

Summary

May 22, 2022

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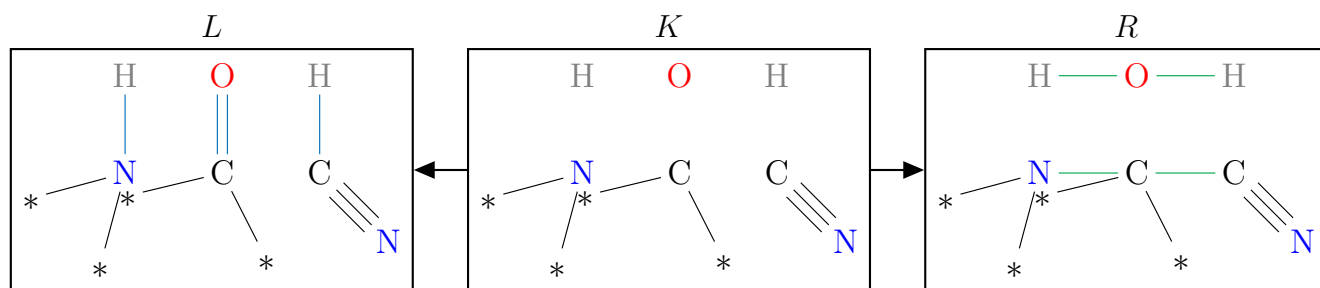
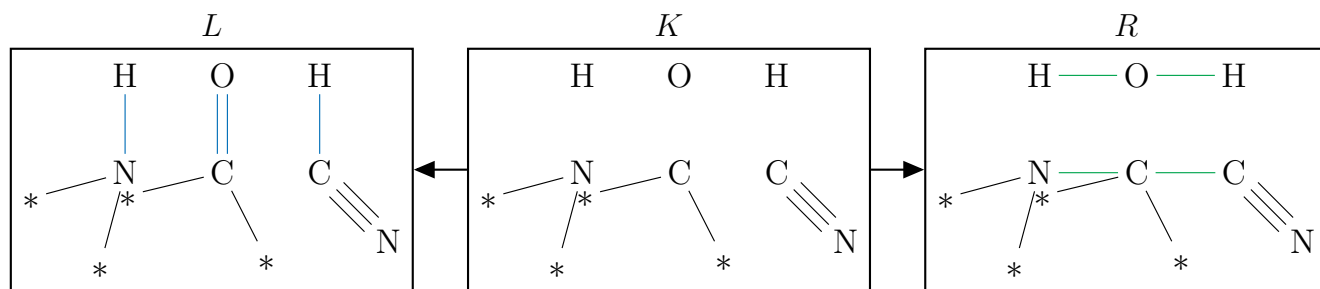
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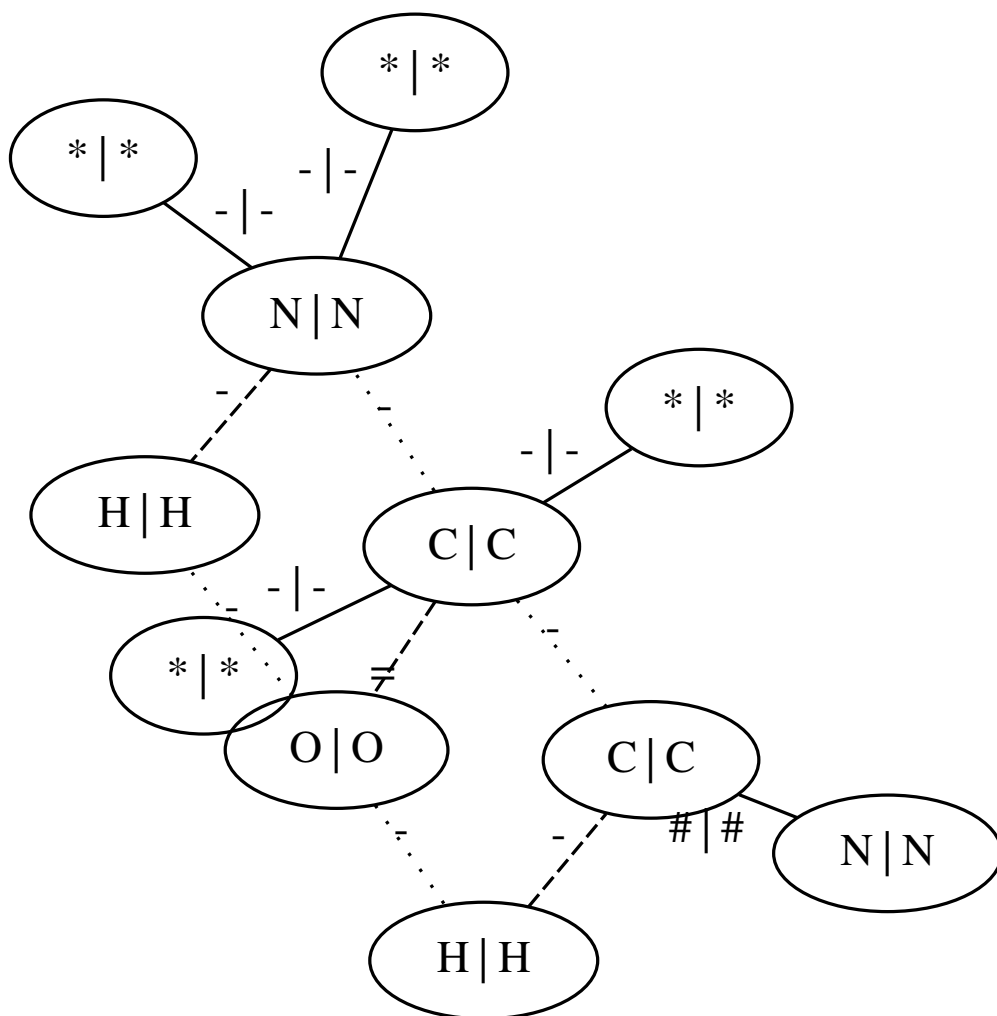
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1 Formose Reaction

