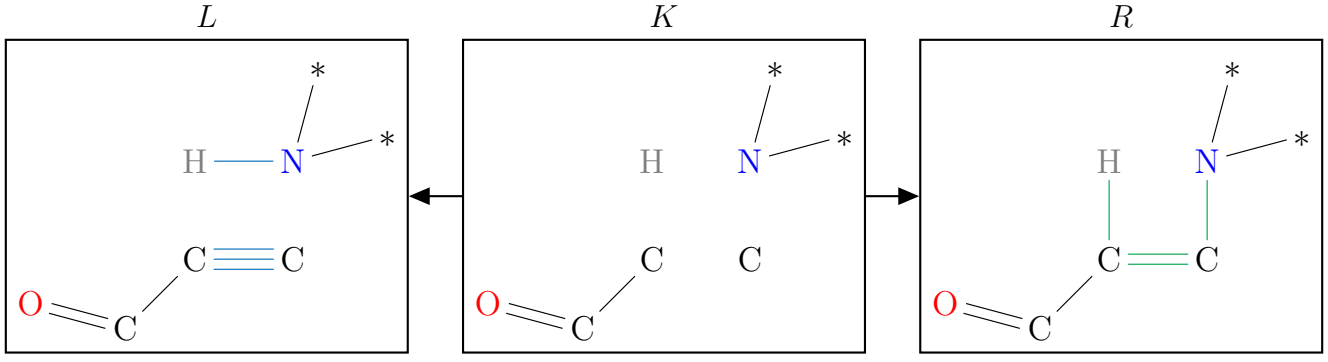
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`='}\}\}| = 0$$

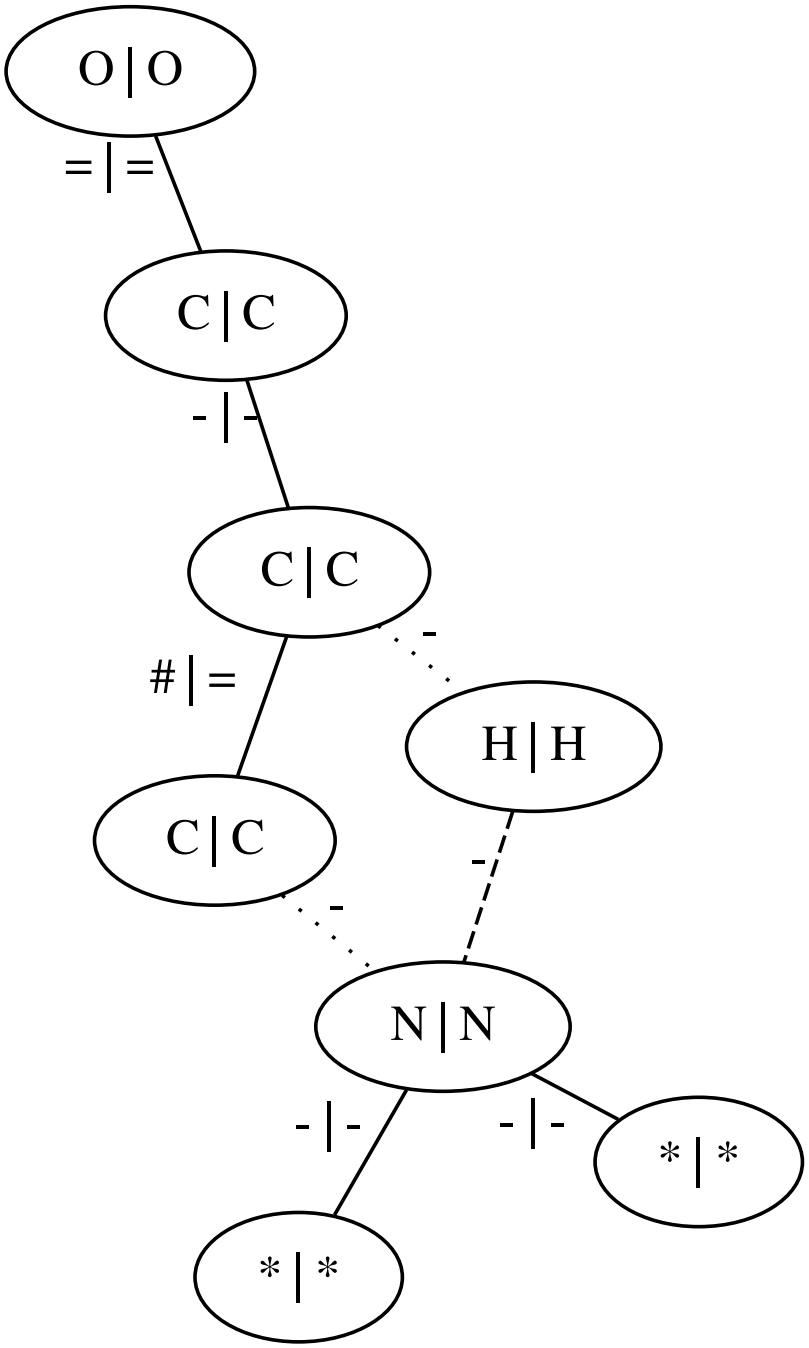
0.0.192 Michael Addition 1,0,



Files: out/955_r_194_10300000_{L, K, R}



Files: out/956_r_194_11300100_{L, K, R}



File: out/957_r_194_combined

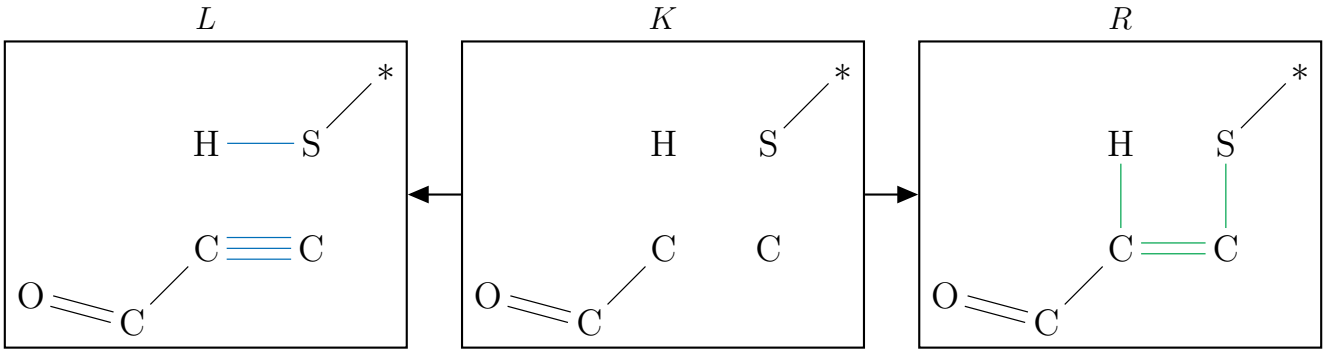
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

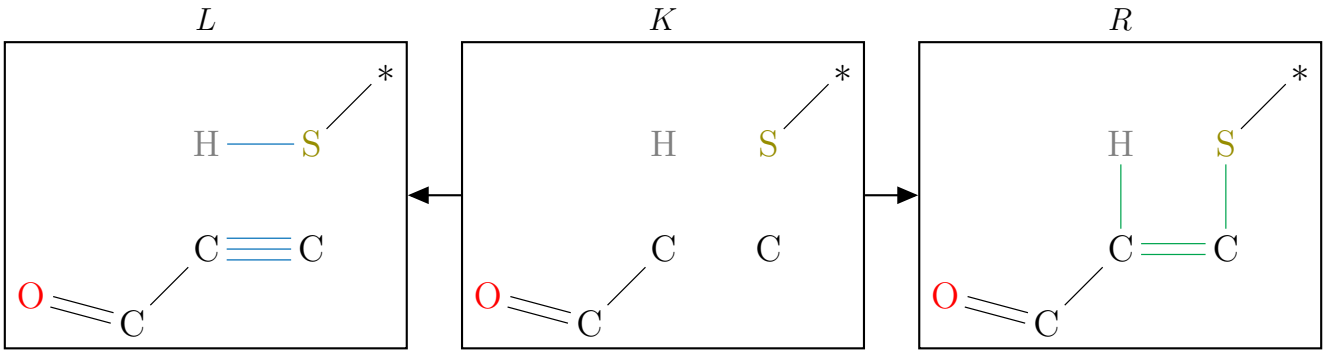
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

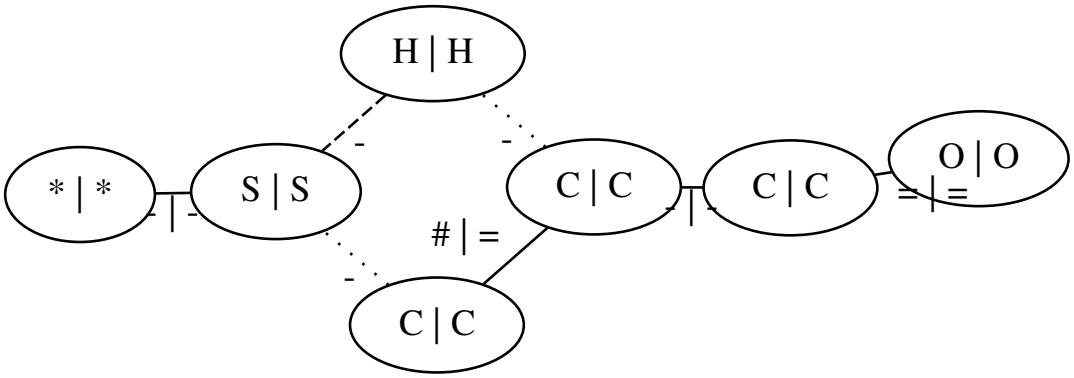
0.0.193 Michael Addition 1,1,



Files: out/960_r_195_10300000_{L, K, R}



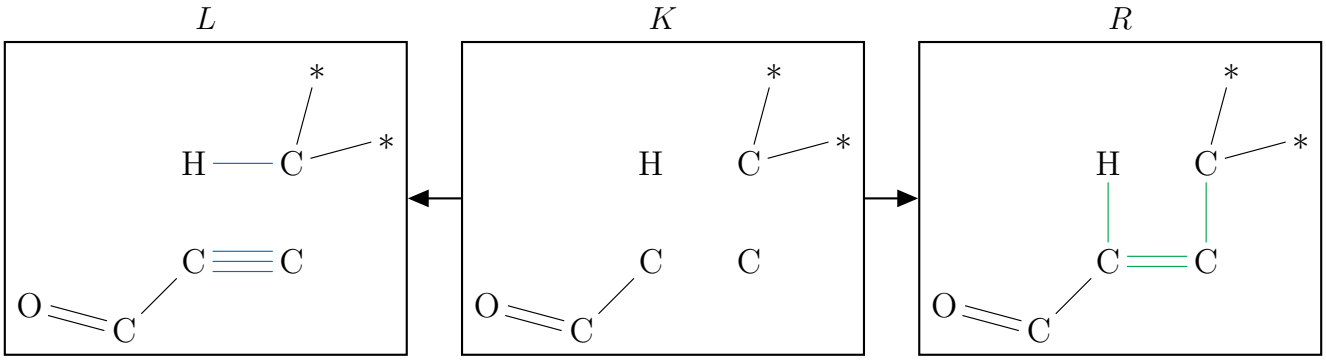
Files: out/961_r_195_11300100_{L, K, R}



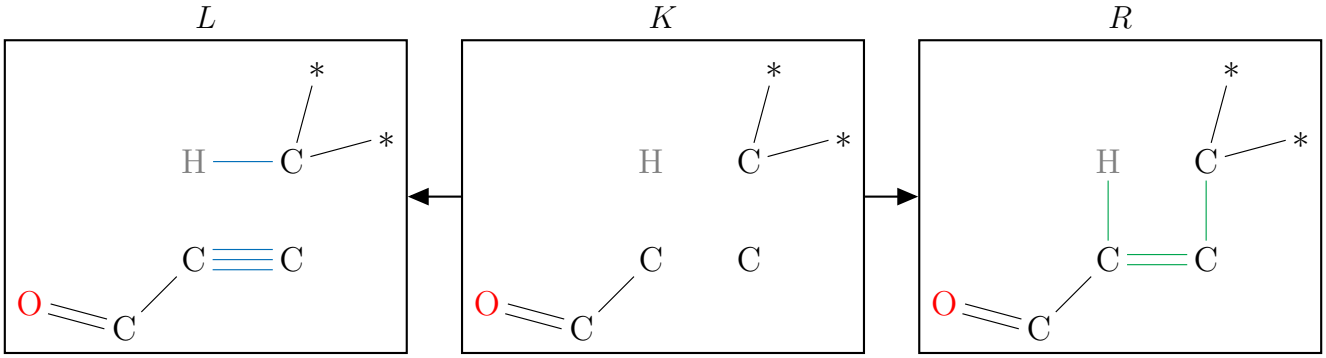
File: out/962_r_195_combined

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

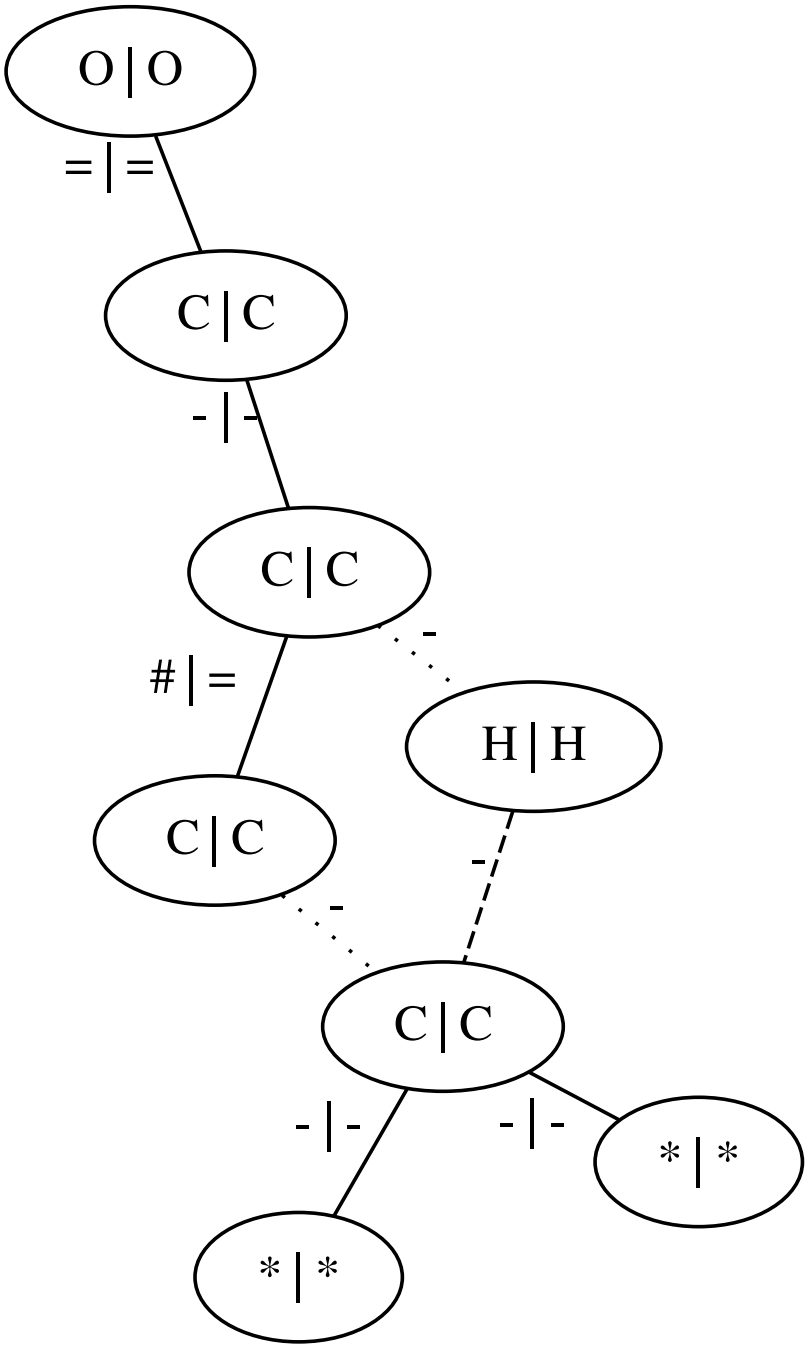
0.0.194 Michael Addition 1,2,



Files: out/965_r_196_10300000_{L, K, R}



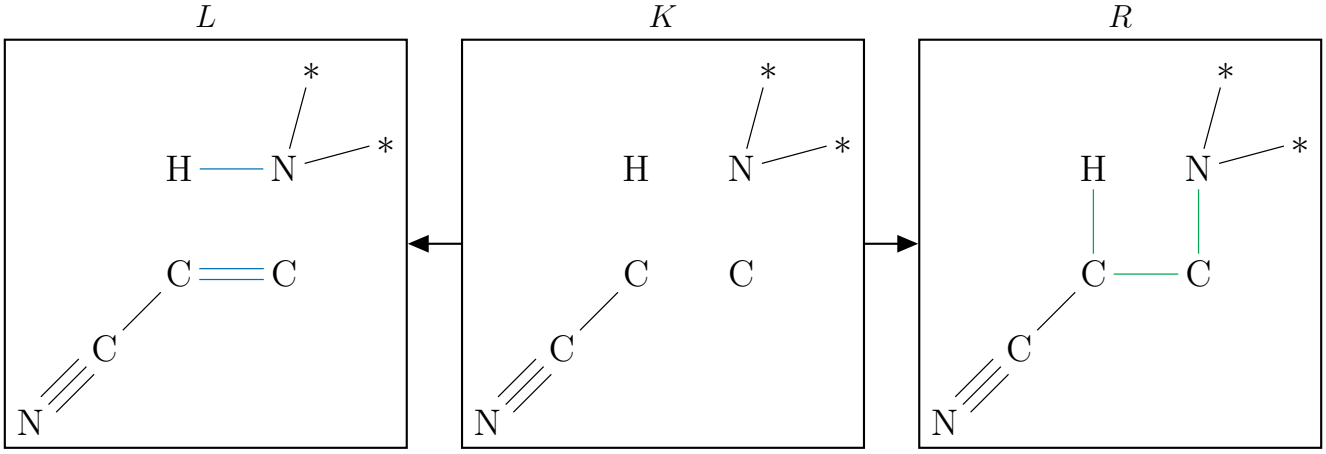
Files: out/966_r_196_11300100_{L, K, R}



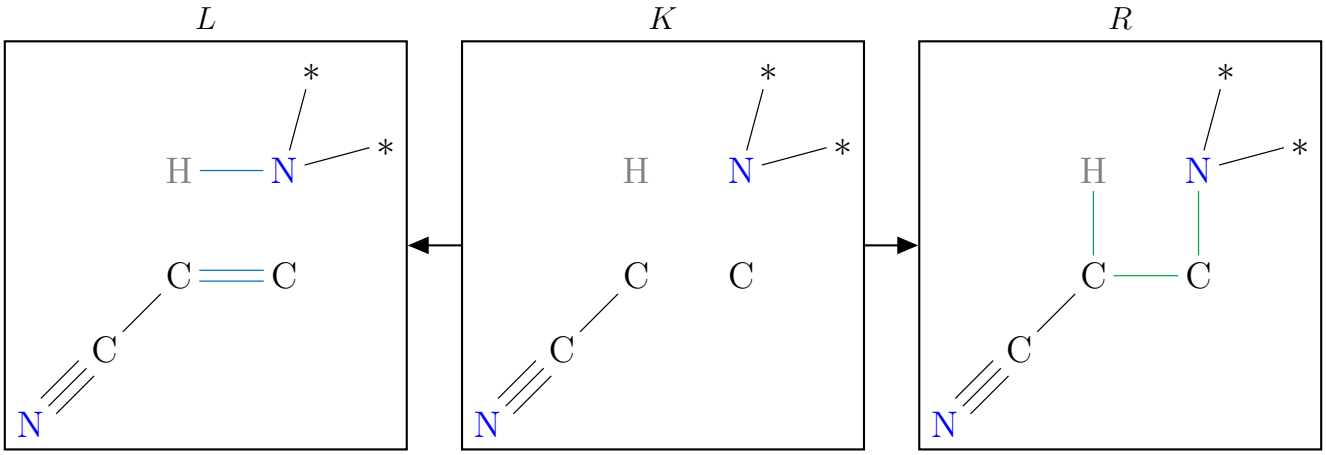
File: out/967_r_196_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 0
\end{aligned}
$$