415

0.0.1 Strecker Synthesis





File: out/003_r_106_combined

```

|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```


$$|\{e \in \text{outEdges}(4) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid$$

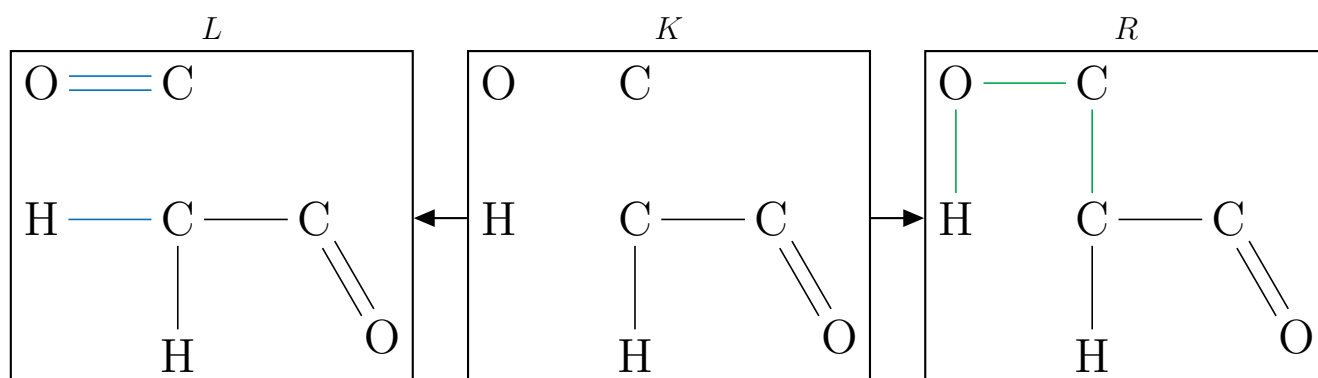
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$$\wedge$$

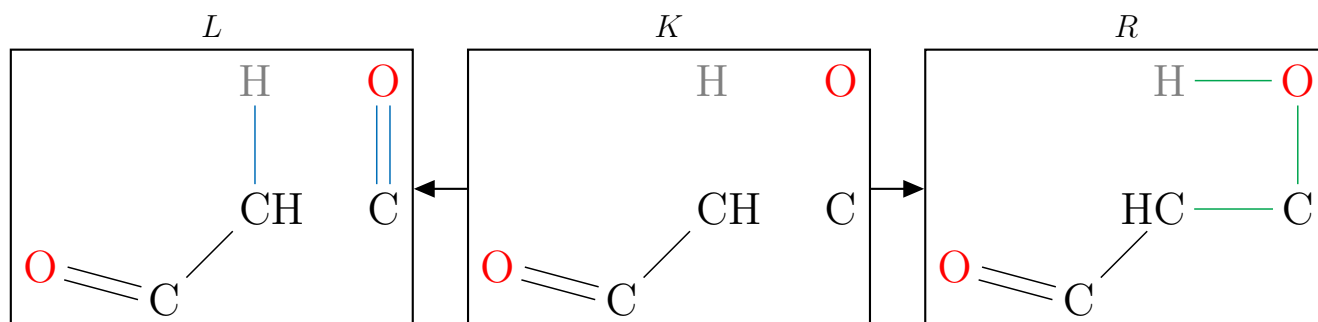
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

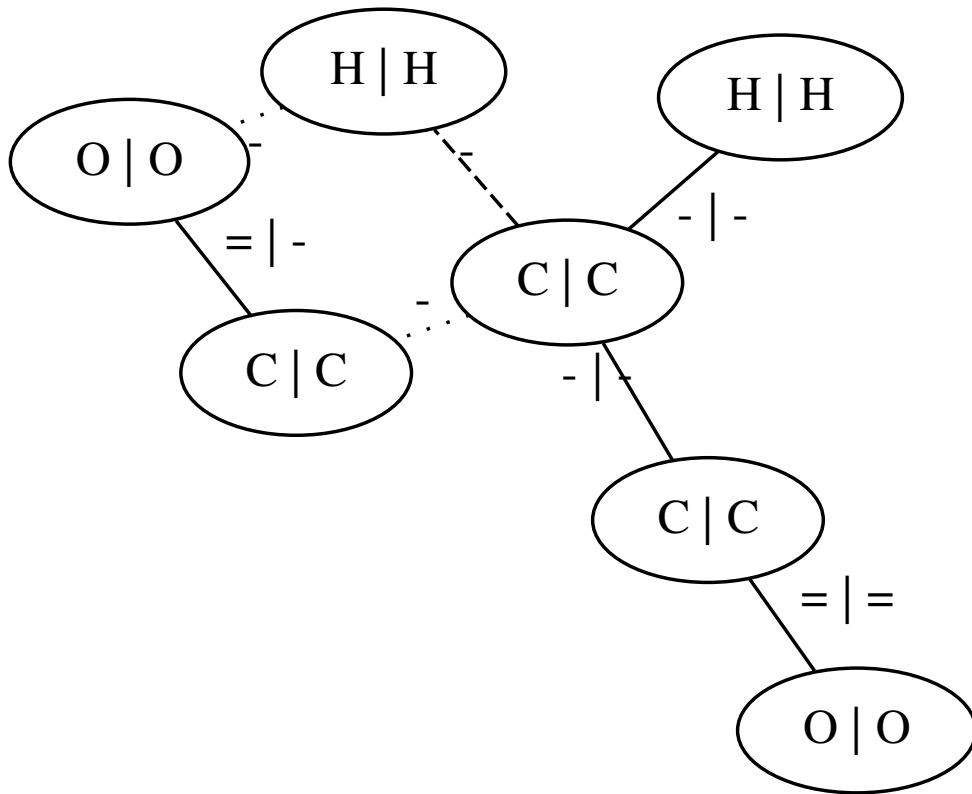
0.0.2 Aldol Condensation



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



Files: out/007_r_0_11300100_{L, K, R}



File: out/008_r_0_combined

```

|{e ∈ outEdges(0) |
  label(target(e)) ∈ {'O', 'N', 'S'}
  ∧
  label(e) ∈ {'-'}
}| = 0

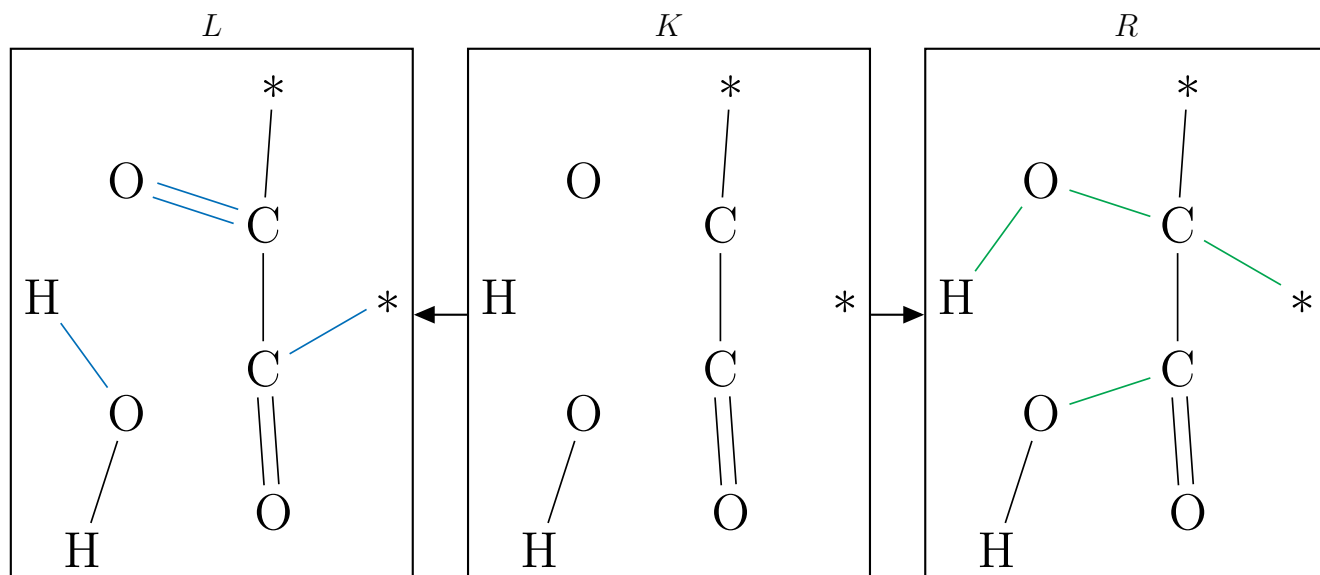
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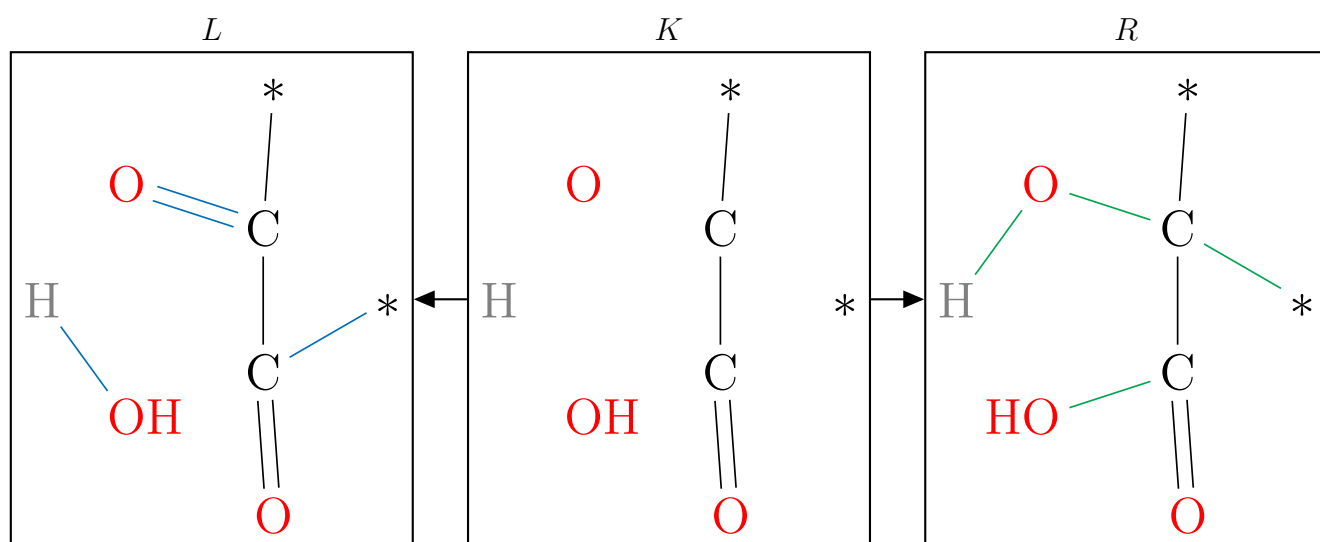
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  label(target(e)) ∈ {'O', 'N', 'S'}
  ∧
  label(e) ∈ {'-'}
}| = 0

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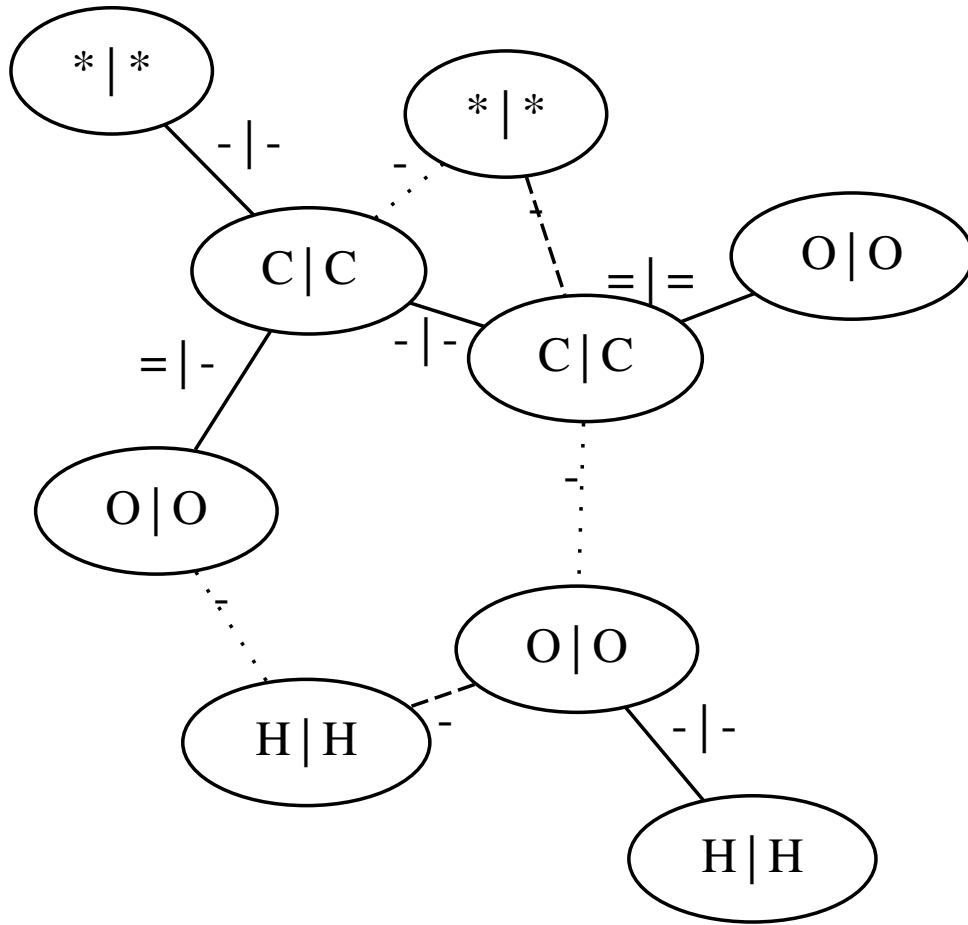
0.0.3 Benzilic Acid Rearrangement