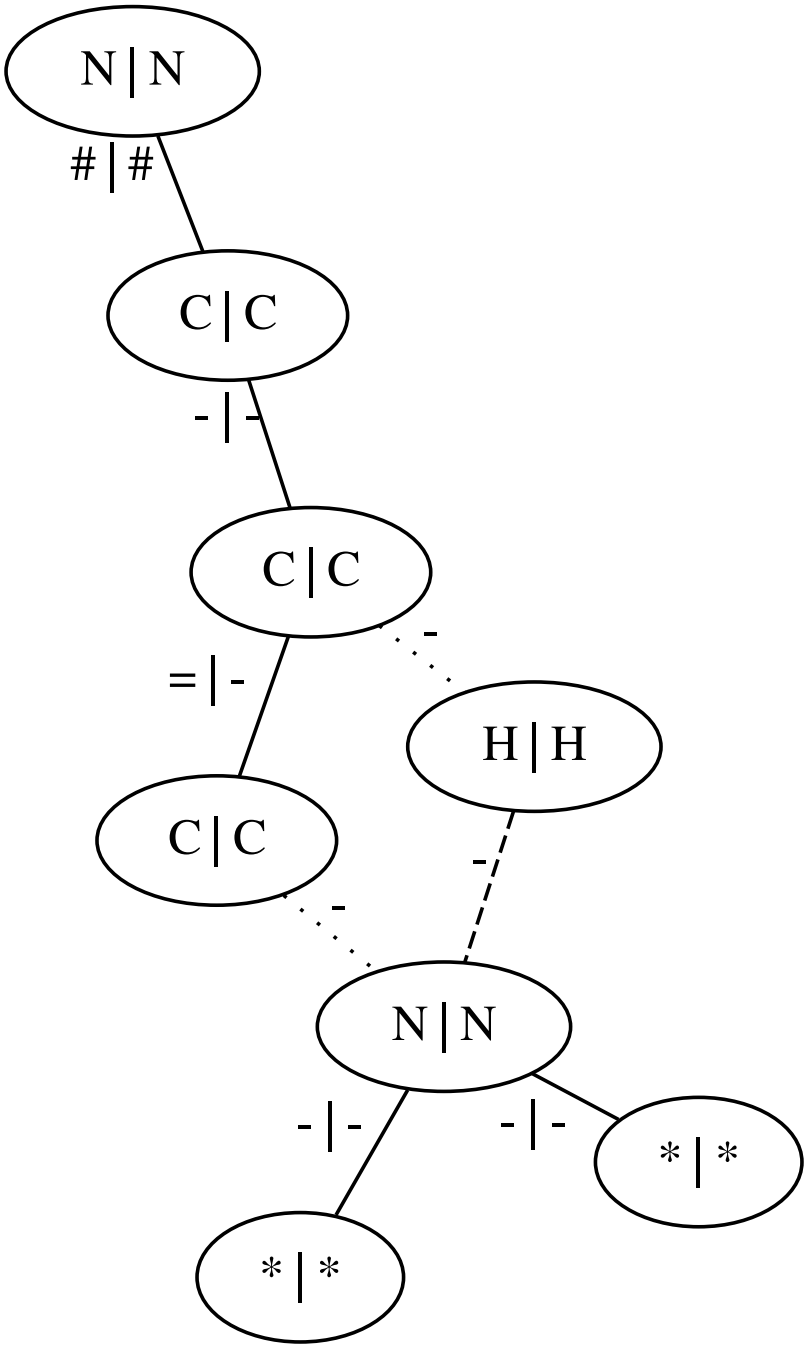
0.0.195 Michael Addition 2,0,



Files: out/970_r_197_10300000_{L, K, R}



Files: out/971_r_197_11300100_{L, K, R}



File: out/972_r_197_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

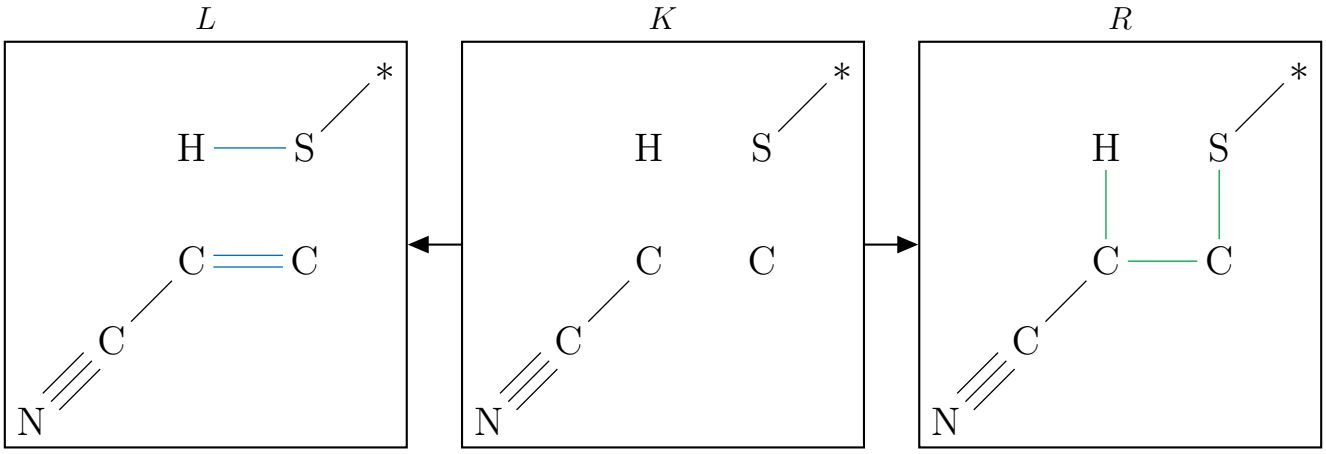
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

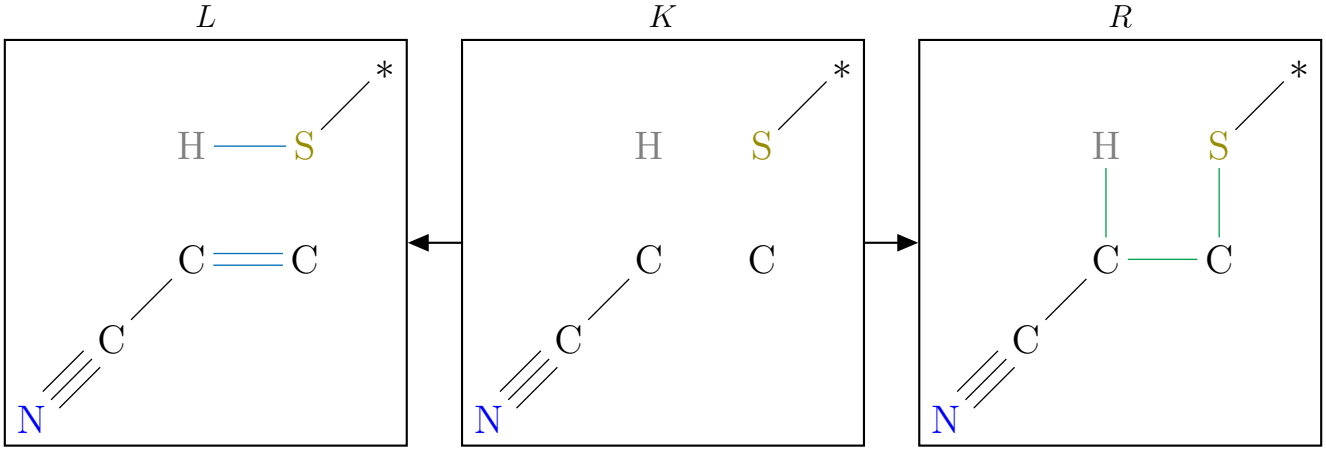
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

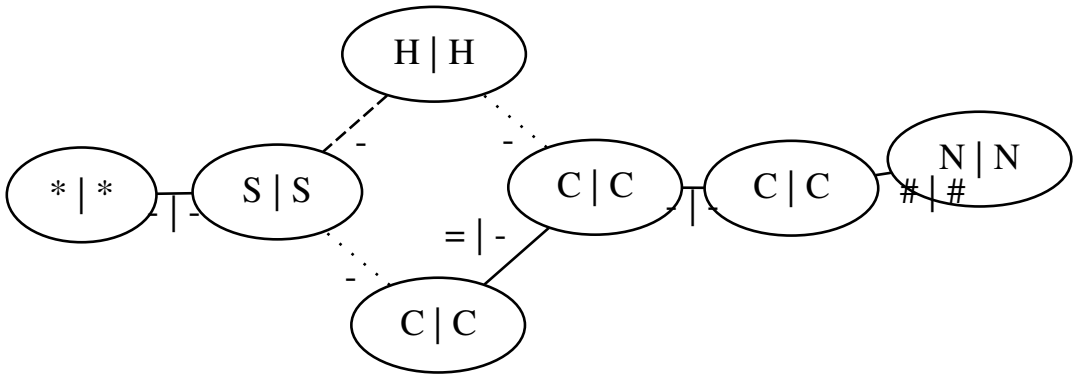
0.0.196 Michael Addition 2,1,



Files: out/975_r_198_10300000_{L, K, R}



Files: out/976_r_198_11300100_{L, K, R}



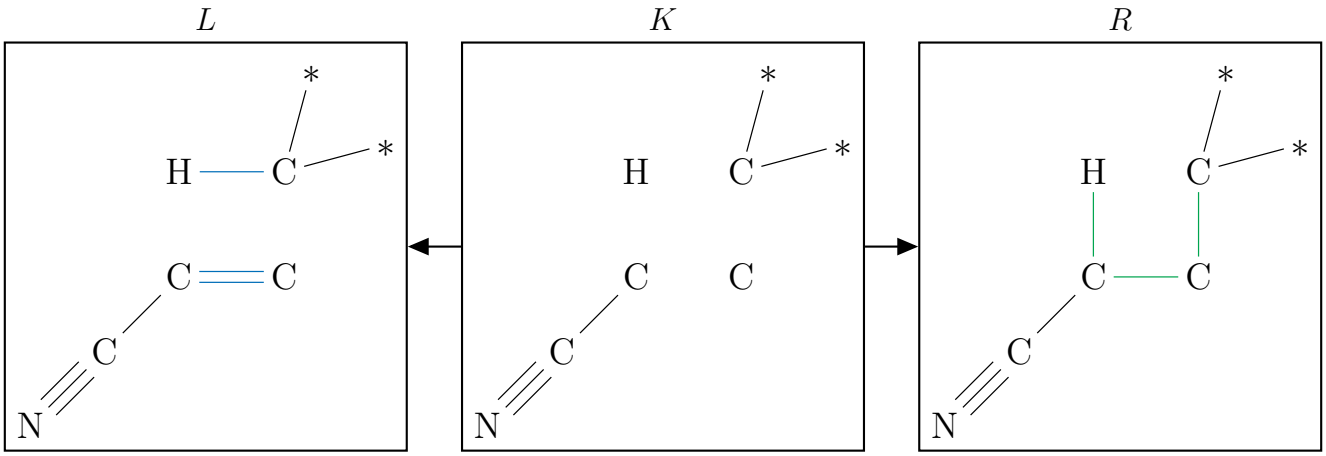
File: out/977_r_198_combined

$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

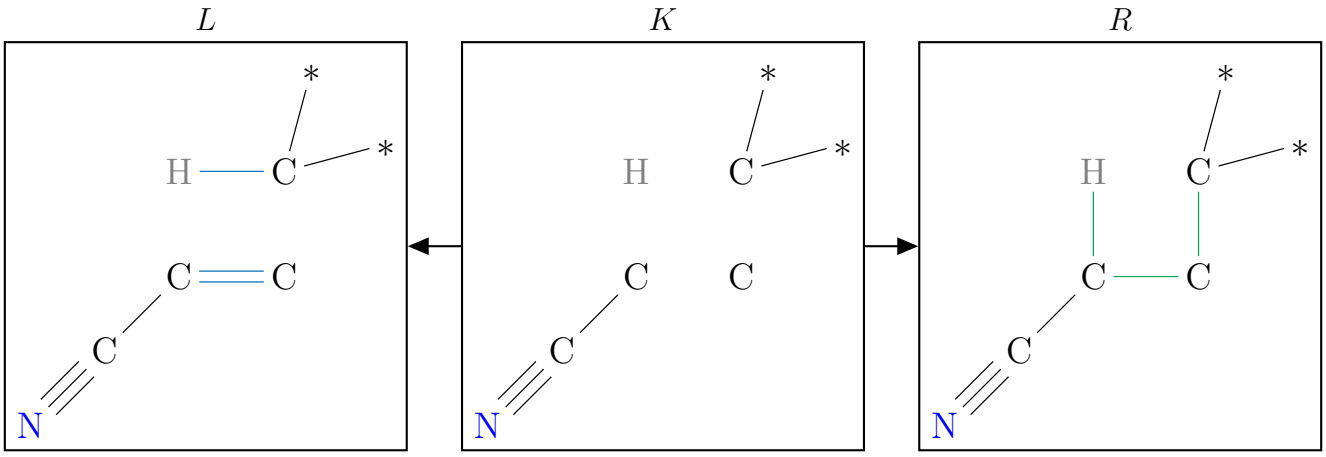
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

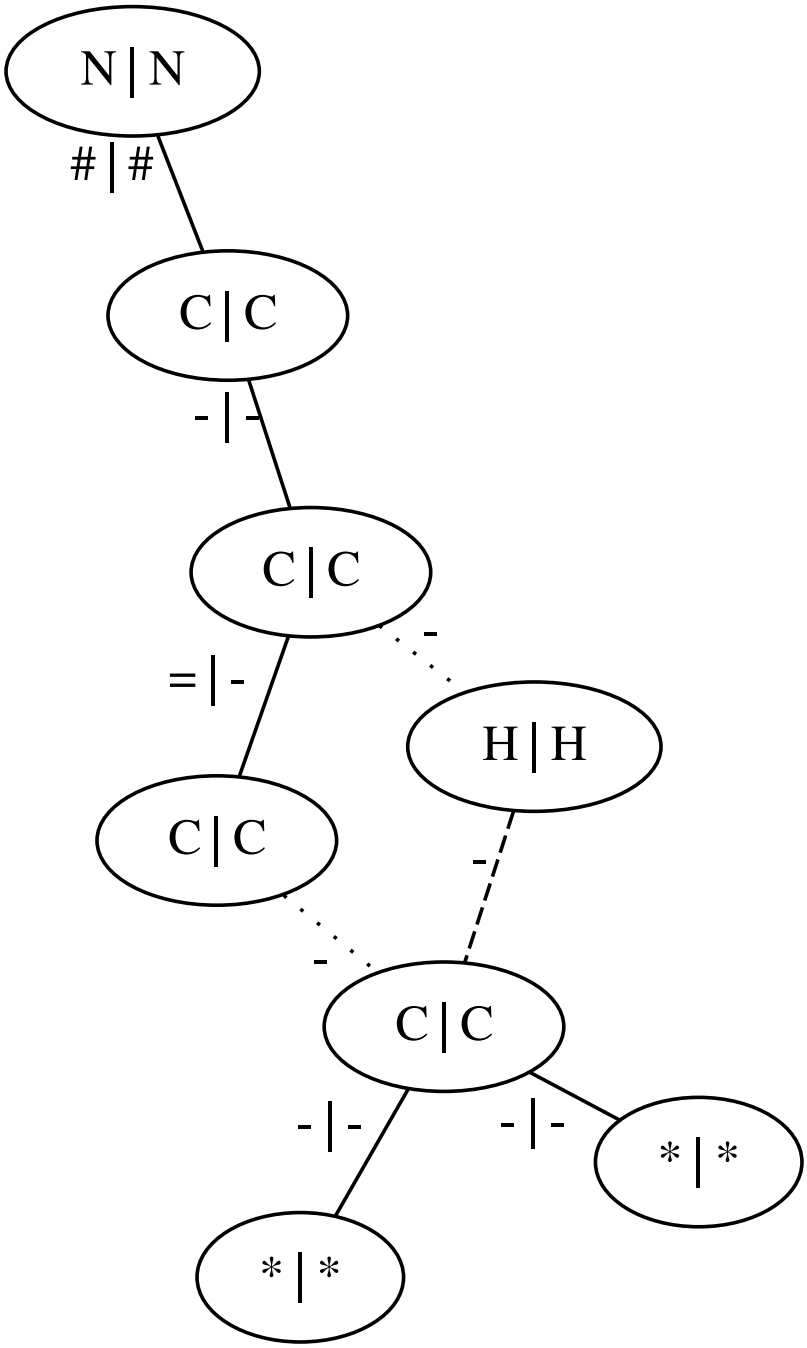
0.0.197 Michael Addition 2,2,



Files: out/980_r_199_10300000_{L, K, R}



Files: out/981_r_199_11300100_{L, K, R}



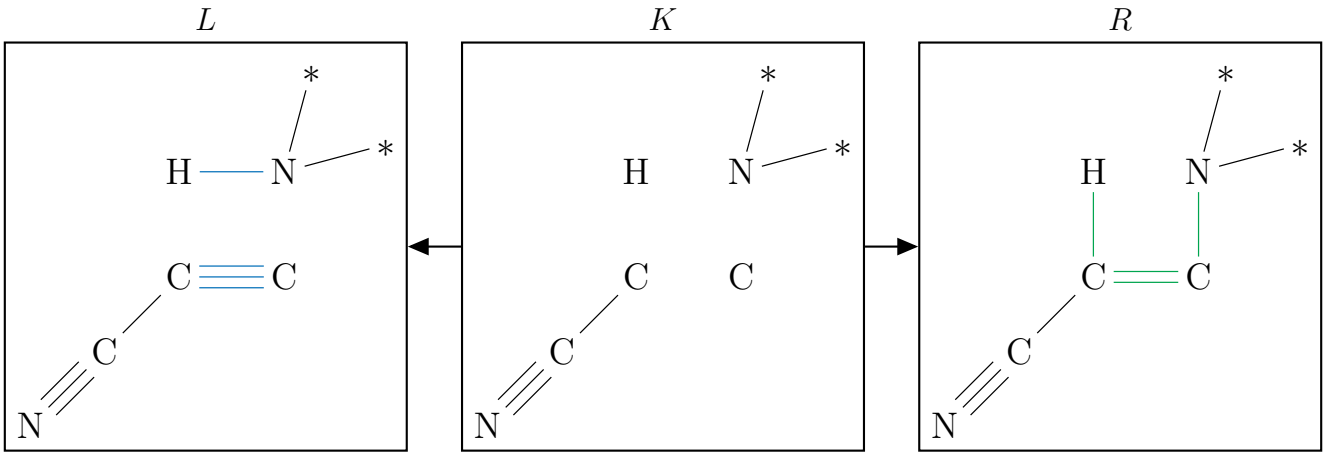
File: out/982_r_199_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

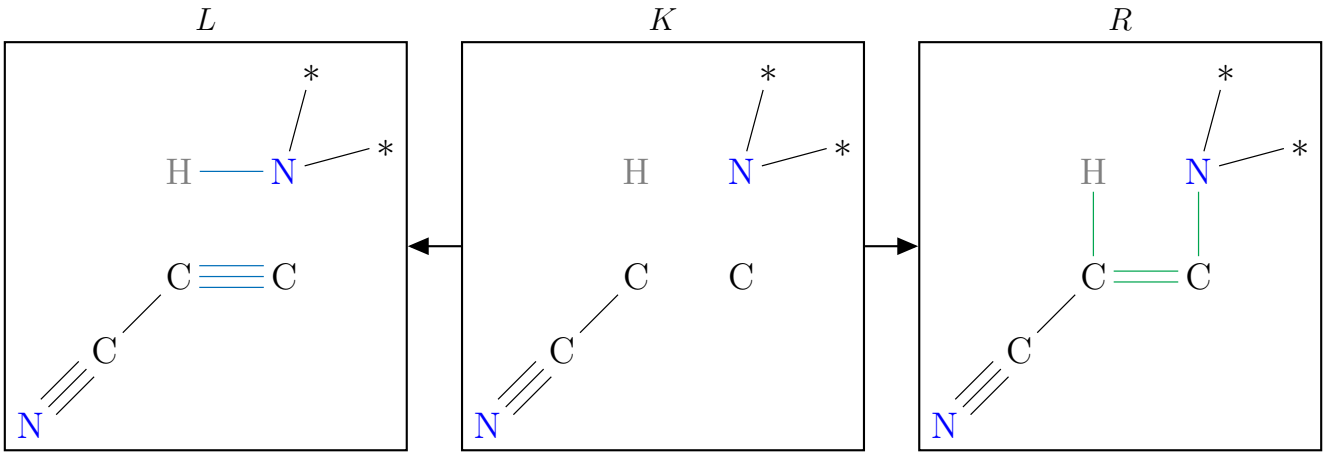
$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 0
\end{aligned}
$$