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



Files: out/012_r_1_11300100_{L, K, R}



File: out/013_r_1_combined

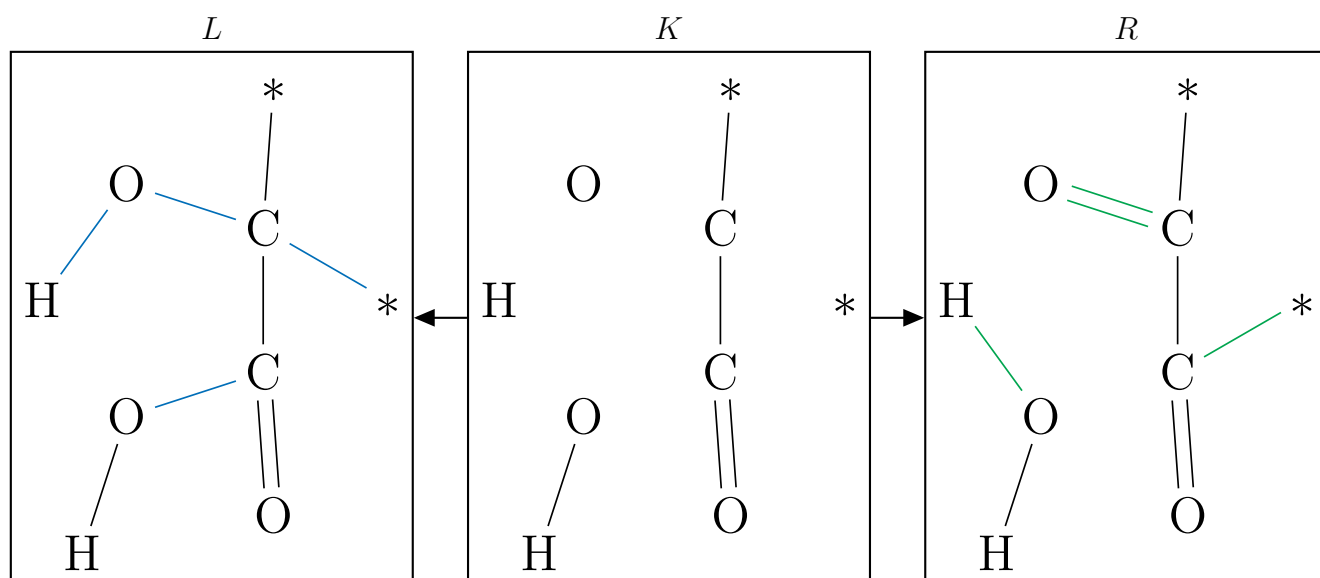
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|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'N', 'O'}
  ∧
  label(e) ∈ {'-'}
}| = 0

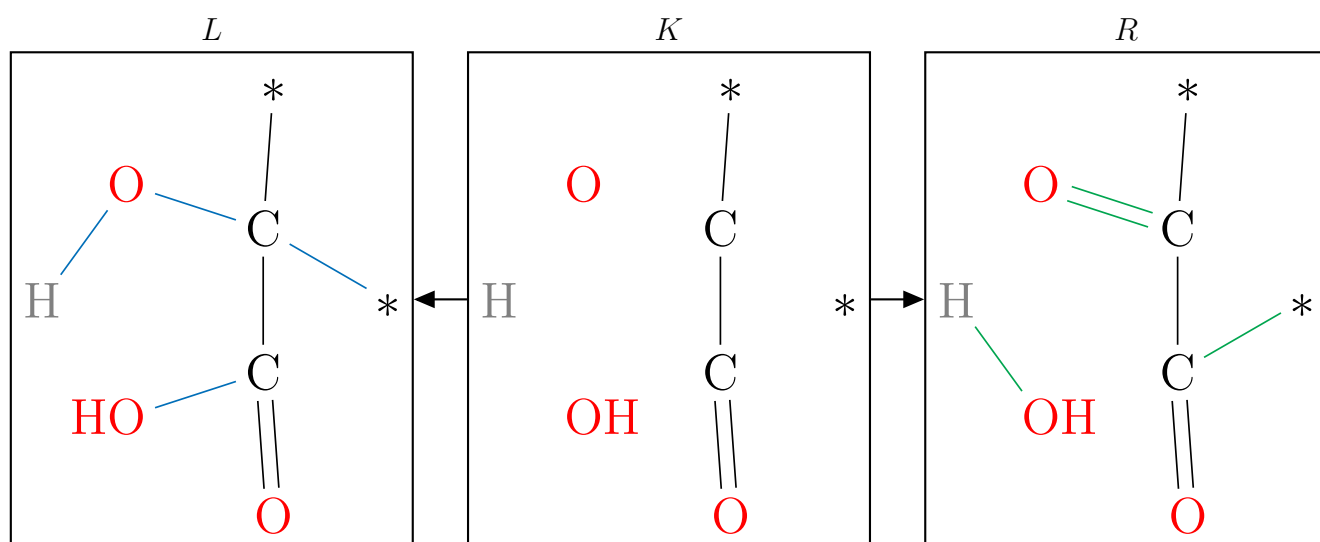
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$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\} = 0
\end{aligned}$$