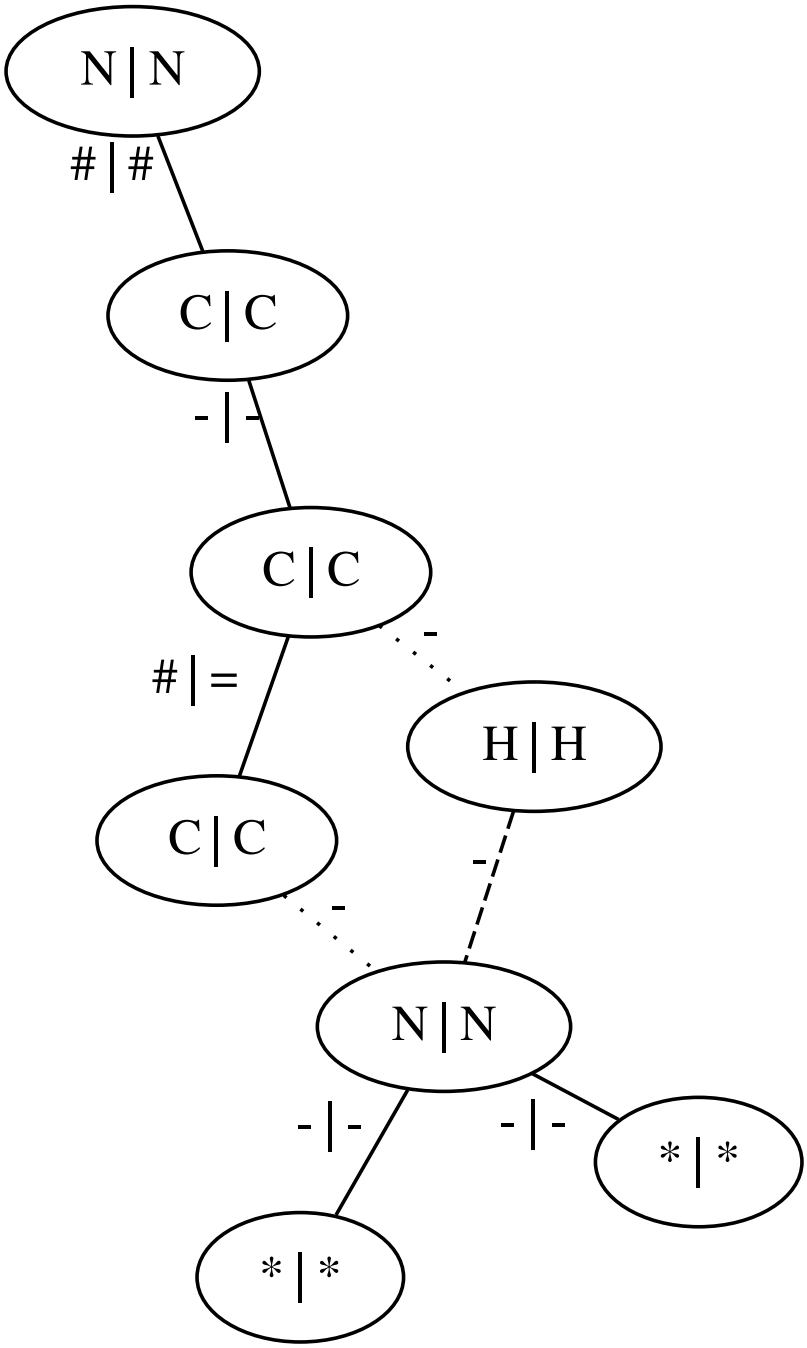
0.0.198 Michael Addition 3,0,



Files: out/985_r_200_10300000_{L, K, R}



Files: out/986_r_200_11300100_{L, K, R}



File: out/987_r_200_combined

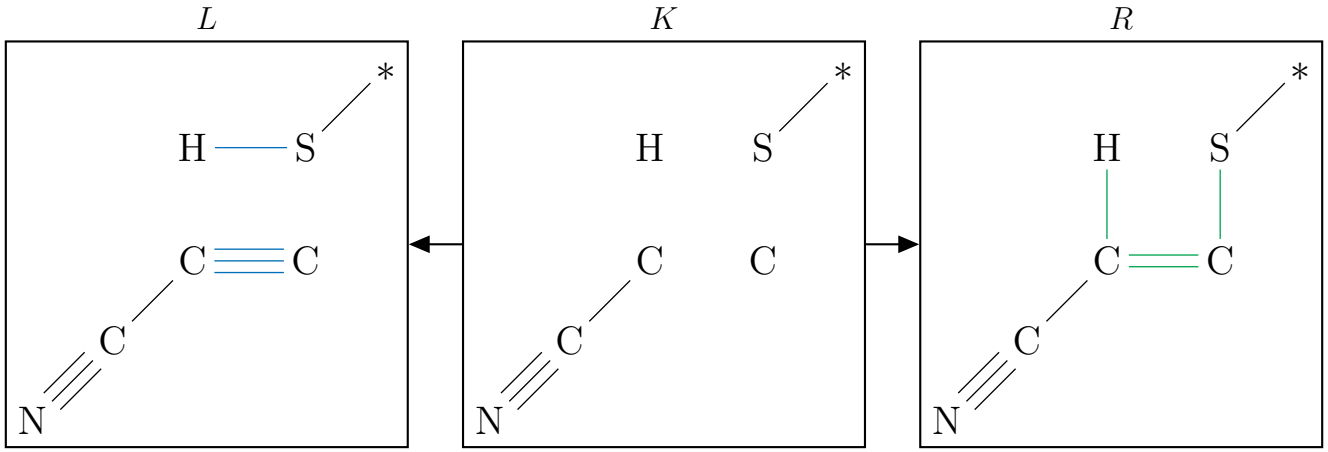
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

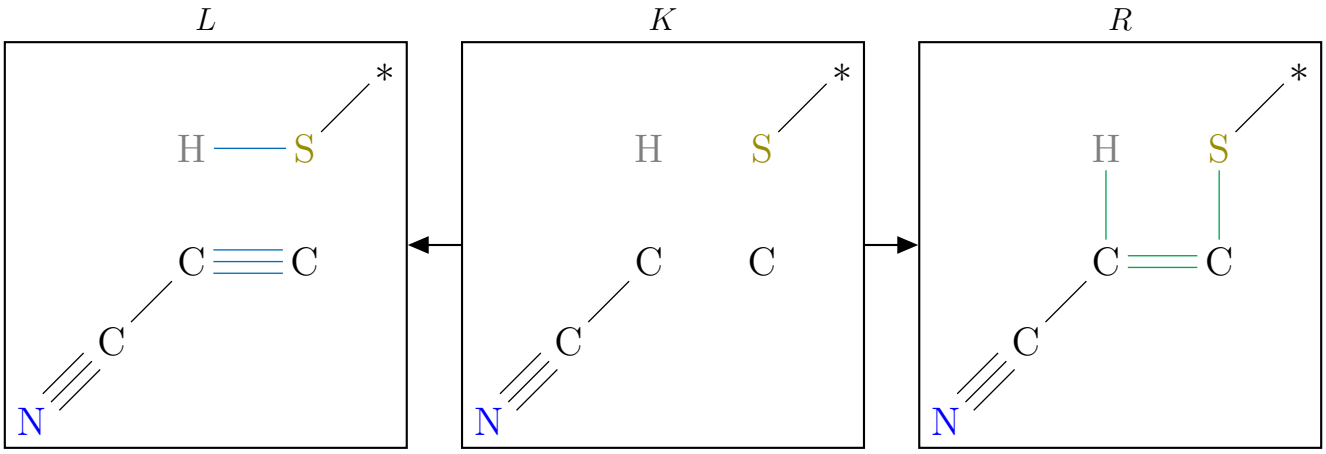
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

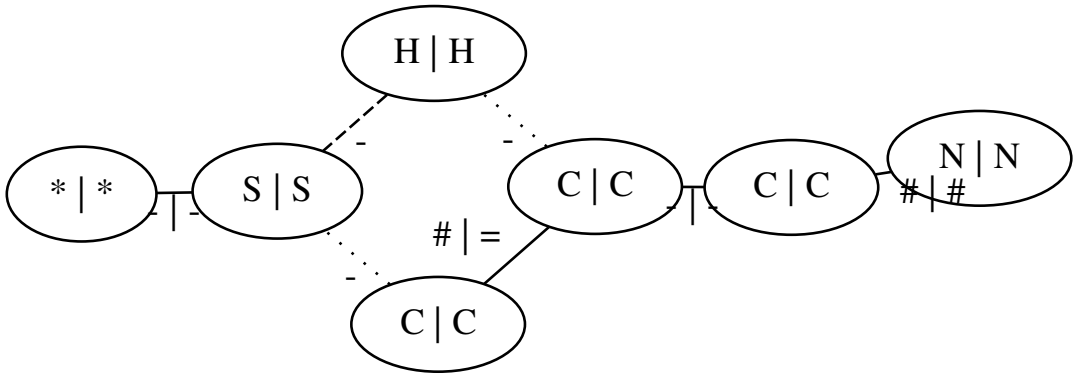
0.0.199 Michael Addition 3,1,



Files: out/990_r_201_10300000_{L, K, R}



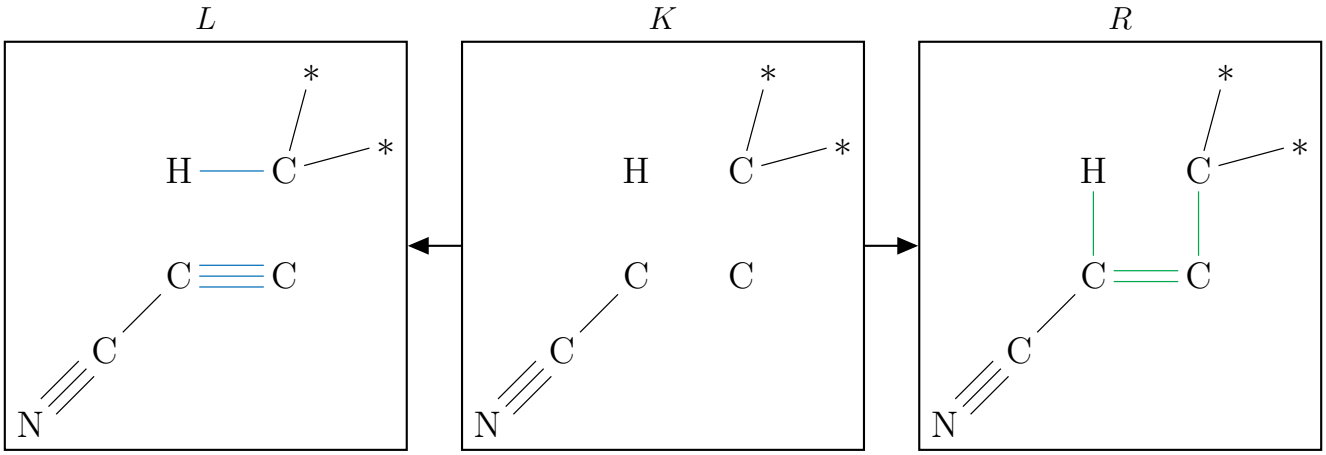
Files: out/991_r_201_11300100_{L, K, R}



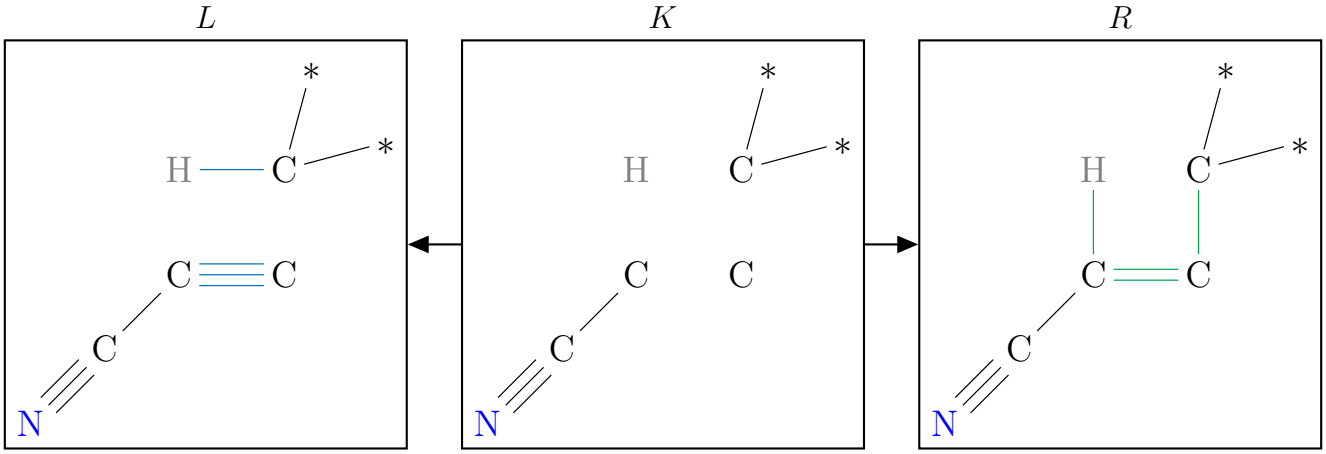
File: out/992_r_201_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

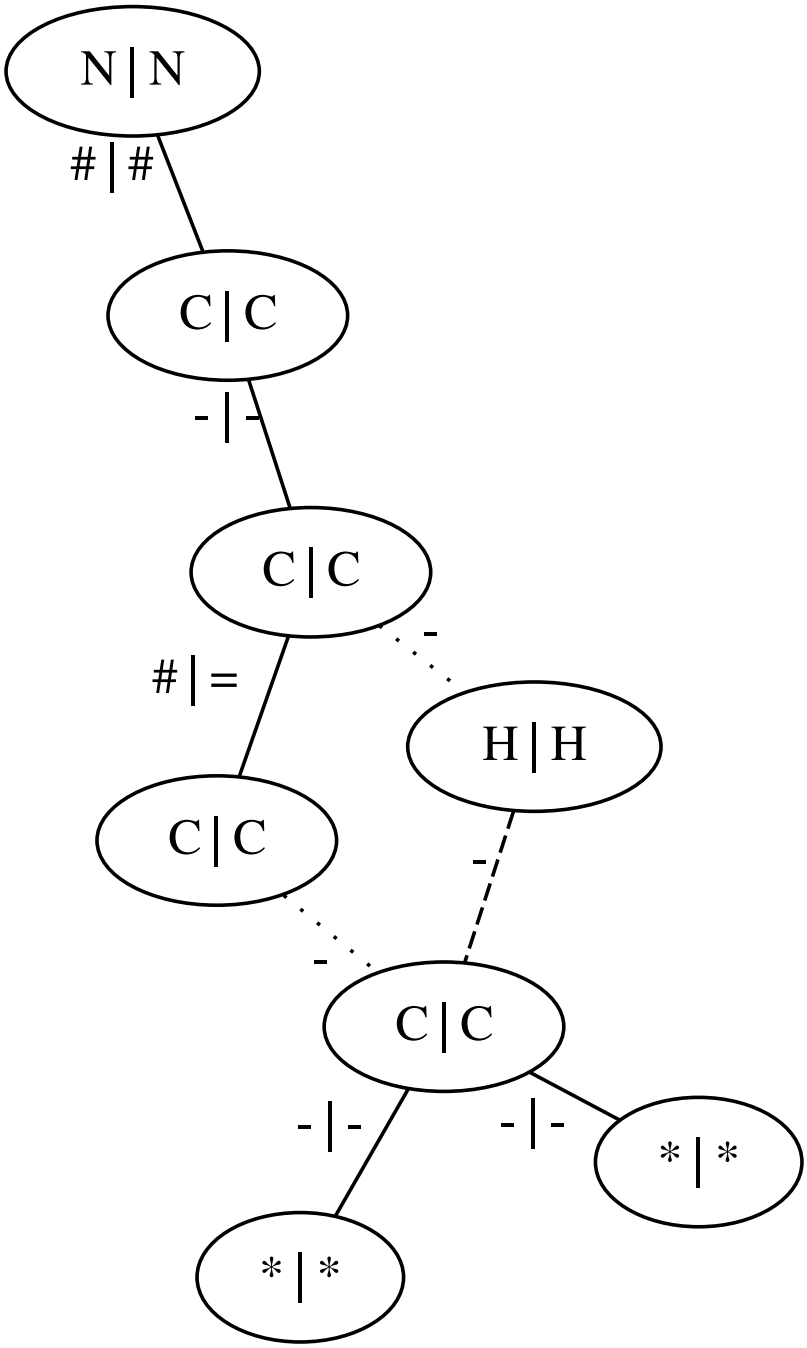
0.0.200 Michael Addition 3,2,



Files: out/995_r_202_10300000_{L, K, R}



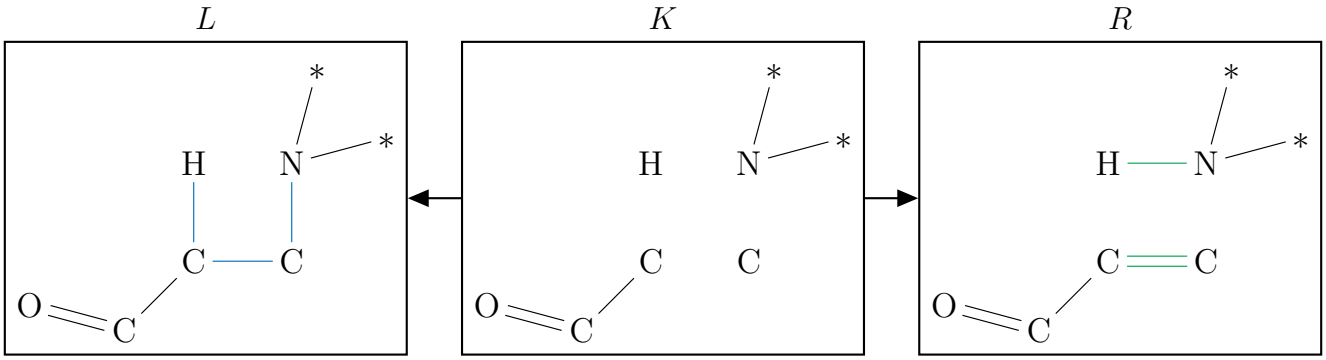
Files: out/996_r_202_11300100_{L, K, R}



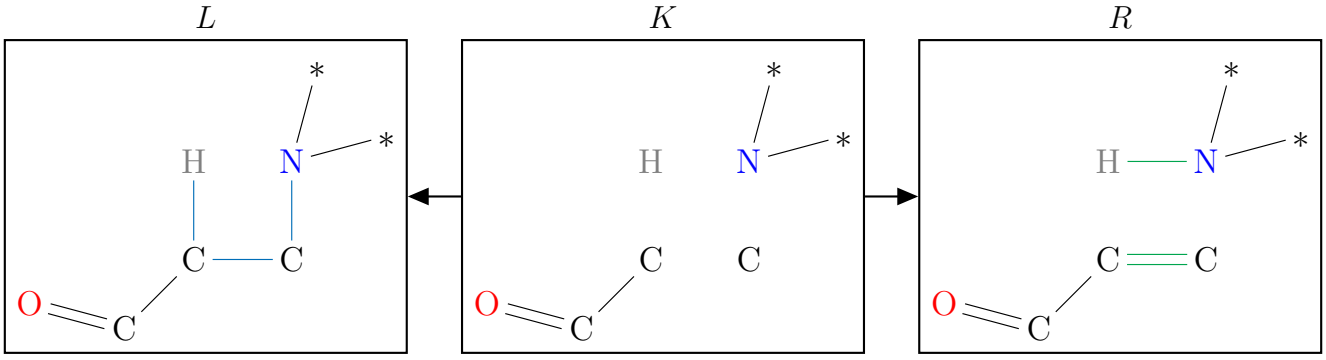
File: out/997_r_202_combined

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \wedge \text{label}(e) \in \{\text{`\#'}, \text{`='}\}\}| = 0$$

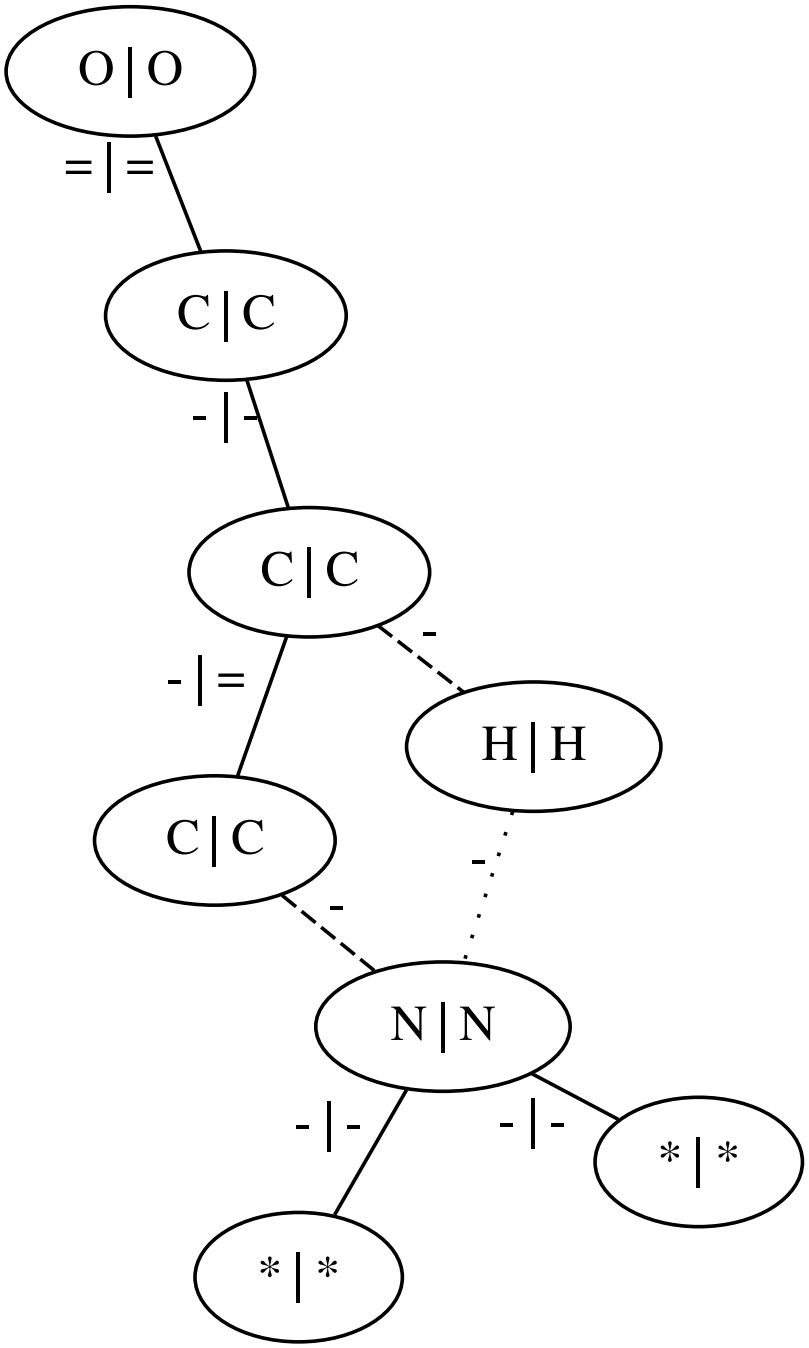
0.0.201 Michael Addition 0,0, (reverse)