0.0.4 Benzilic Acid Rearrangement (inverse)



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

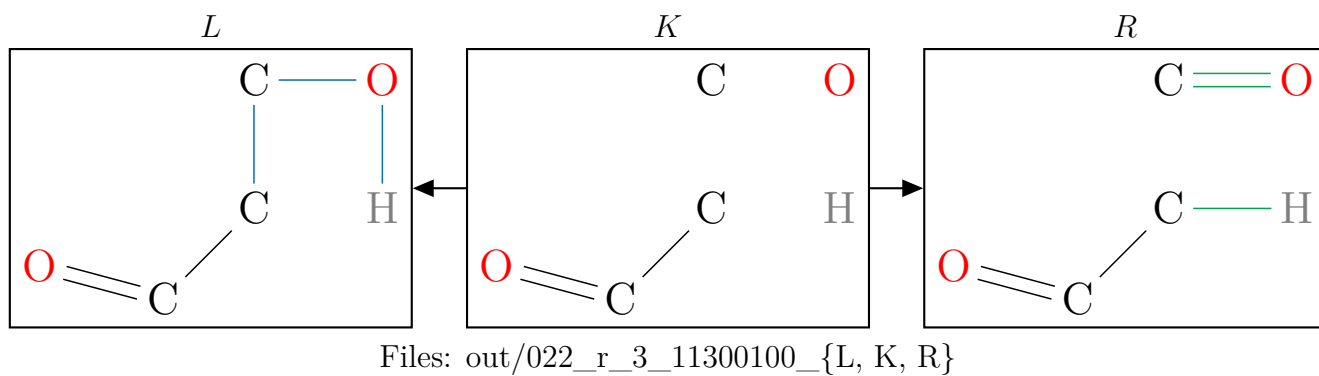
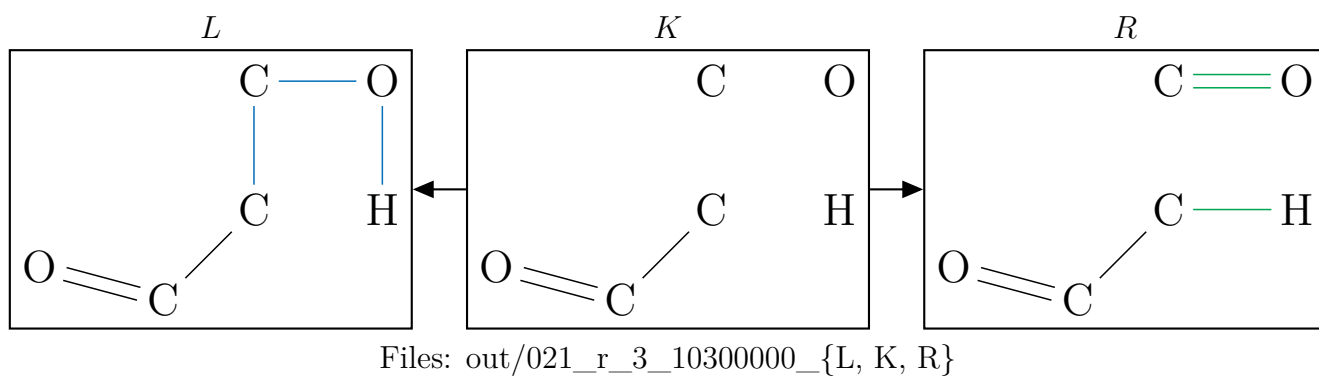