Files: out/1000_r_203_10300000_{L, K, R}



Files: out/1001_r_203_11300100_{L, K, R}



File: out/1002_r_203_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

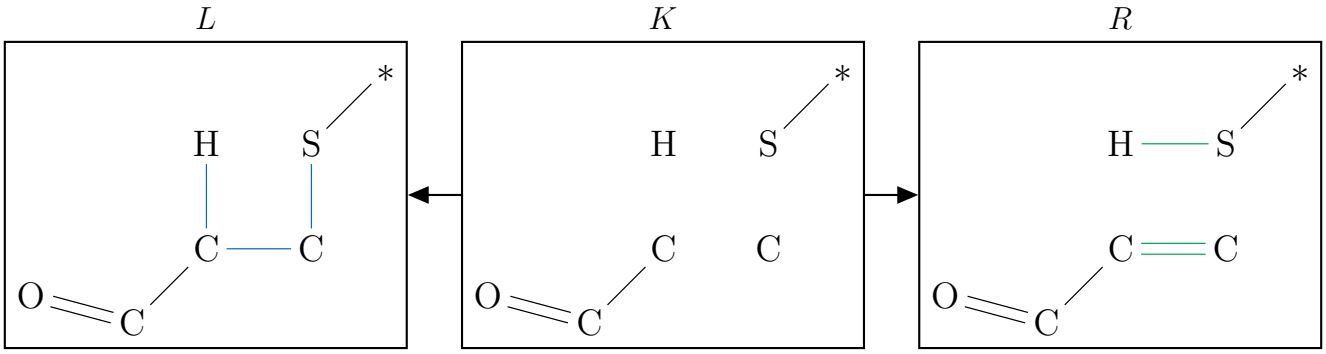
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

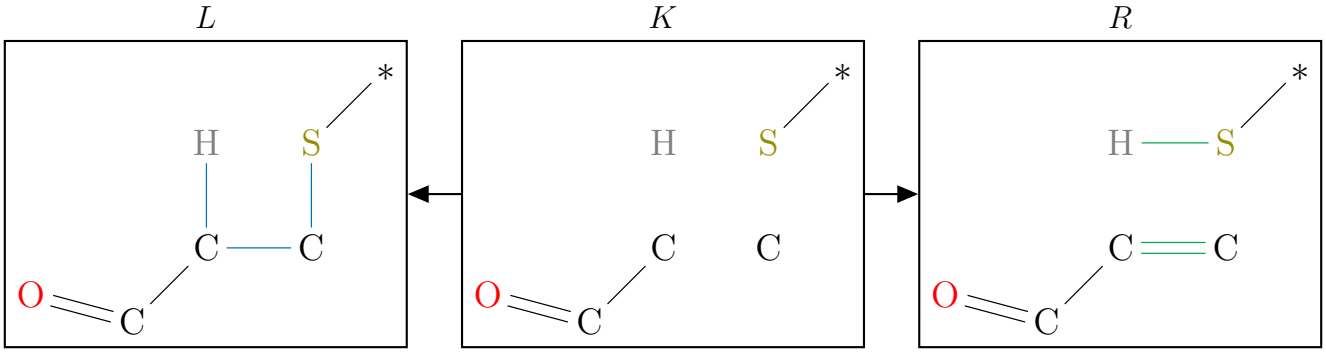
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

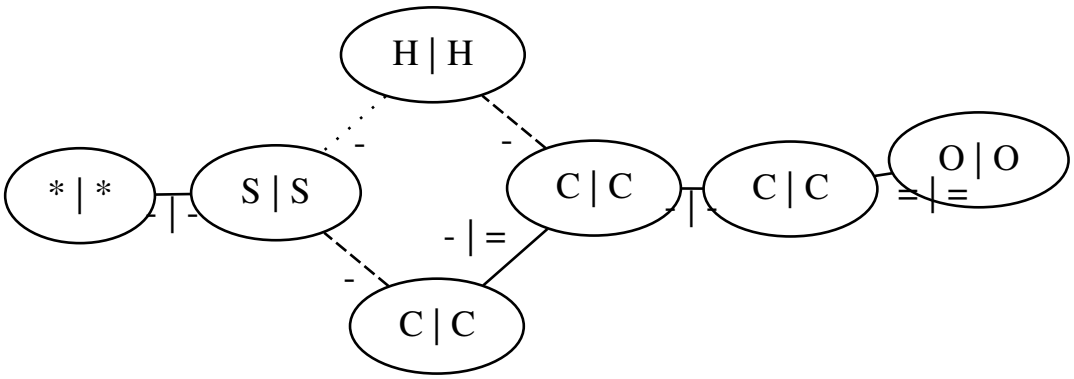
0.0.202 Michael Addition 0,1, (reverse)



Files: out/1005_r_204_10300000_{L, K, R}



Files: out/1006_r_204_11300100_{L, K, R}



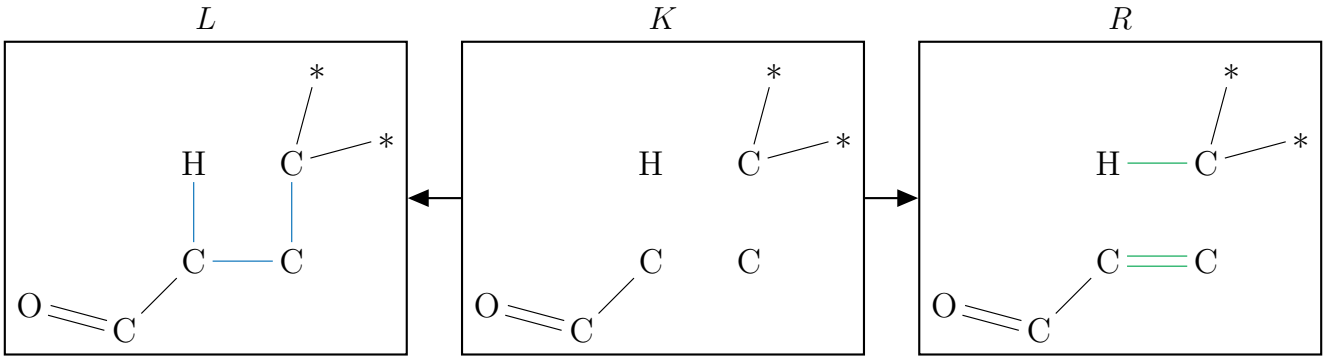
File: out/1007_r_204_combined

$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

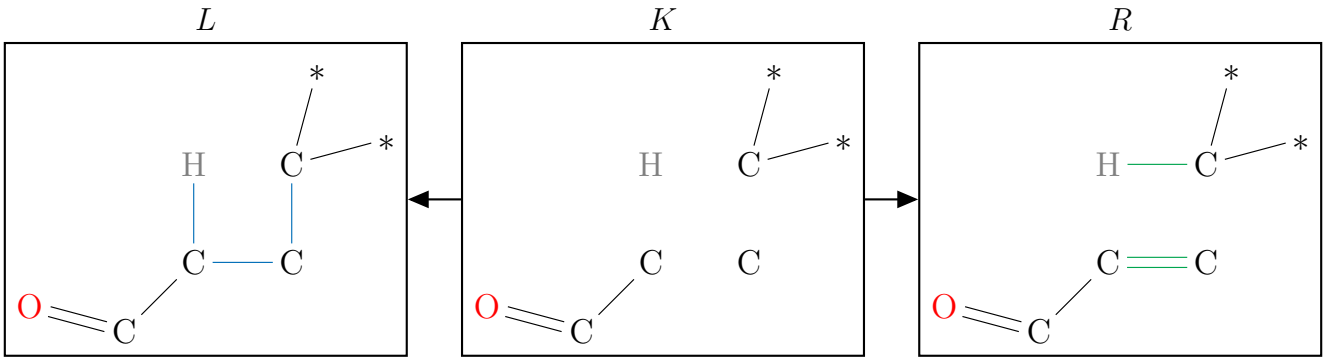
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`-'}\}\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\} \wedge \text{label}(e) \in \{\text{`='}\}\}| = 0$$

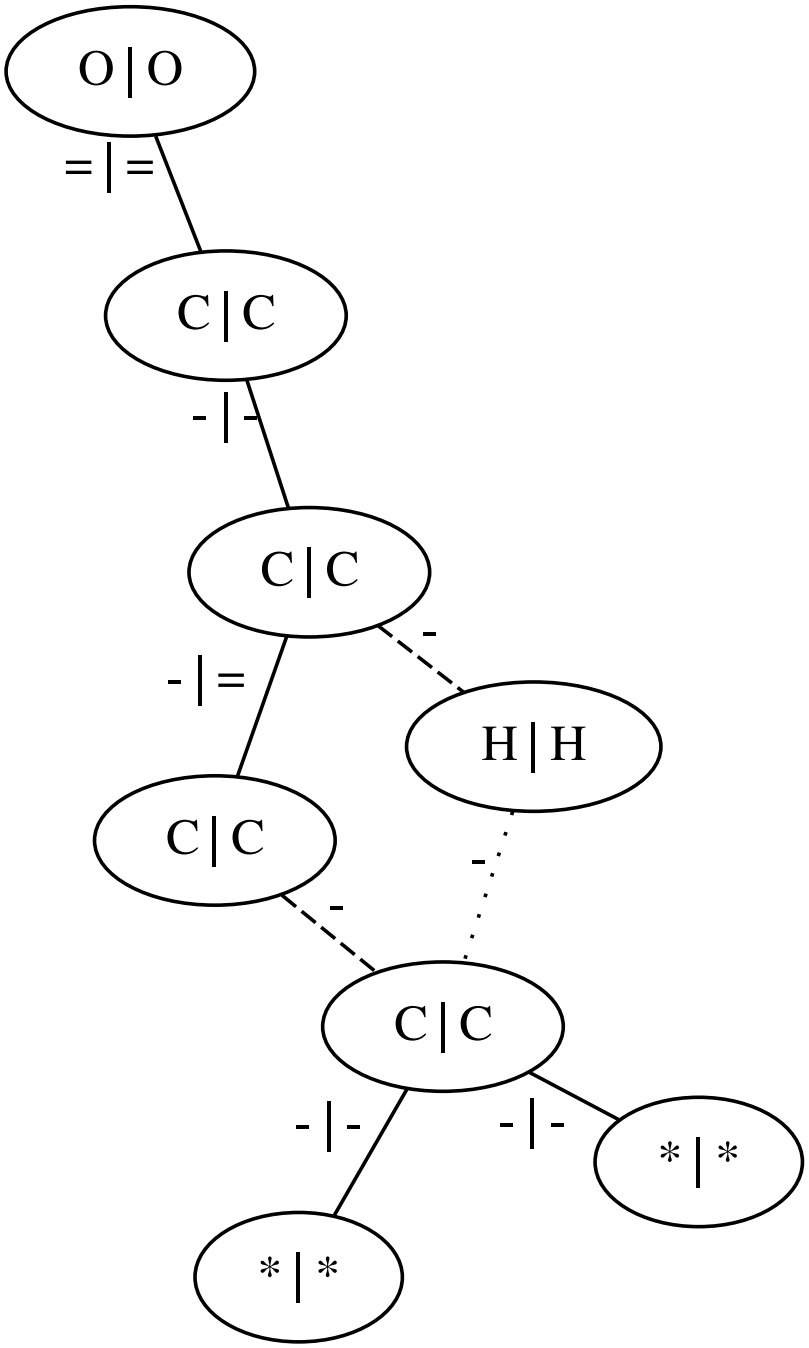
0.0.203 Michael Addition 0,2, (reverse)



Files: out/1010_r_205_10300000_{L, K, R}



Files: out/1011_r_205_11300100_{L, K, R}



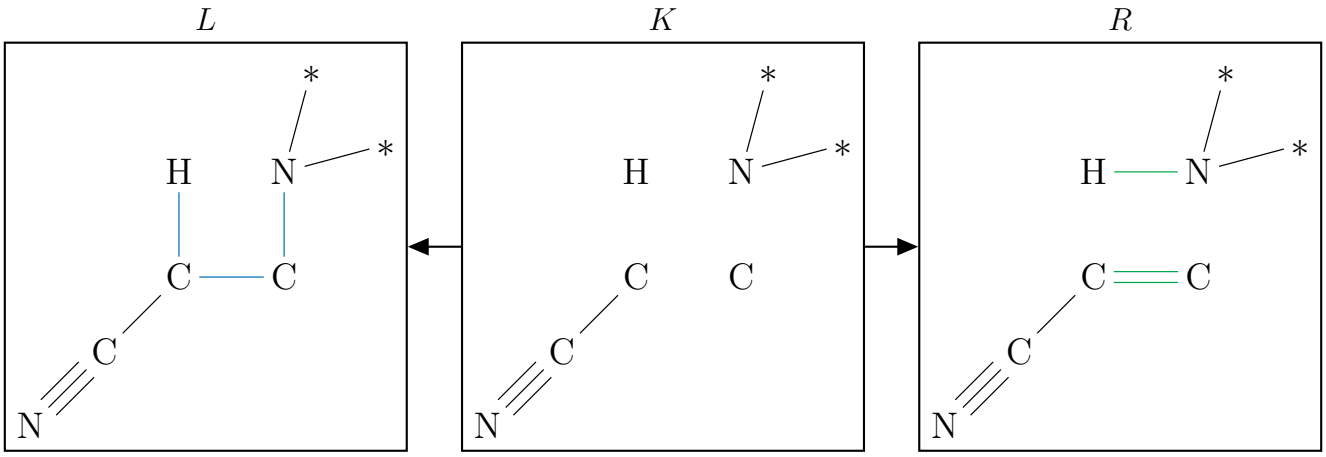
File: out/1012_r_205_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

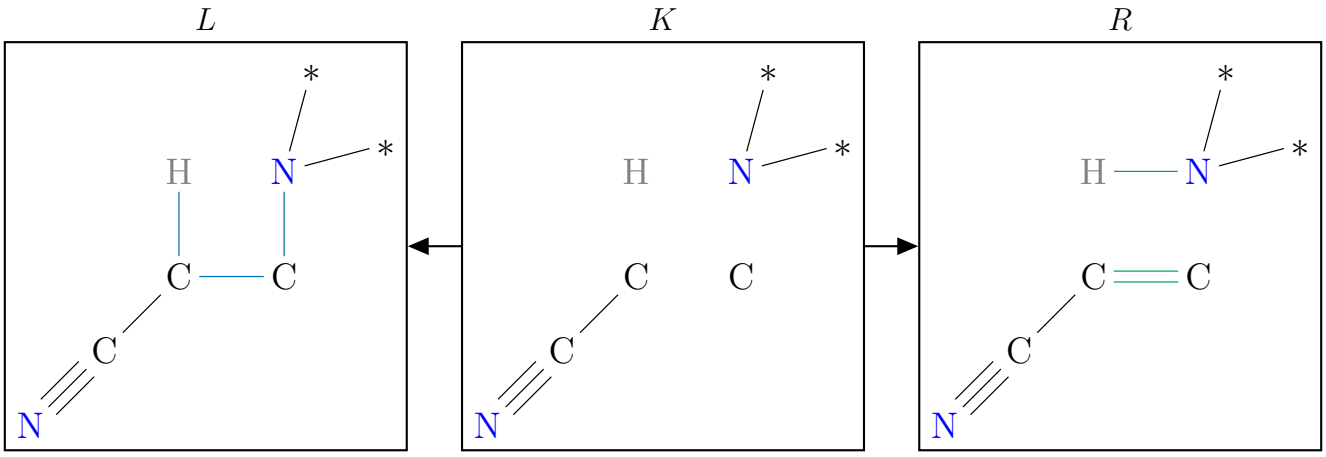
$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 0
\end{aligned}
$$

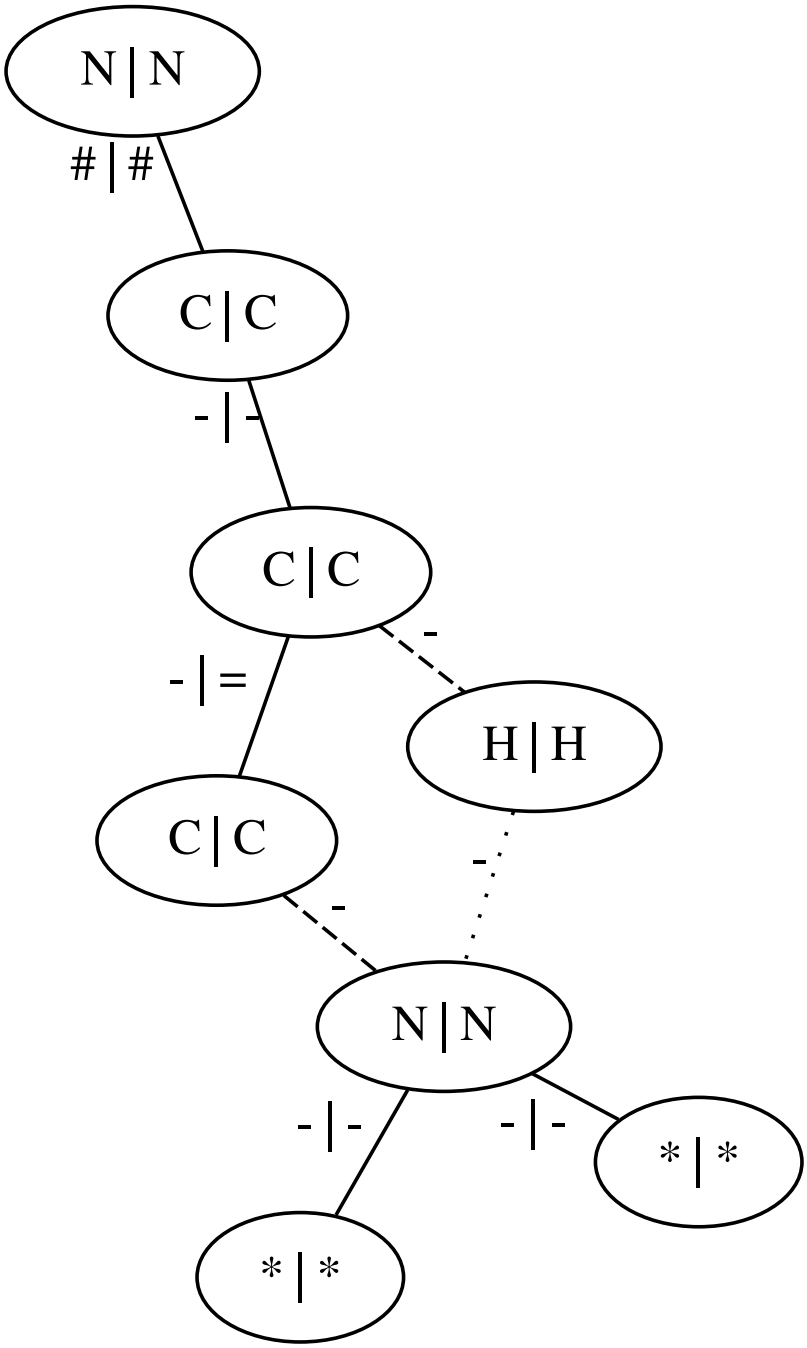
0.0.204 Michael Addition 2,0, (reverse)



Files: out/1015_r_206_10300000_{L, K, R}



Files: out/1016_r_206_11300100_{L, K, R}



File: out/1017_r_206_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

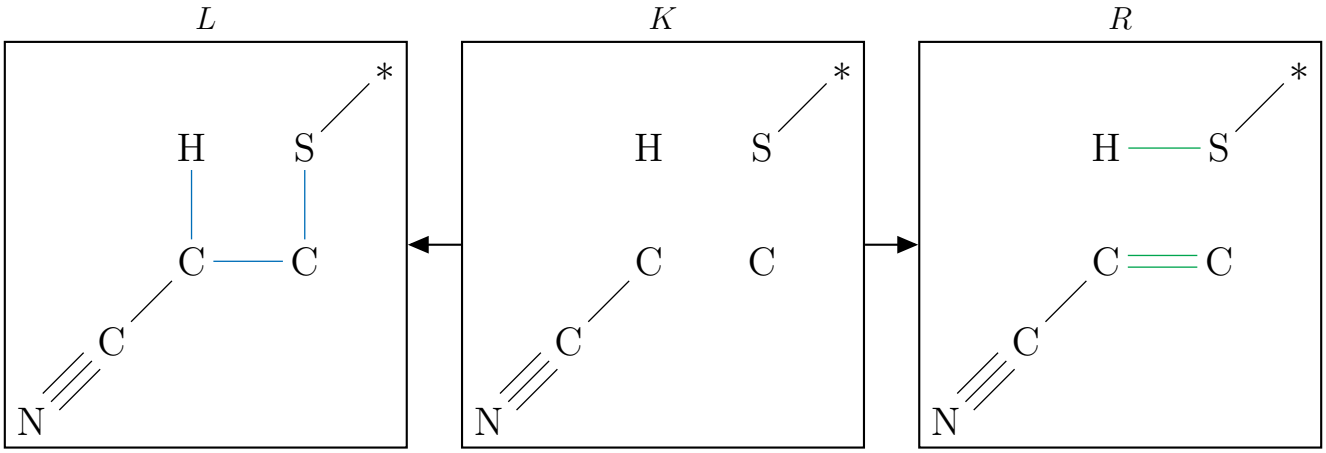
$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

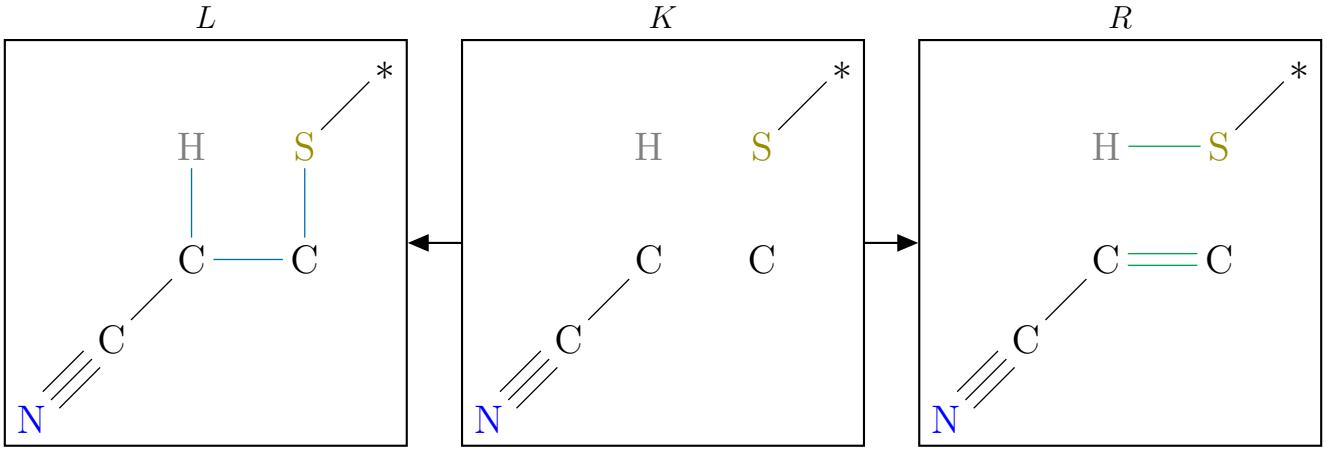
$$
\begin{aligned}
&|\{e \in \text{outEdges}(7) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(5) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`S'}, \text{`O'}, \text{`N'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

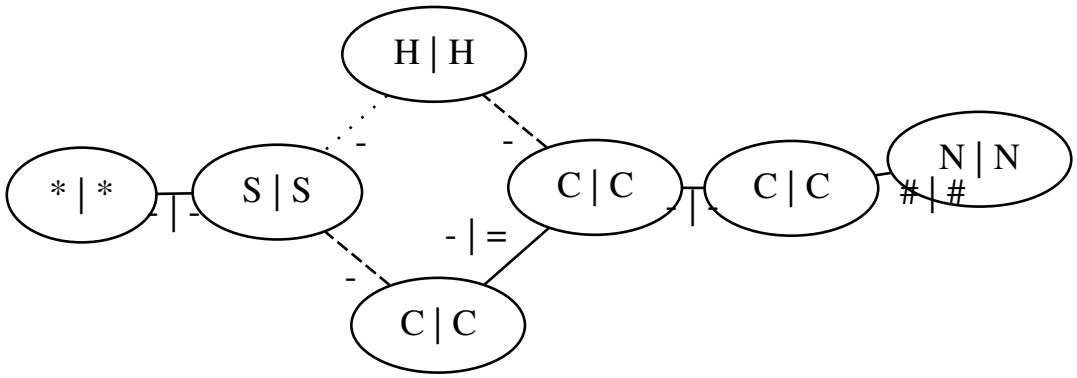
0.0.205 Michael Addition 2,1, (reverse)



Files: out/1020_r_207_10300000_{L, K, R}



Files: out/1021_r_207_11300100_{L, K, R}



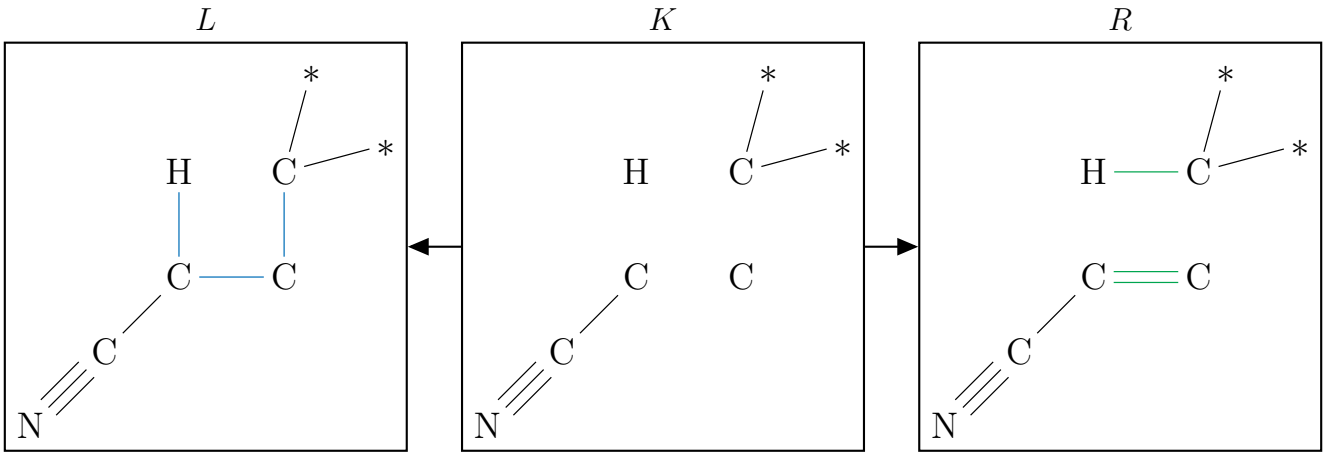
File: out/1022_r_207_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

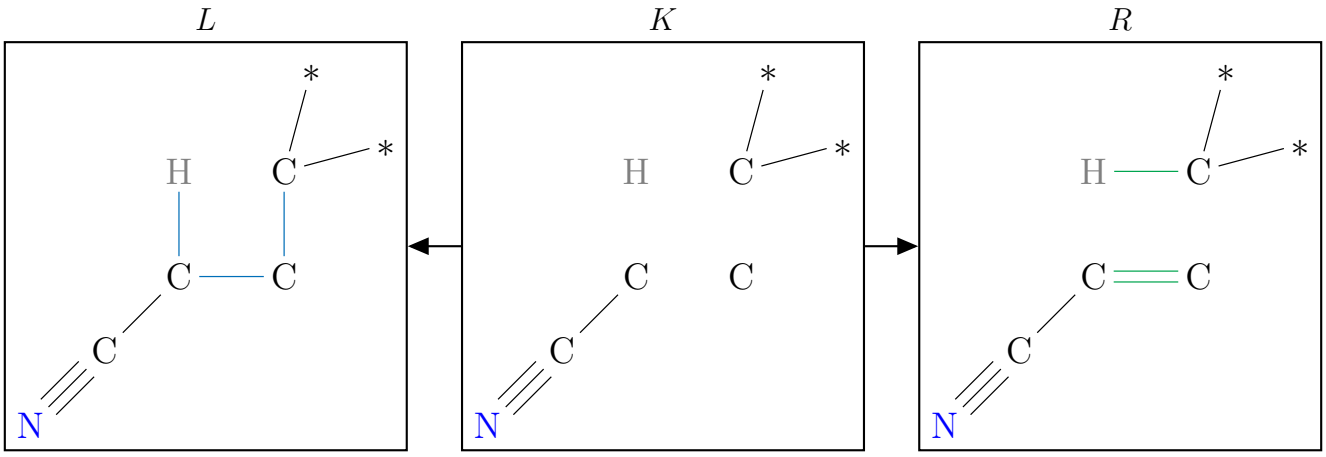
$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

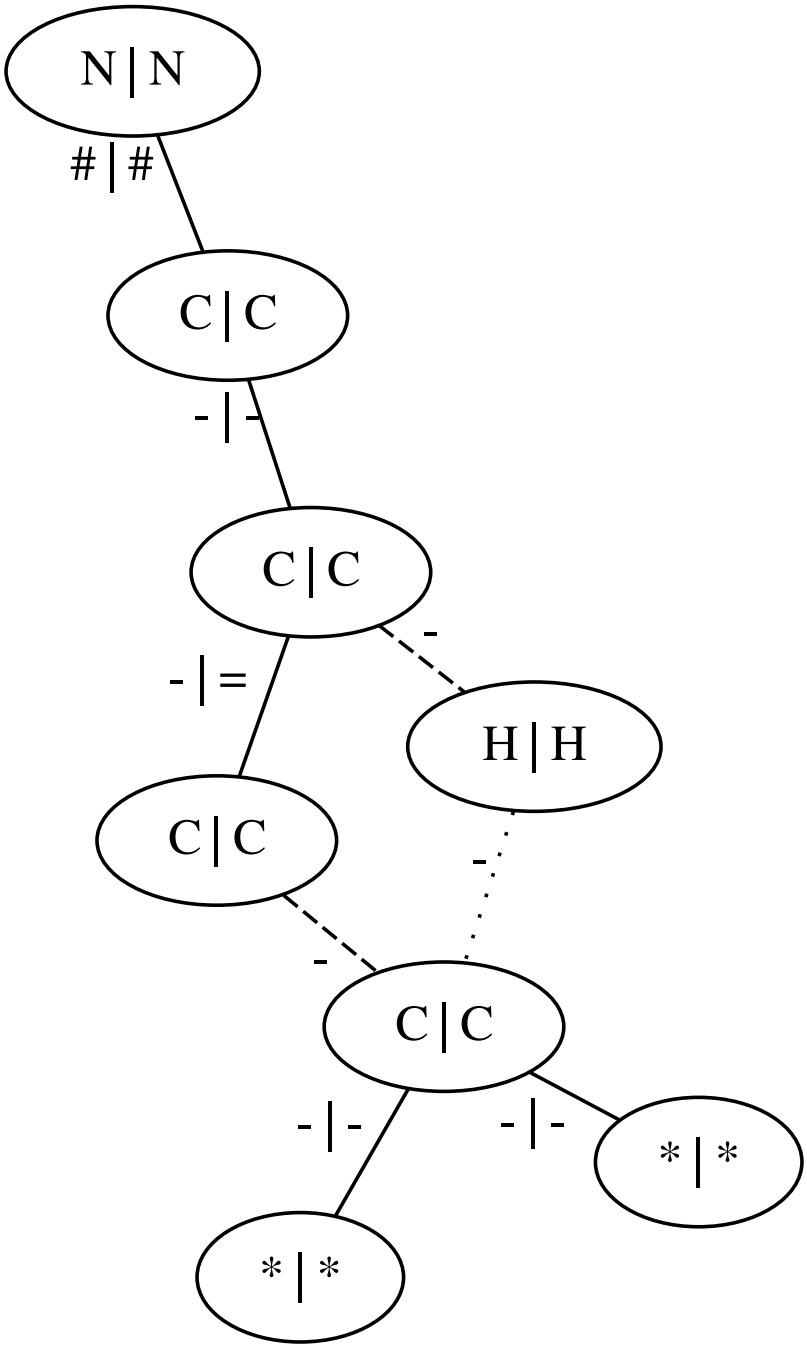
0.0.206 Michael Addition 2,2, (reverse)



Files: out/1025_r_208_10300000_{L, K, R}



Files: out/1026_r_208_11300100_{L, K, R}



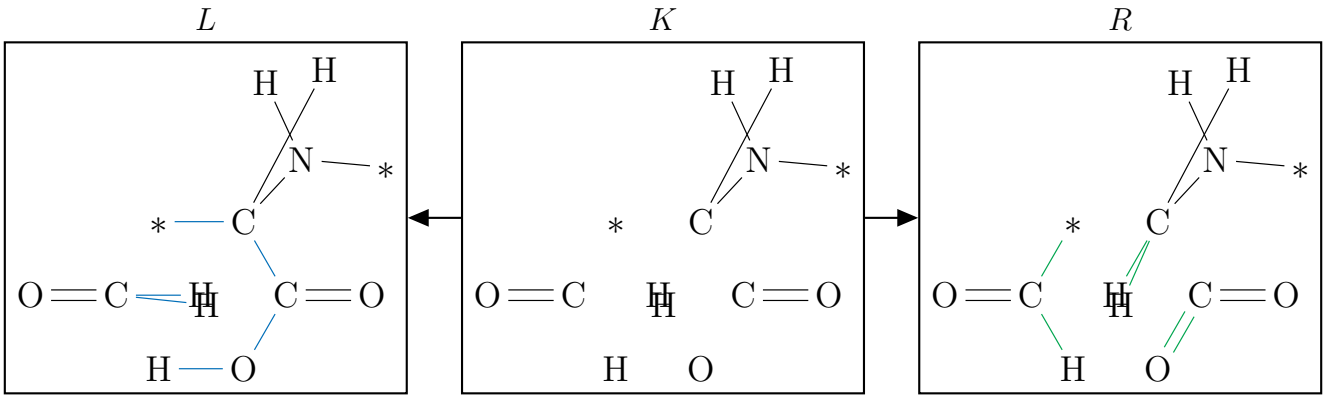
File: out/1027_r_208_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(0) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

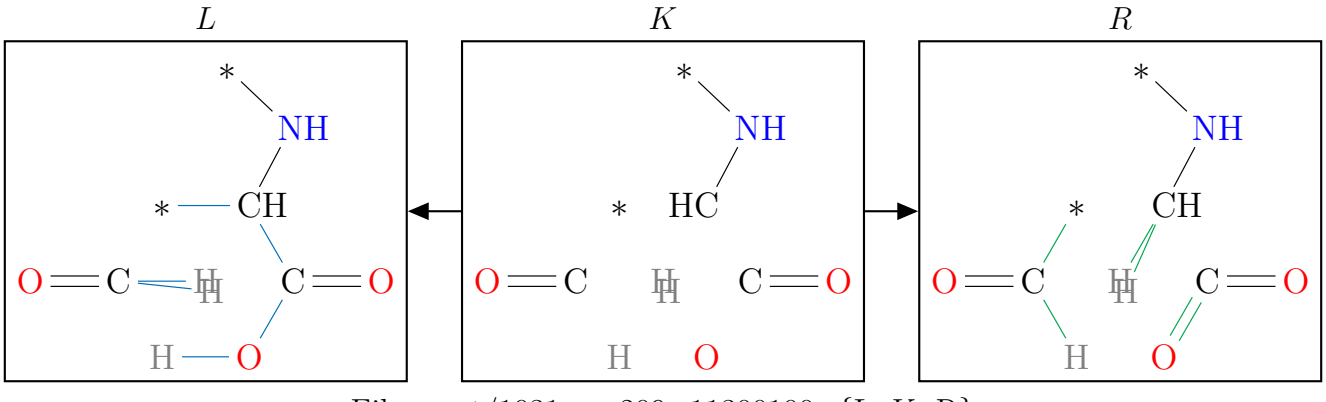
$$
\begin{aligned}
&|\{e \in \text{outEdges}(1) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`-'}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`N'}, \text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`\#'}, \text{`='}\} \\
&\}| = 0
\end{aligned}
$$