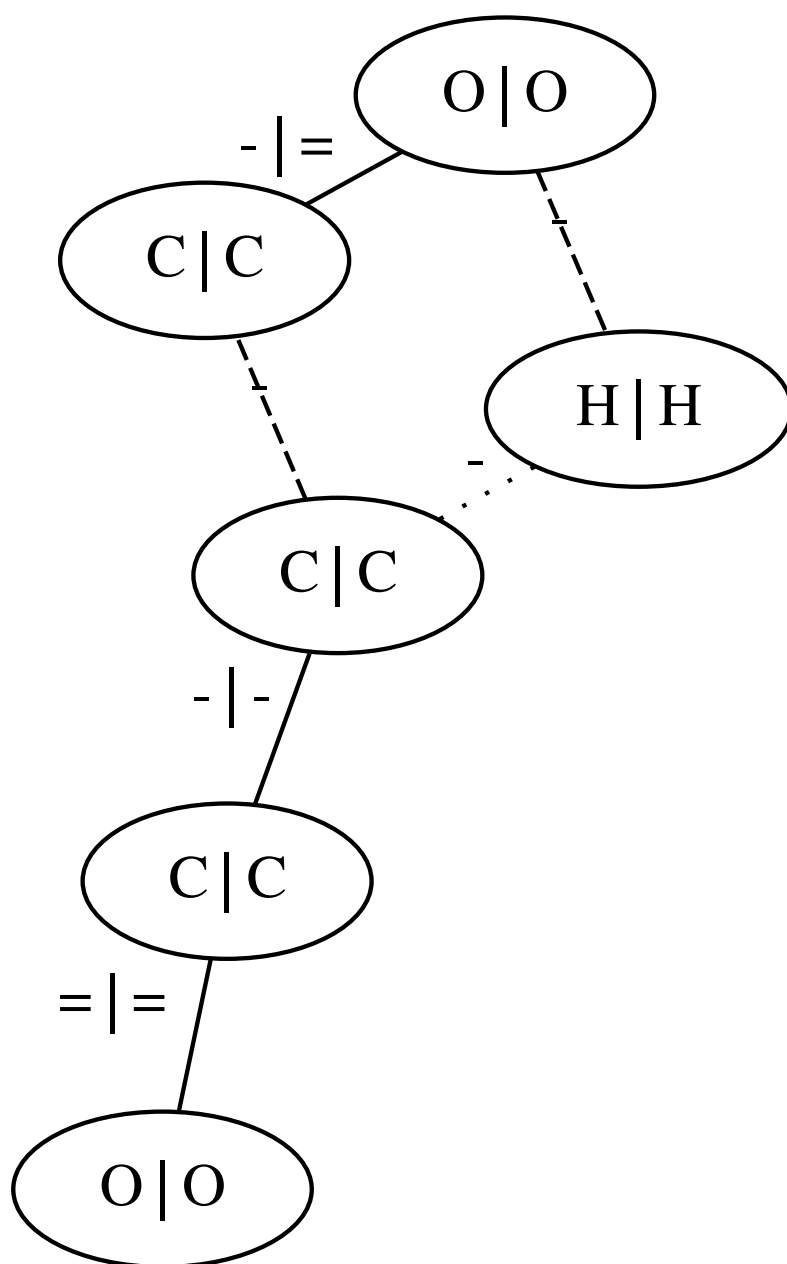
Files: out/017_r_2_11300100_{L, K, R}

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

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

0.0.5 Retro Aldol



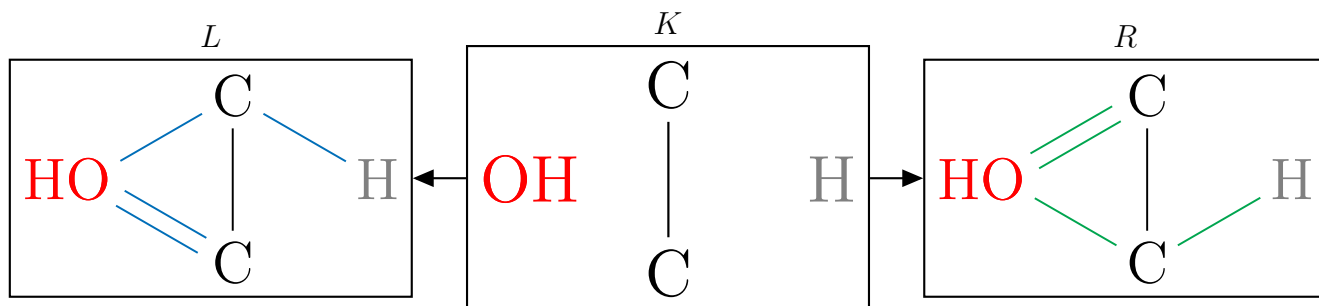
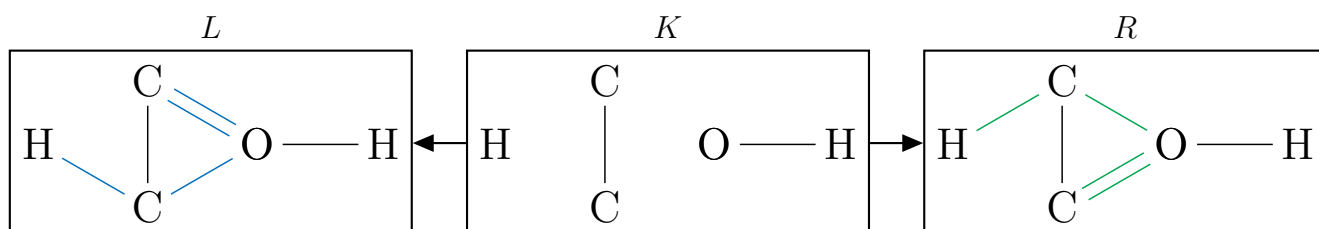


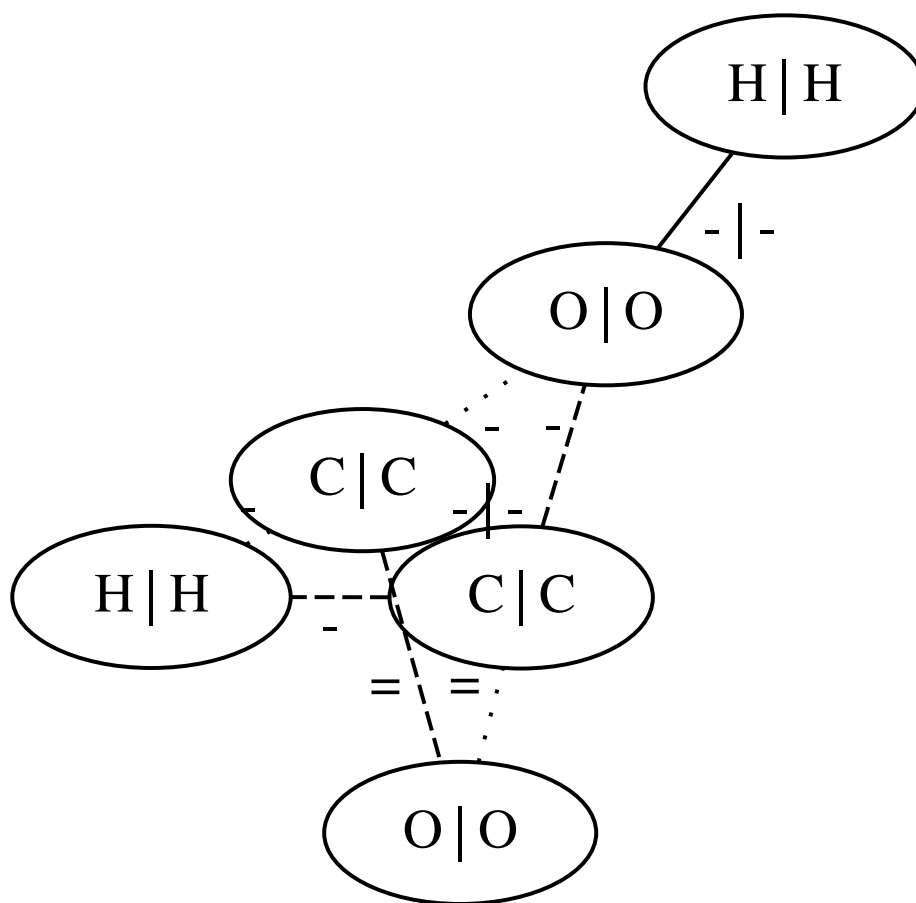
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$$\begin{aligned}
& |\{e \in \text{outEdges}(3) \mid \\
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& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
& \quad \}\} = 0
\end{aligned}$$