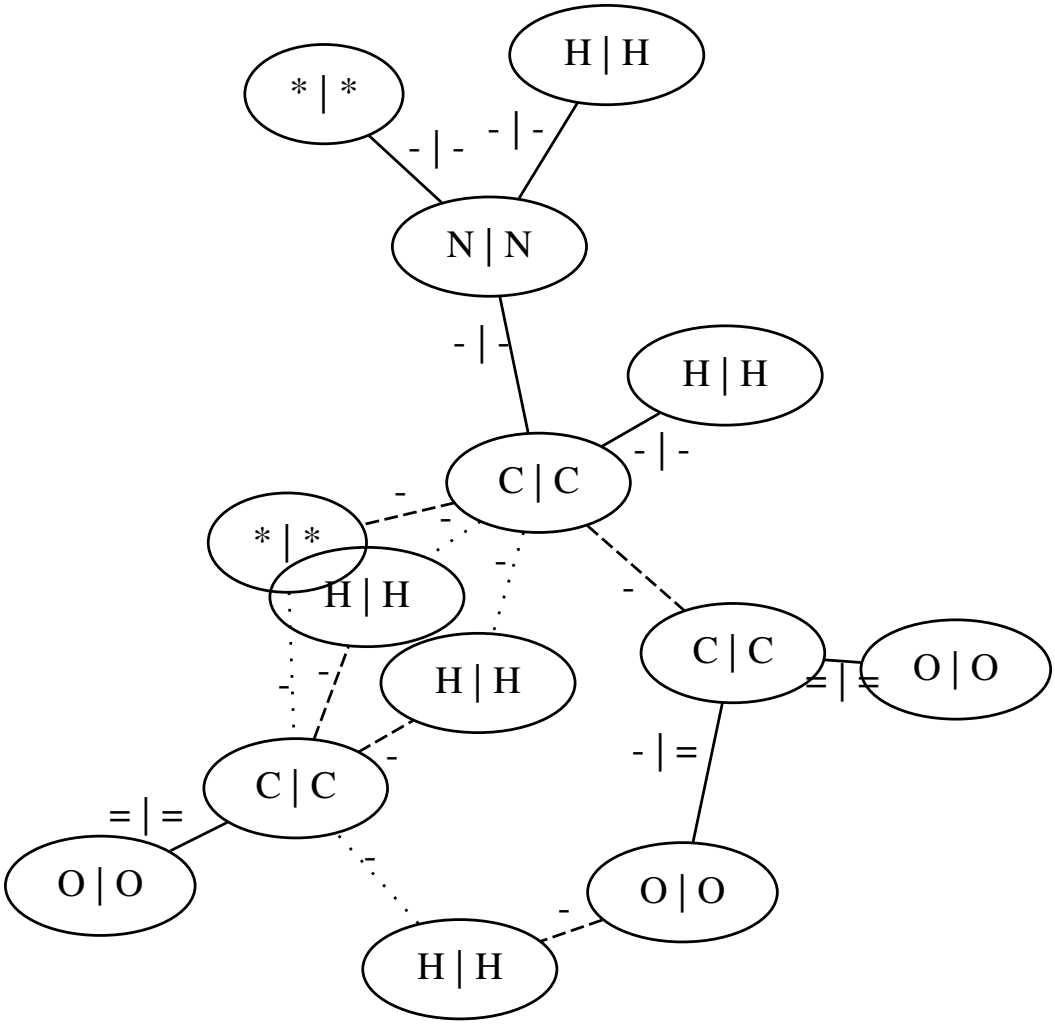
0.0.207 Strecker Degradation, HH



Files: out/1030_r_209_10300000_{L, K, R}

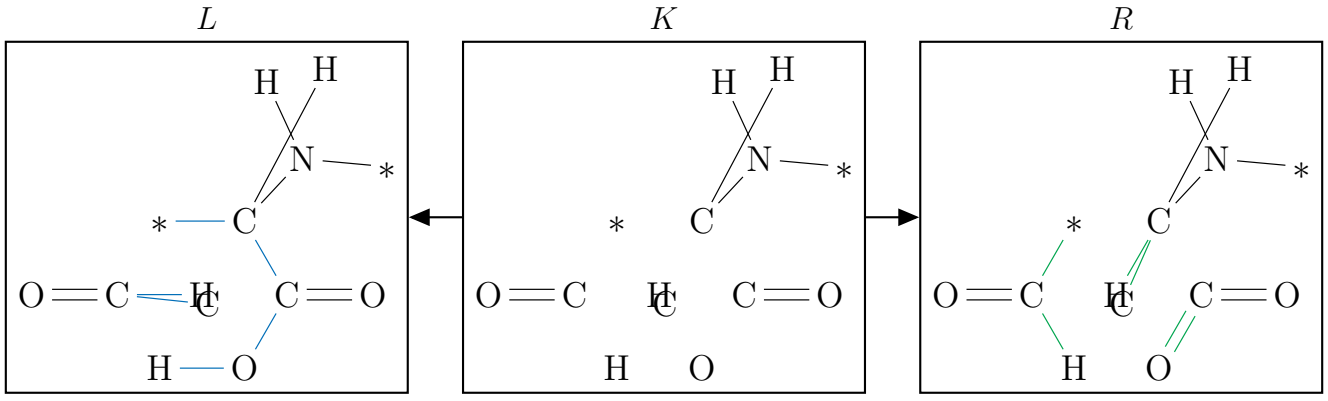


Files: out/1031_r_209_11300100_{L, K, R}

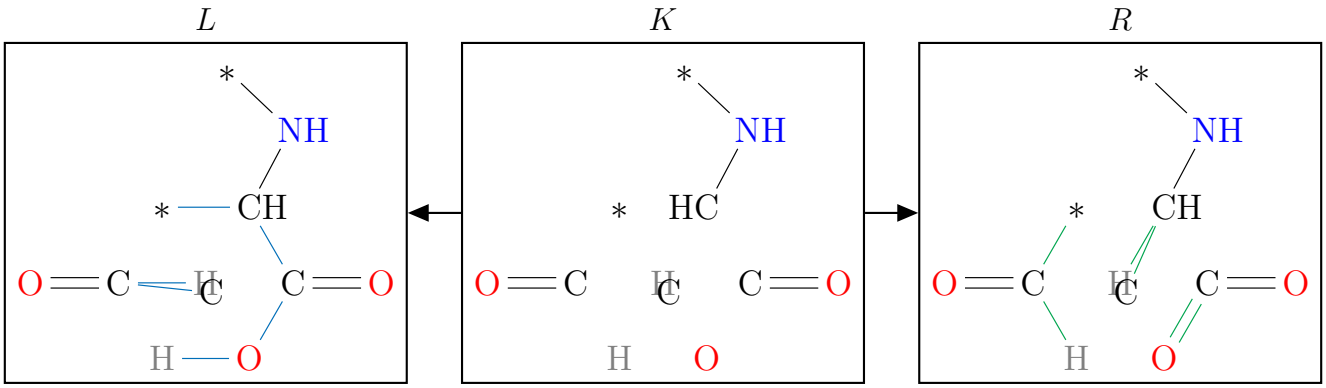


File: out/1032_r_209_combined

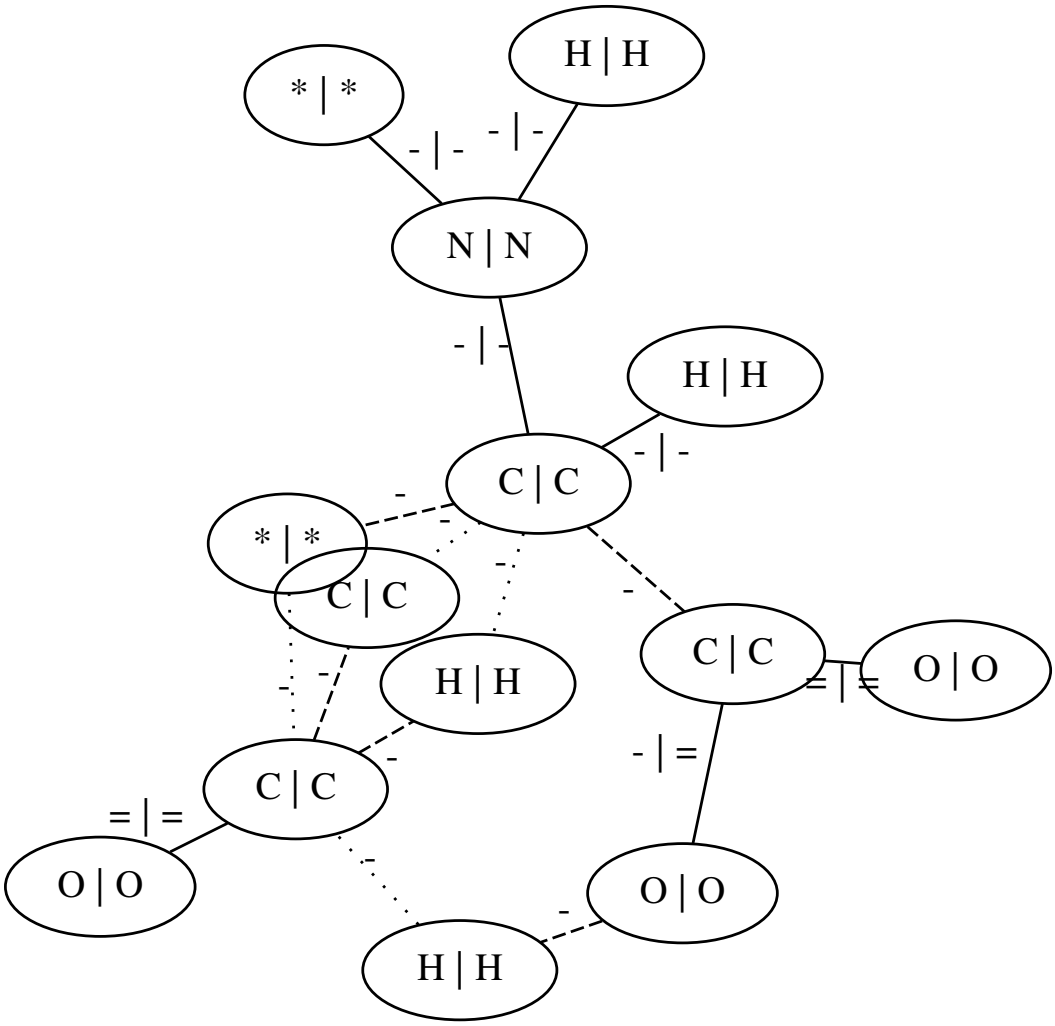
0.0.208 Strecker Degradation, HC



Files: out/1035_r_210_10300000_{L, K, R}



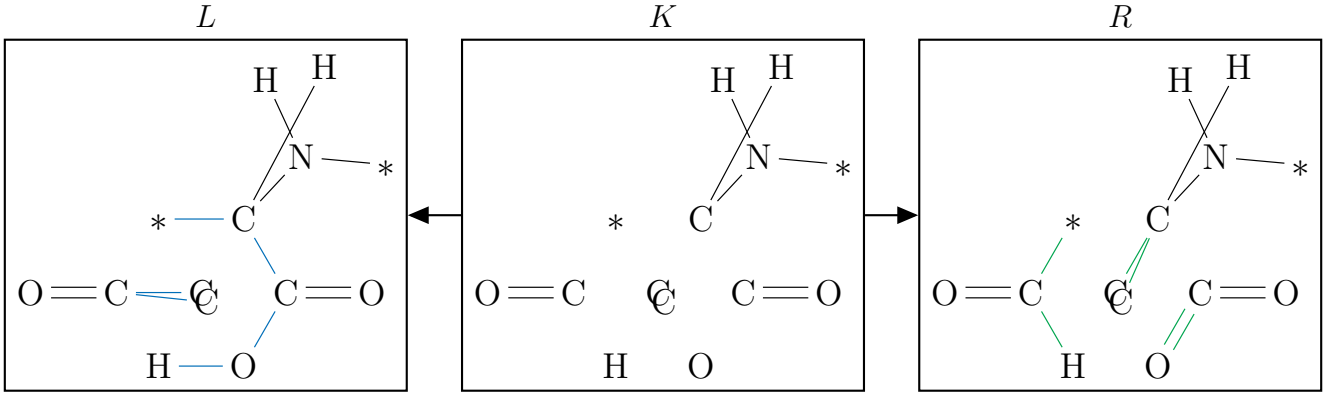
Files: out/1036_r_210_11300100_{L, K, R}



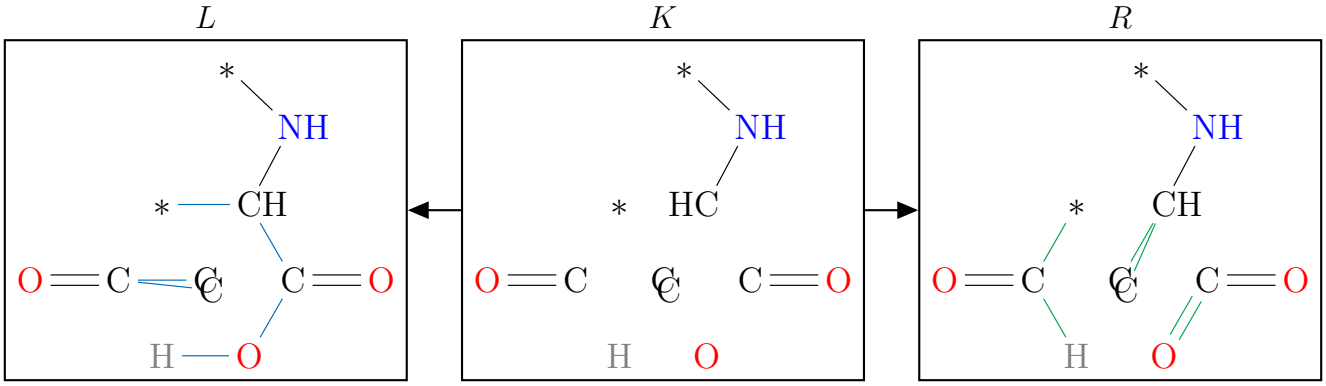
File: out/1037_r_210_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(13) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

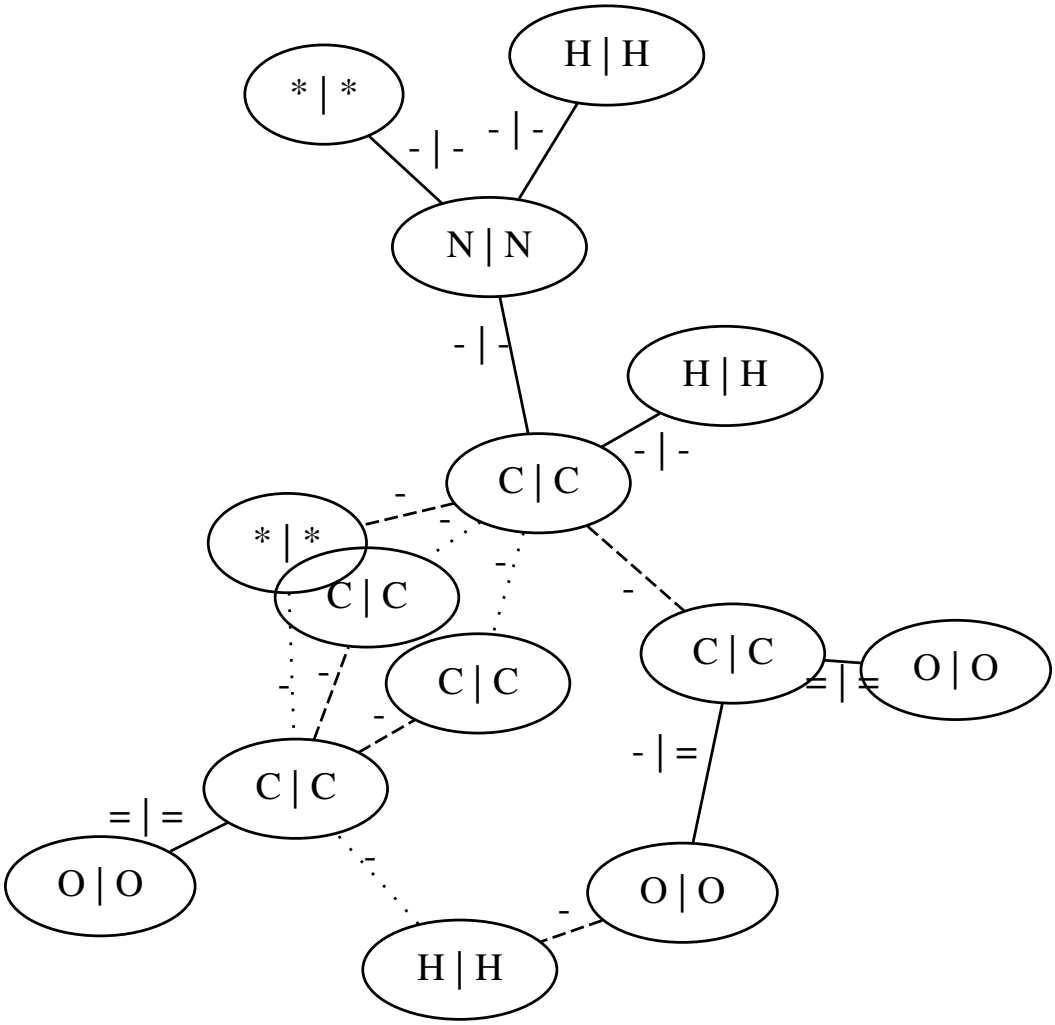
0.0.209 Strecker Degradation, CC



Files: out/1040_r_211_10300000_{L, K, R}



Files: out/1041_r_211_11300100_{L, K, R}

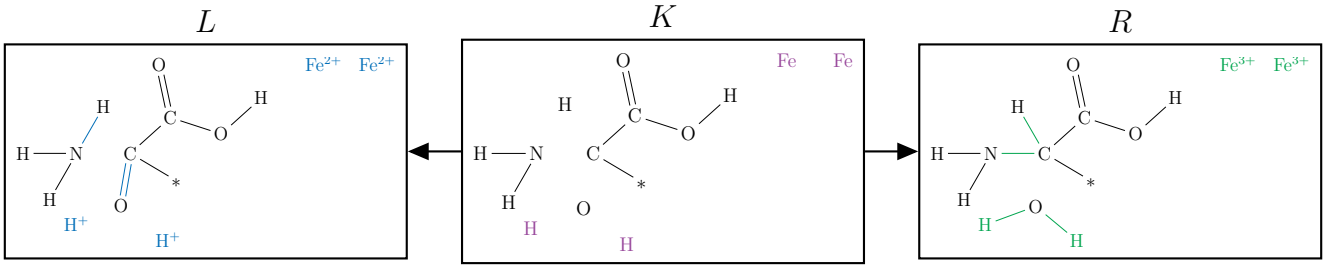


File: out/1042_r_211_combined

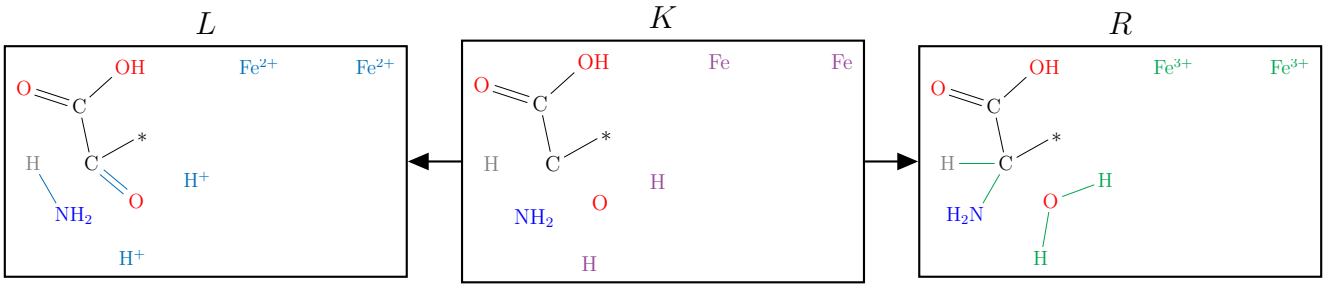
$$
\begin{aligned}
&|\{e \in \text{outEdges}(12) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

$$
\begin{aligned}
&|\{e \in \text{outEdges}(13) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

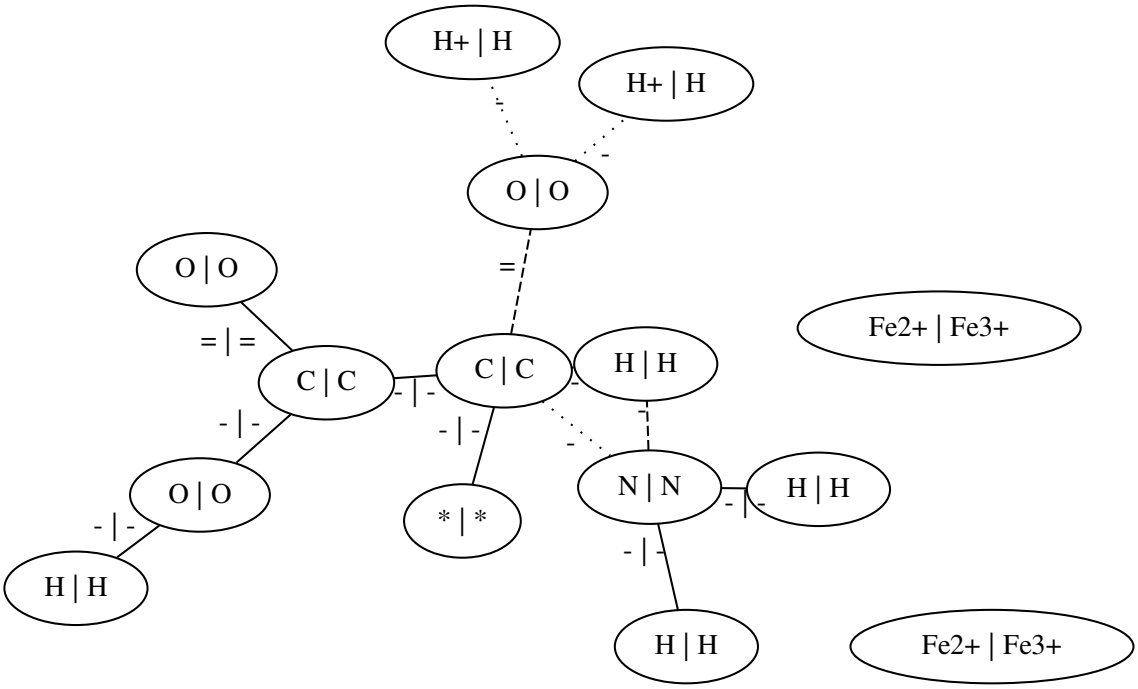
0.0.210 Fe2 —> Fe3 Alpha Keto Reduction, conversion to amino acid



Files: out/1045_r_212_10300000_{L, K, R}

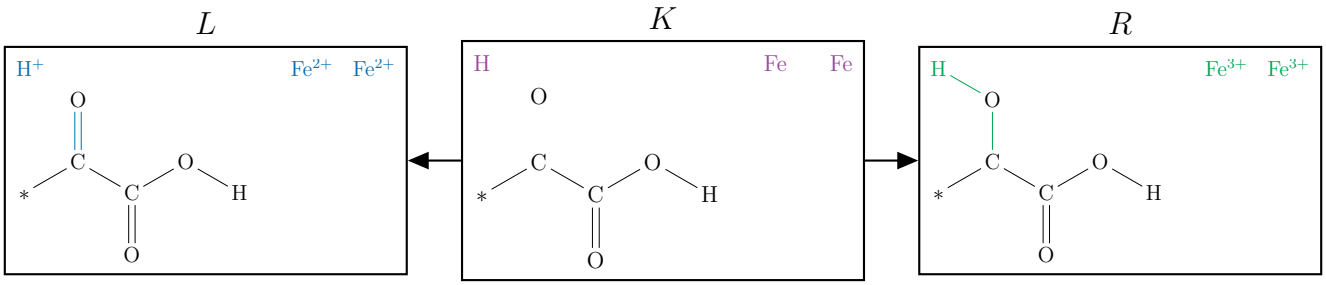


Files: out/1046_r_212_11300100_{L, K, R}

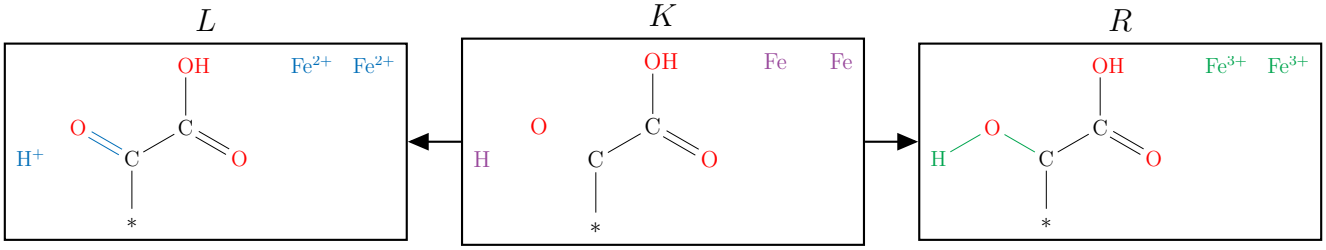


File: out/1047_r_212_combined

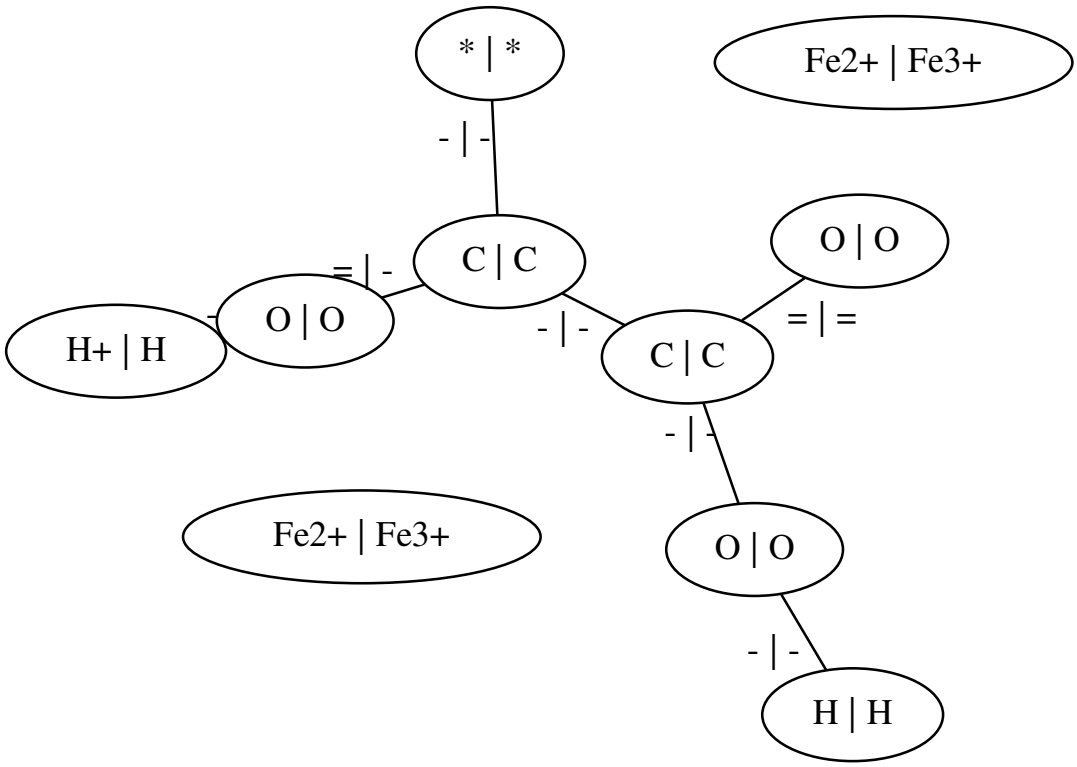
0.0.211 Fe2 —> Fe3 Alpha Keto Reduction of a Carboxylic Acid (Fe2+ to Fe3+)



Files: out/1050_r_213_10300000_{L, K, R}

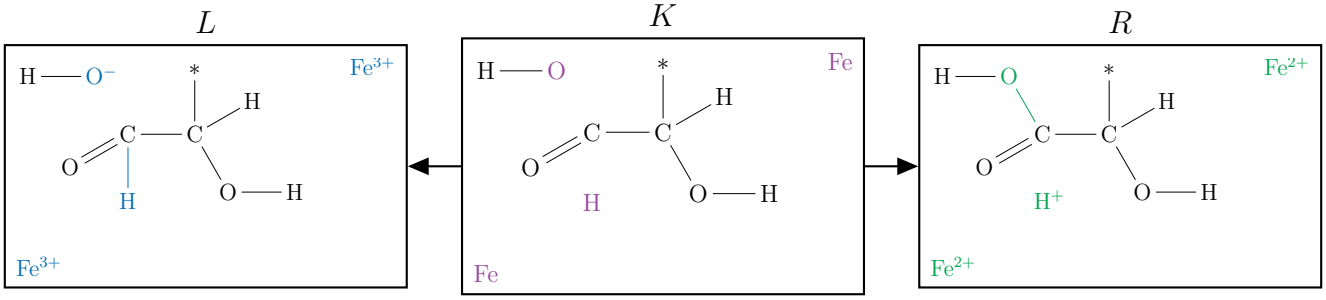


Files: out/1051_r_213_11300100_{L, K, R}

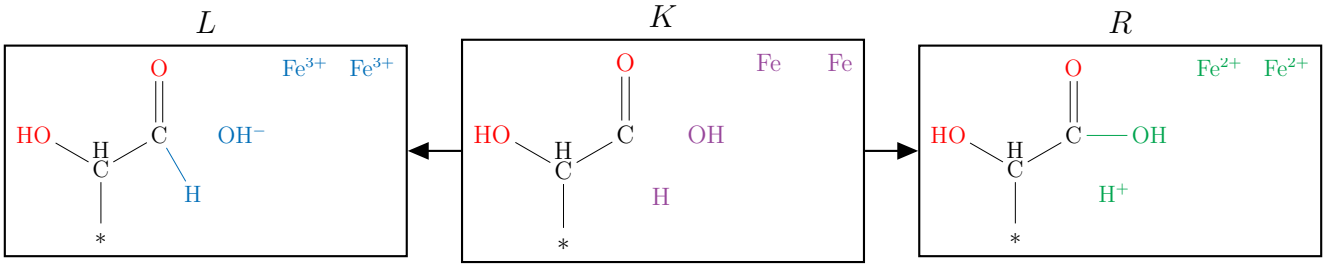


File: out/1052_r_213_combined

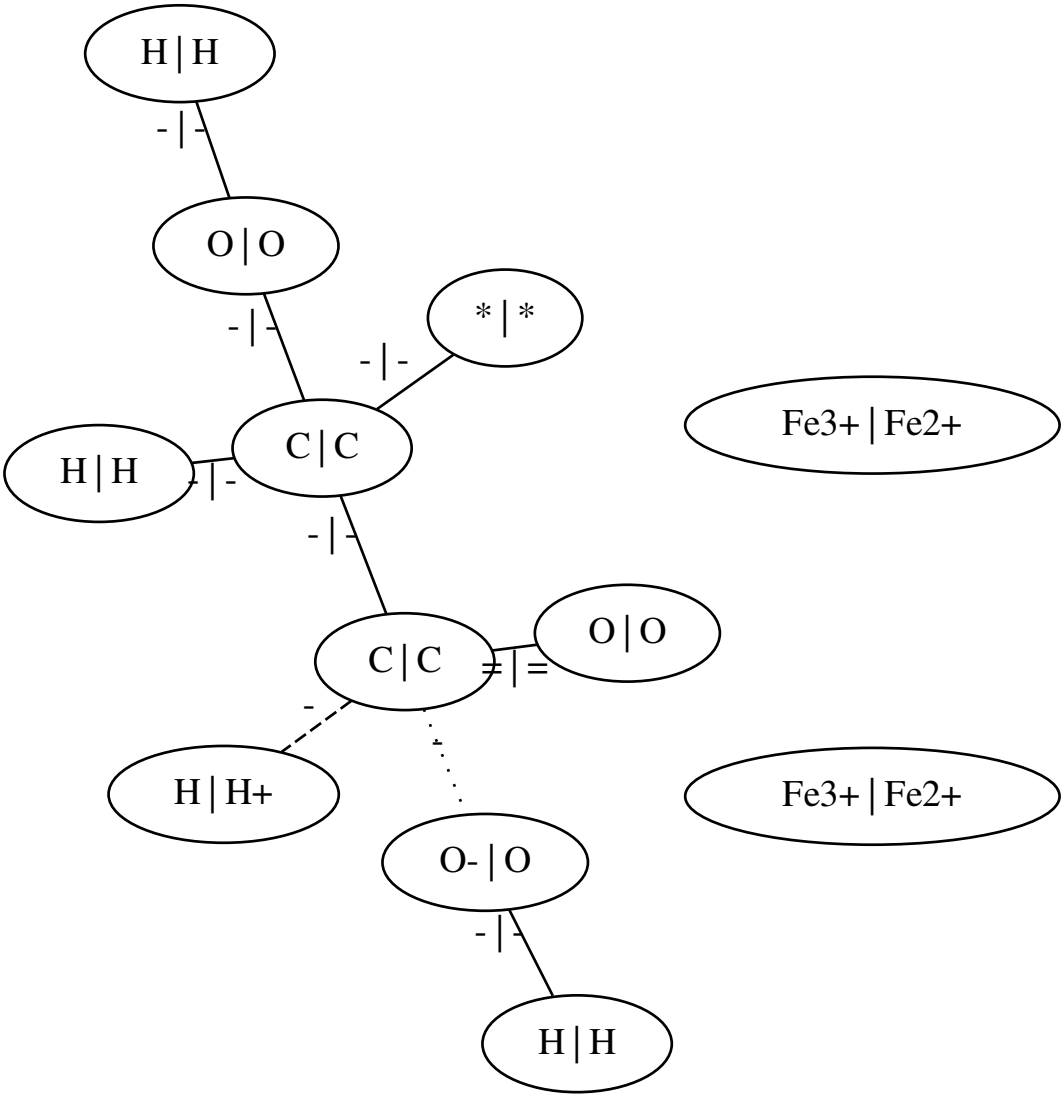
0.0.212 Fe3 —> Fe2 Aldehyde to acid



Files: out/1055_r_214_10300000_{L, K, R}

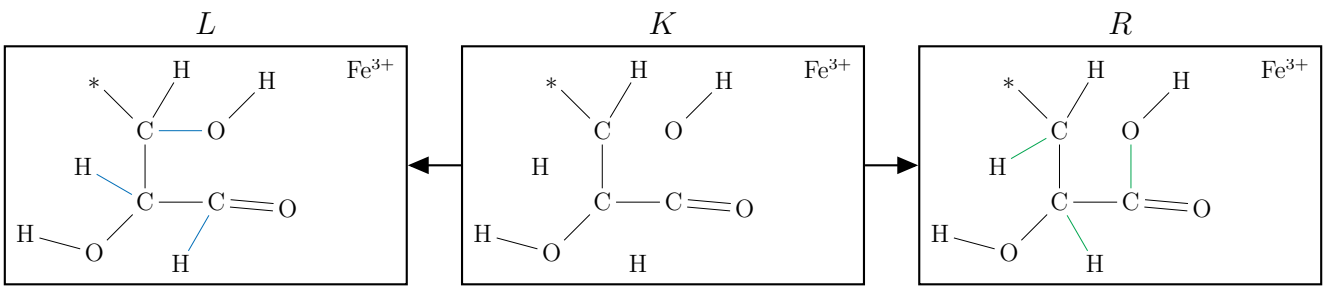


Files: out/1056_r_214_11300100_{L, K, R}

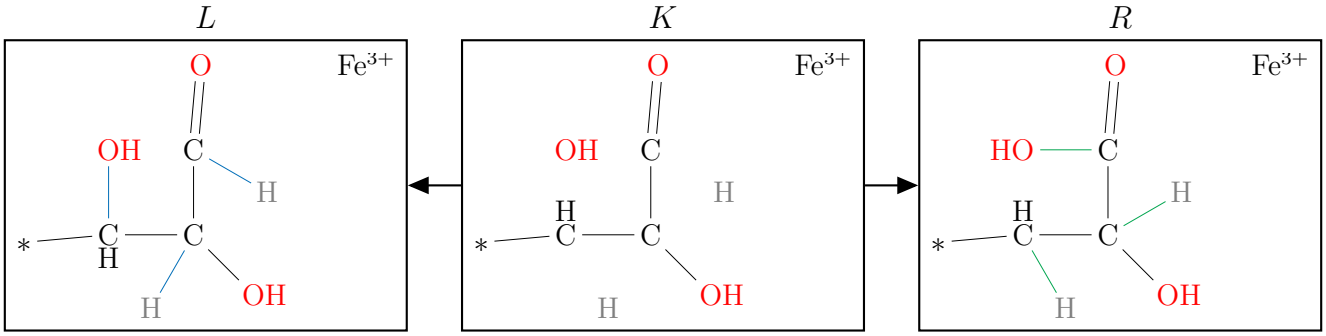


File: out/1057_r_214_combined

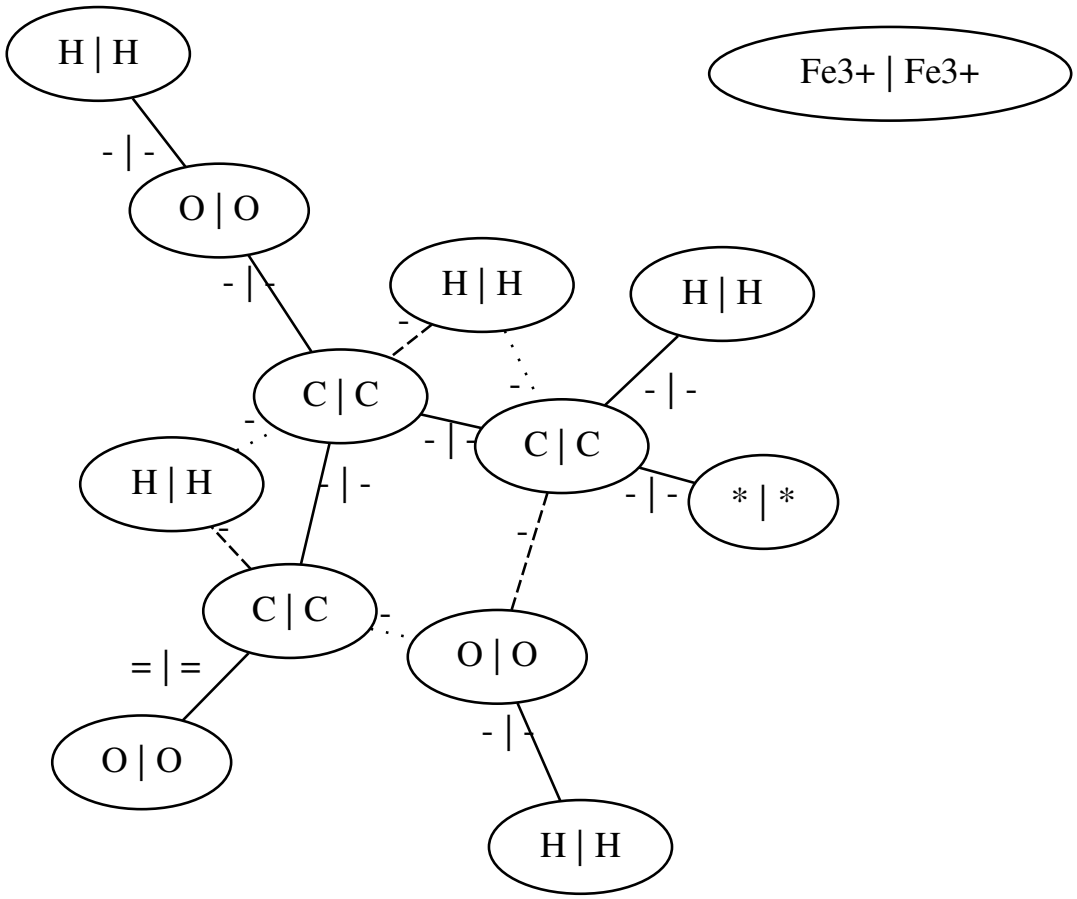
0.0.213 Fe3 Complex Beta elimination from a sugar and Conversion to Acid



Files: out/1060_r_215_10300000_{L, K, R}

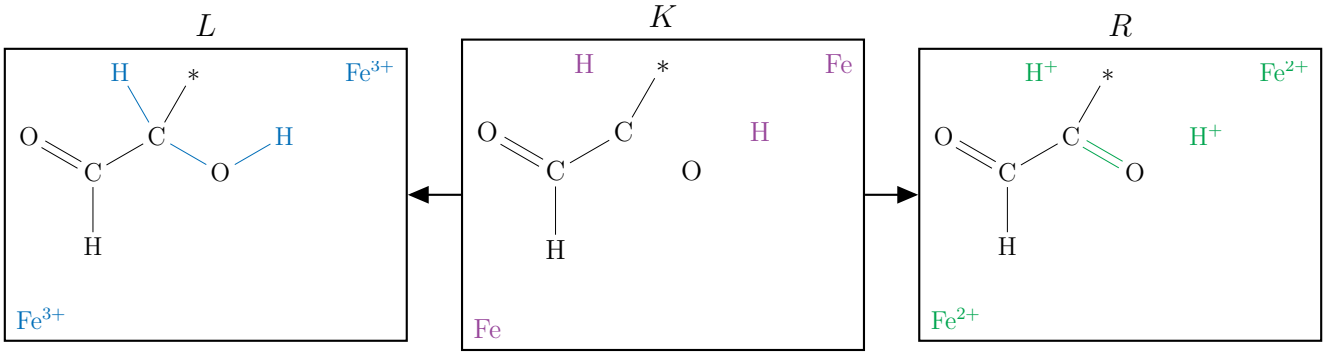


Files: out/1061_r_215_11300100_{L, K, R}

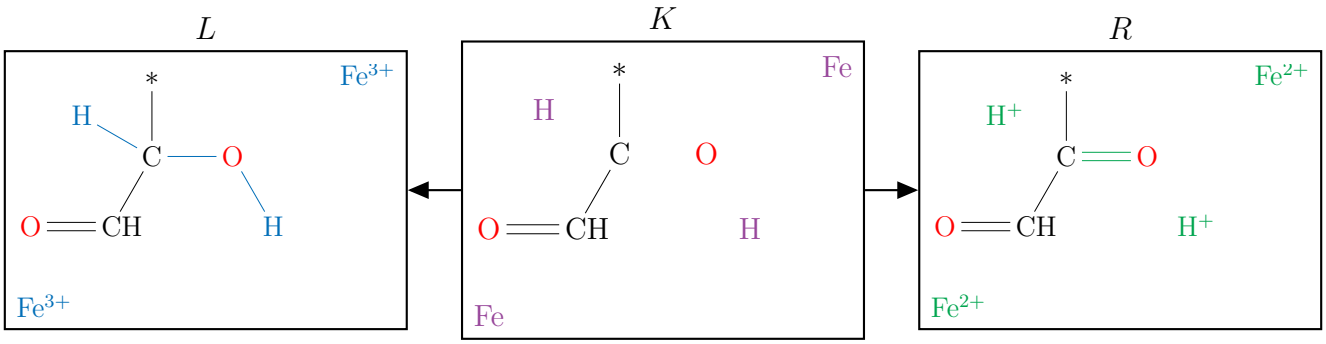


File: out/1062_r_215_combined

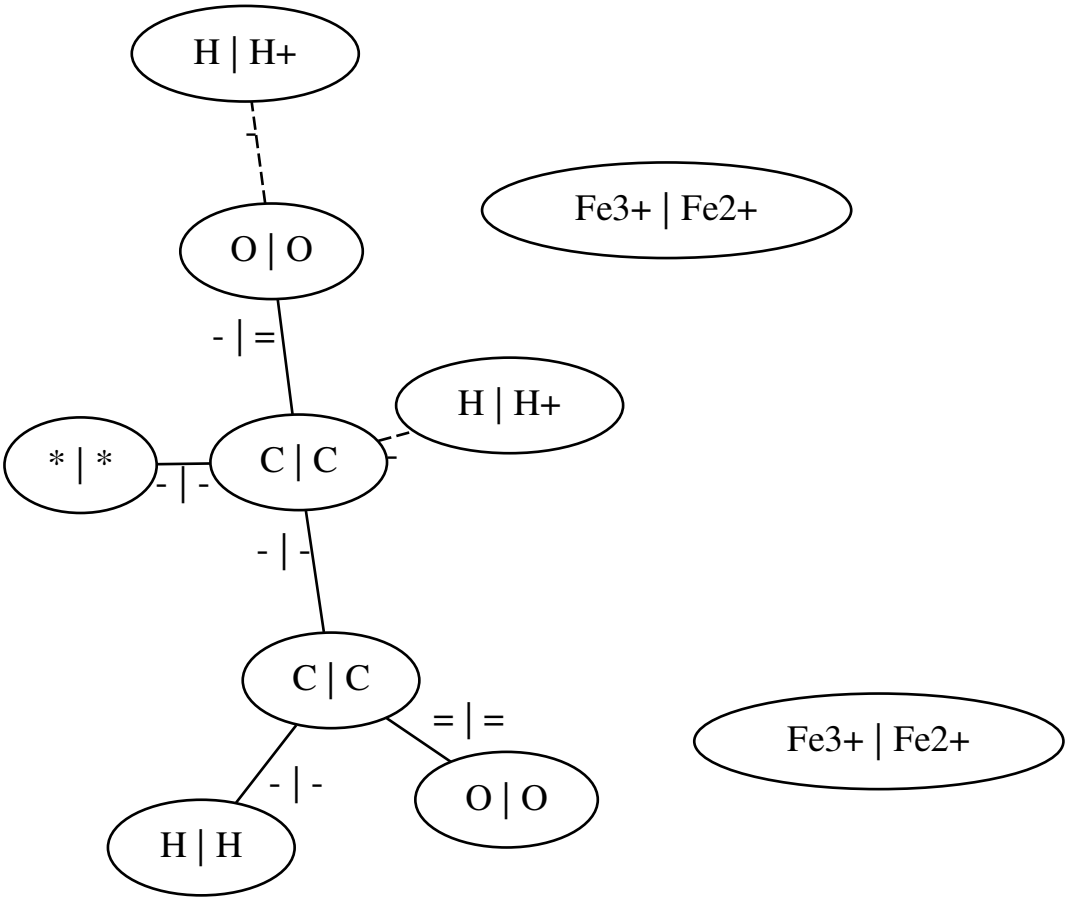
0.0.214 Fe3 —> Fe2 Conversion of Alpha Hydroxy Group of an aldehyde to Alpha Keto group