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

0.0.6 Keto-enol migration twice

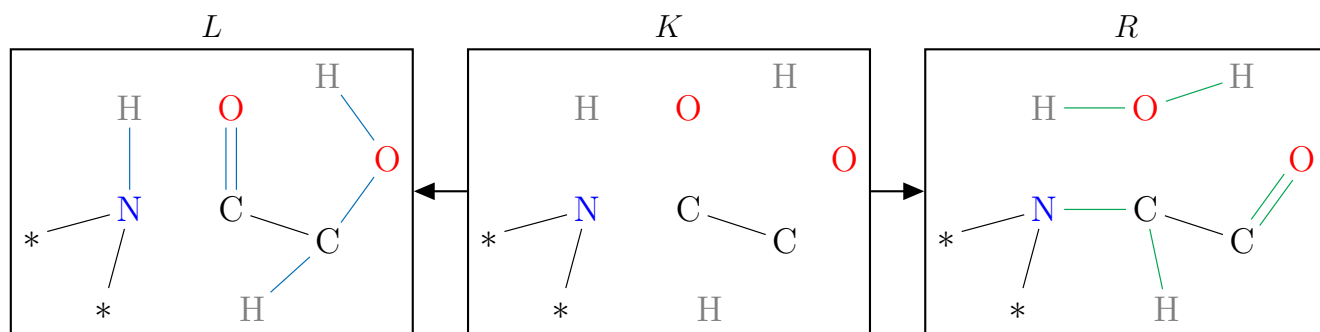
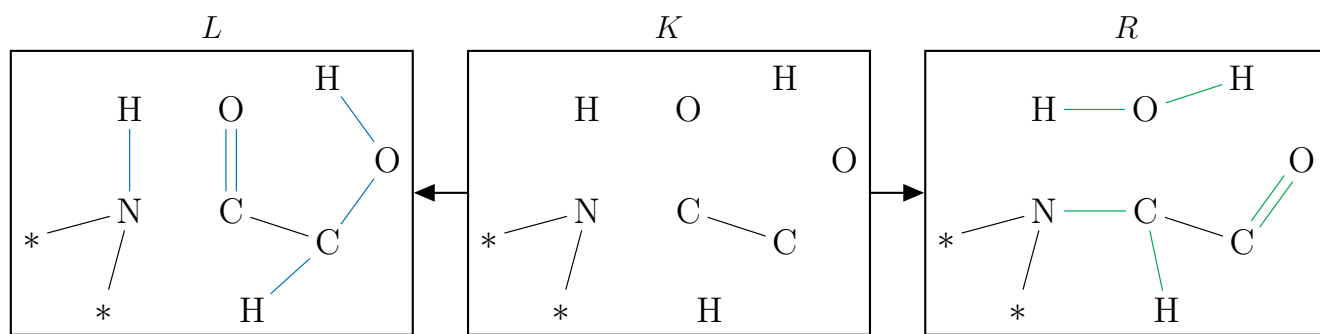


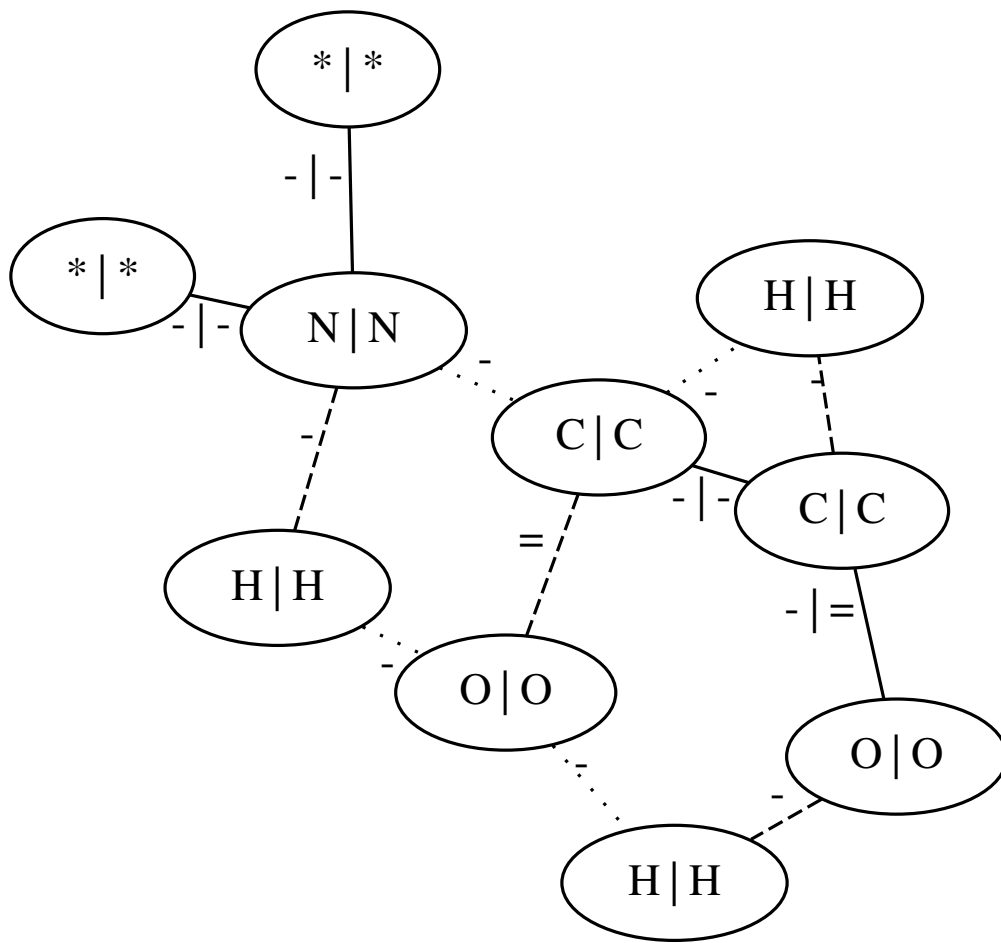


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$$\begin{aligned}
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 &\quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\}\mid = 0
 \end{aligned}$$

0.0.7 Amadori/Heyns Rearrangement





File: out/033_r_5_combined

$$|\{e \in \text{outEdges}(1) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$| = 0$$

$$|\{e \in \text{outEdges}(2) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