Files: out/1065_r_216_10300000_{L, K, R}



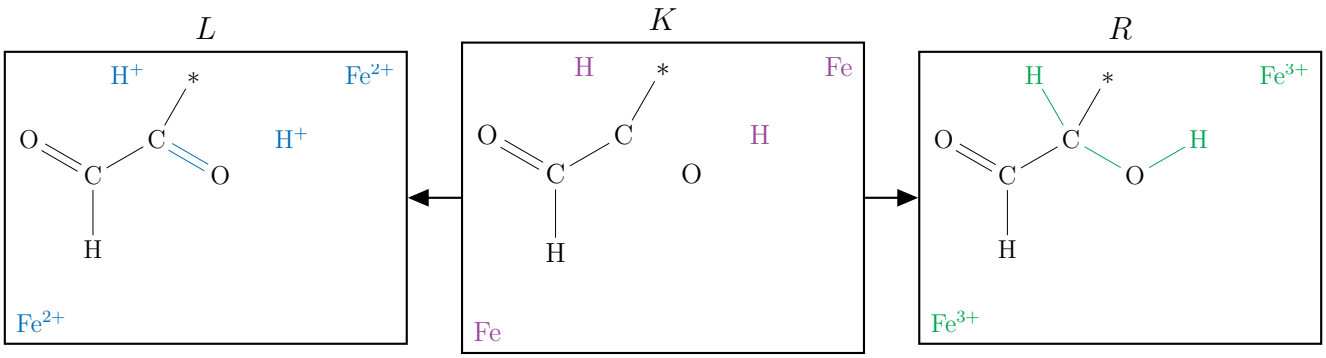
Files: out/1066_r_216_11300100_{L, K, R}



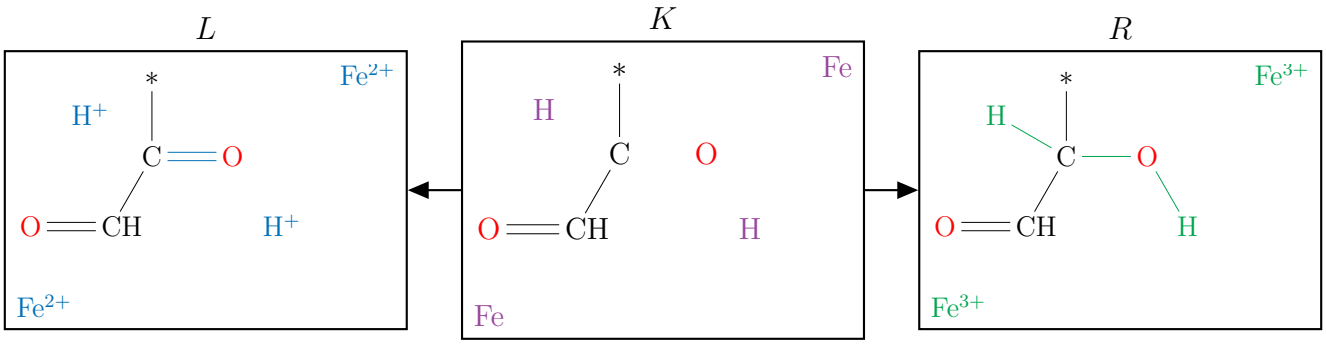
File: out/1067_r_216_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

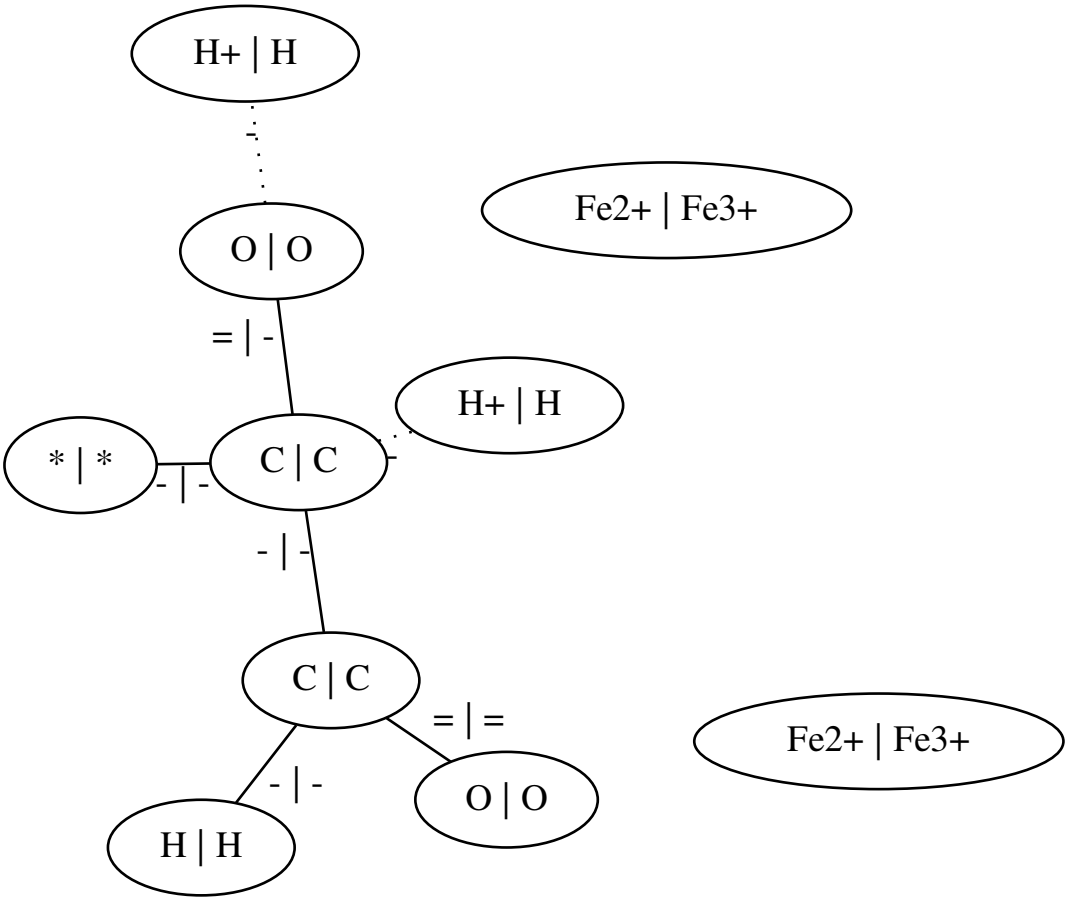
0.0.215 Fe2 —> Fe3 Conversion of Alpha Hydroxy Group of an aldehyde to Alpha Keto group, inverse



Files: out/1070_r_217_10300000_{L, K, R}



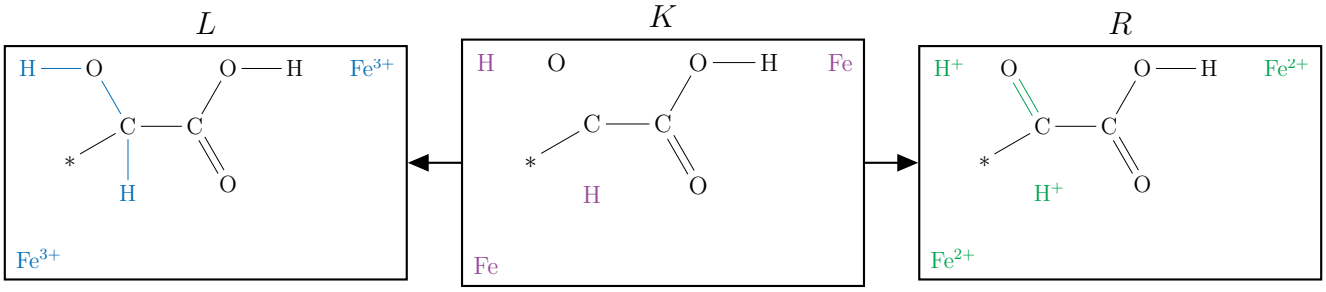
Files: out/1071_r_217_11300100_{L, K, R}



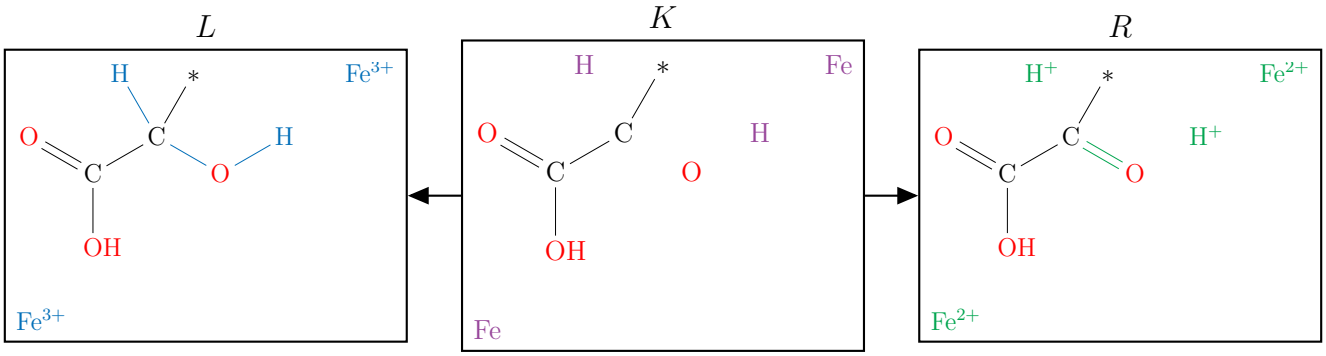
File: out/1072_r_217_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`}\texttt{O}\text{'}, \text{`}\texttt{N}\text{'}, \text{`}\texttt{S}\text{'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`}\texttt{=}\text{'}\} \\
&\}| = 0
\end{aligned}
$$

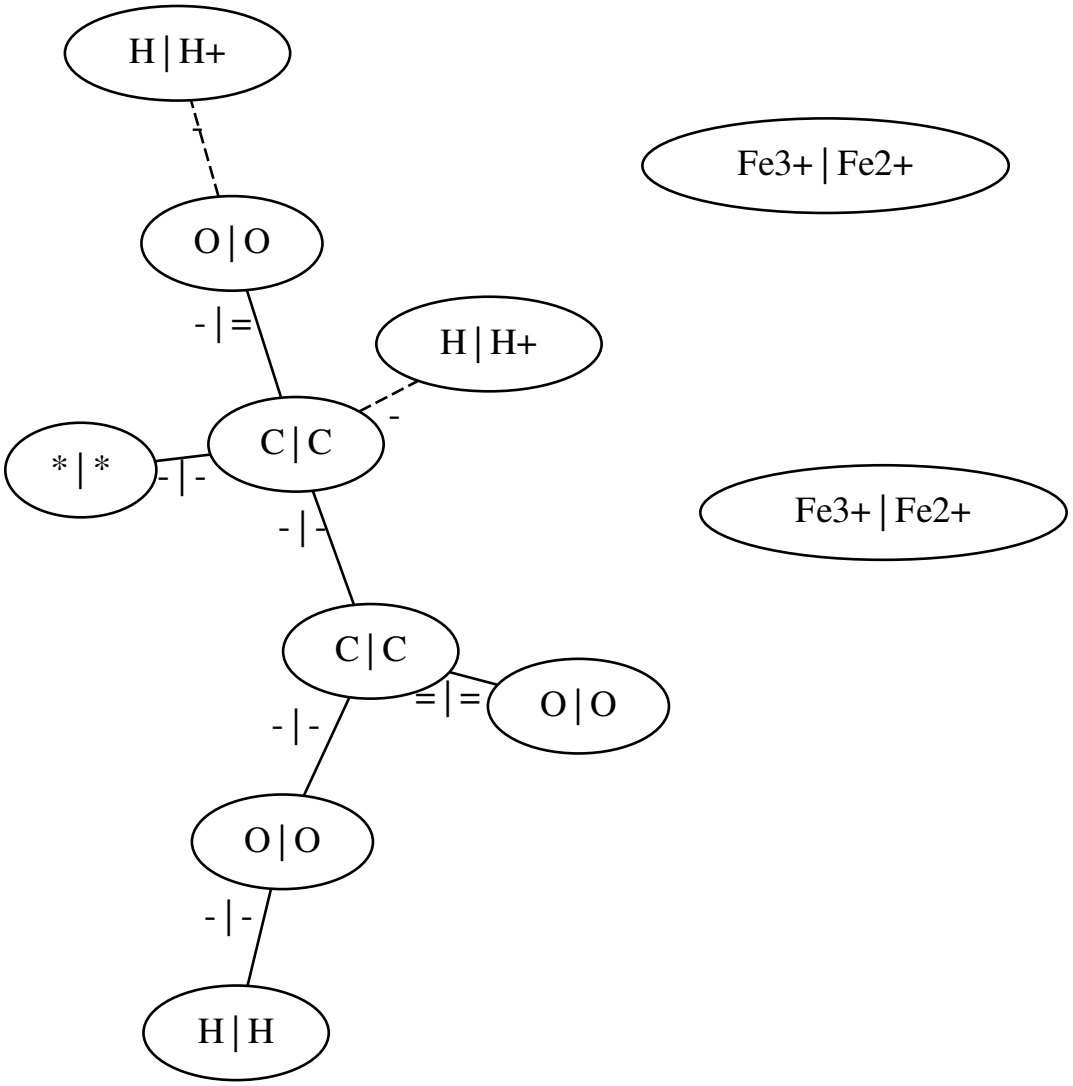
0.0.216 Fe3 —> Fe2 Conversion of Alpha Hydro Group of an ACID to Alpha Keto group



Files: out/1075_r_218_10300000_{L, K, R}



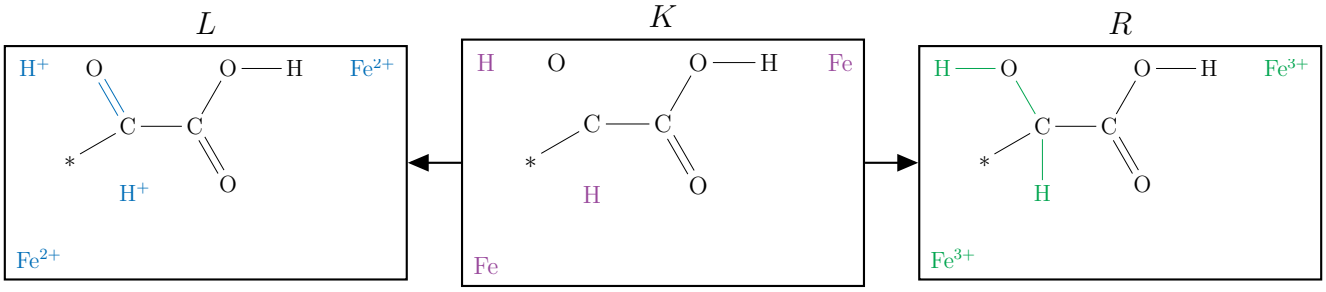
Files: out/1076_r_218_11300100_{L, K, R}



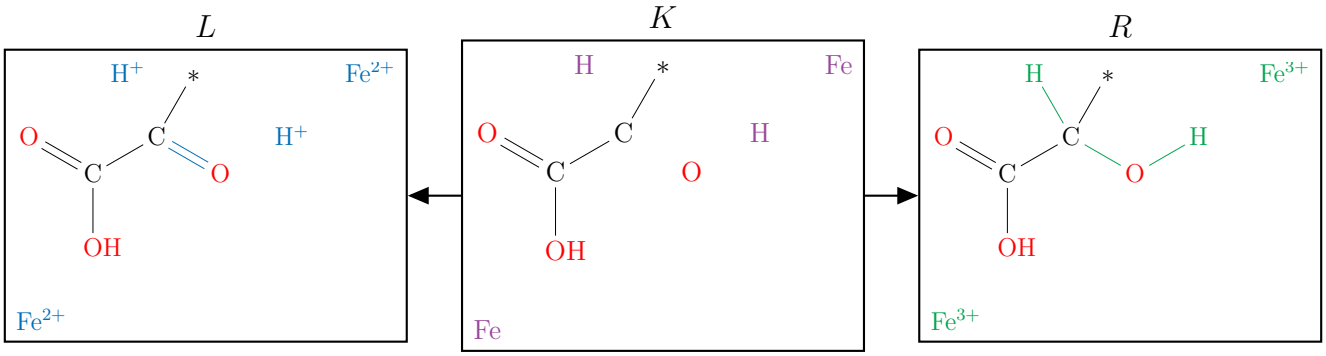
File: out/1077_r_218_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

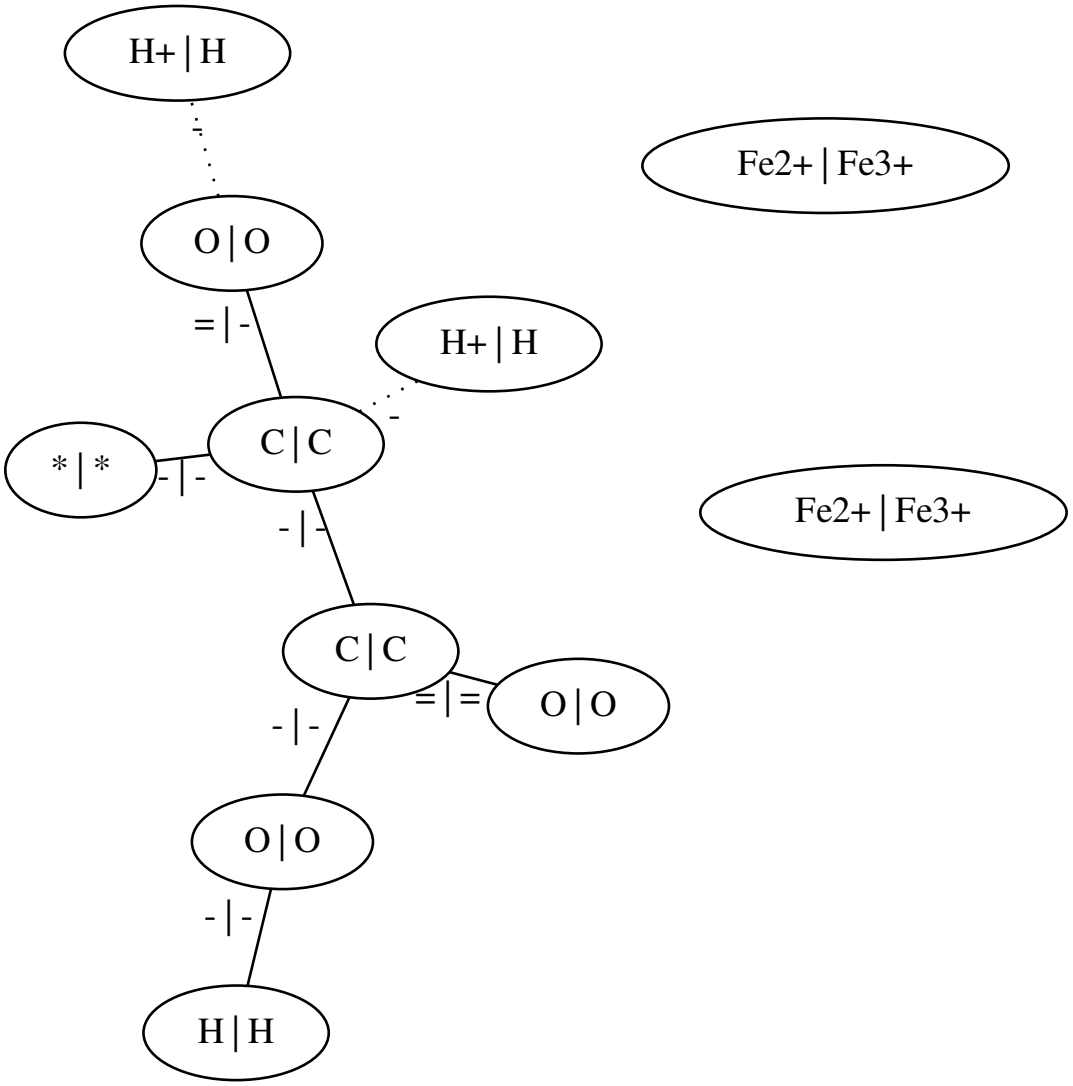
0.0.217 Fe2 —> Fe3 Conversion of Alpha Keto Group of an ACID to Alpha Hydro group



Files: out/1080_r_219_10300000_{L, K, R}



Files: out/1081_r_219_11300100_{L, K, R}



File: out/1082_r_219_combined

$$
\begin{aligned}
&|\{e \in \text{outEdges}(6) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{`O'}, \text{`N'}, \text{`S'}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{`='}\} \\
&\}| = 0
\end{aligned}
$$

Chapter 1

Formose Reaction