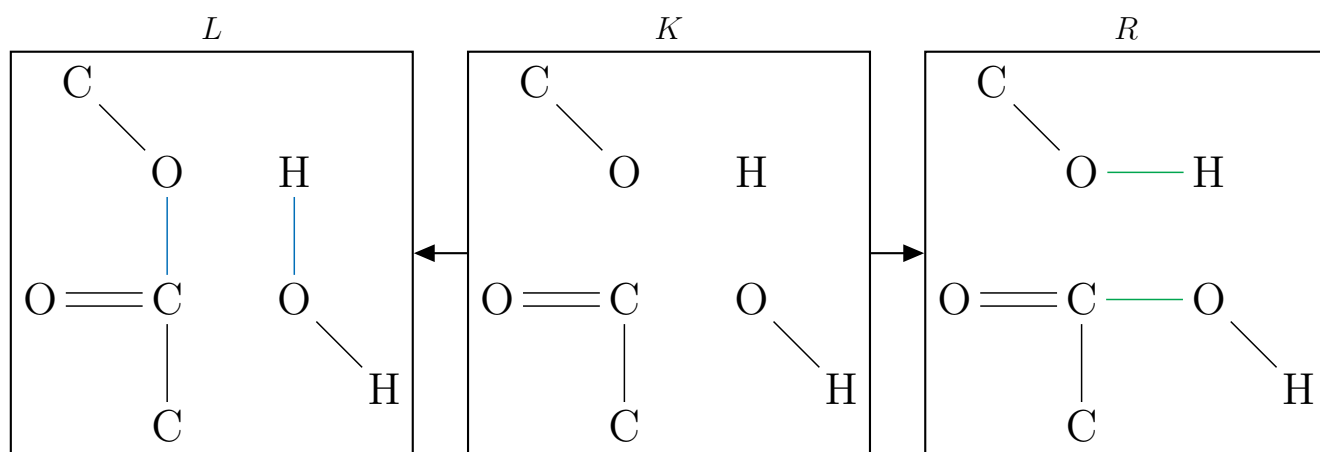
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$$\text{label}(e) \in \{'=\'}\}$$

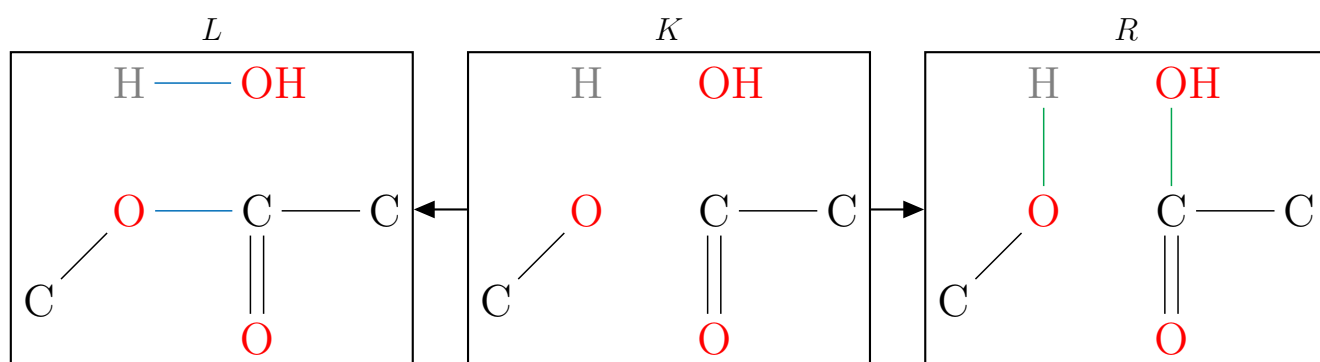
$$| = 0$$

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

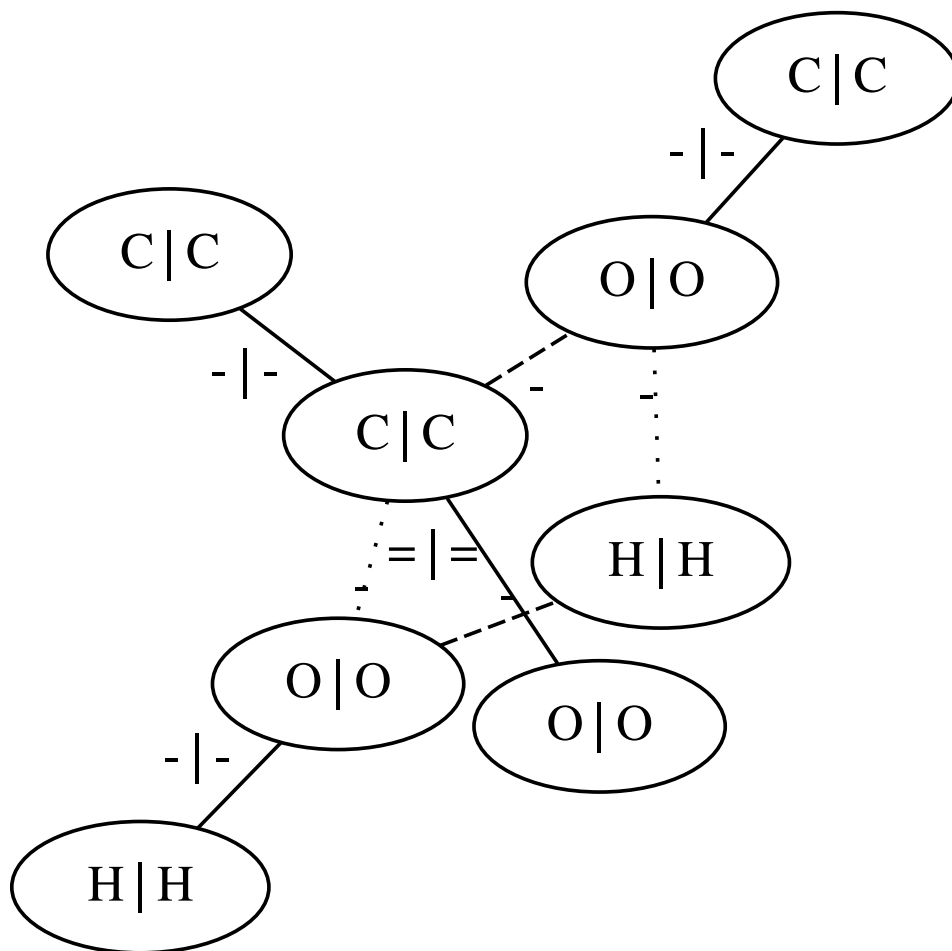
0.0.8 Ester Hydrolysis



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



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



File: out/038_r_6_combined

$$|\{e \in \text{outEdges}(4) \mid$$

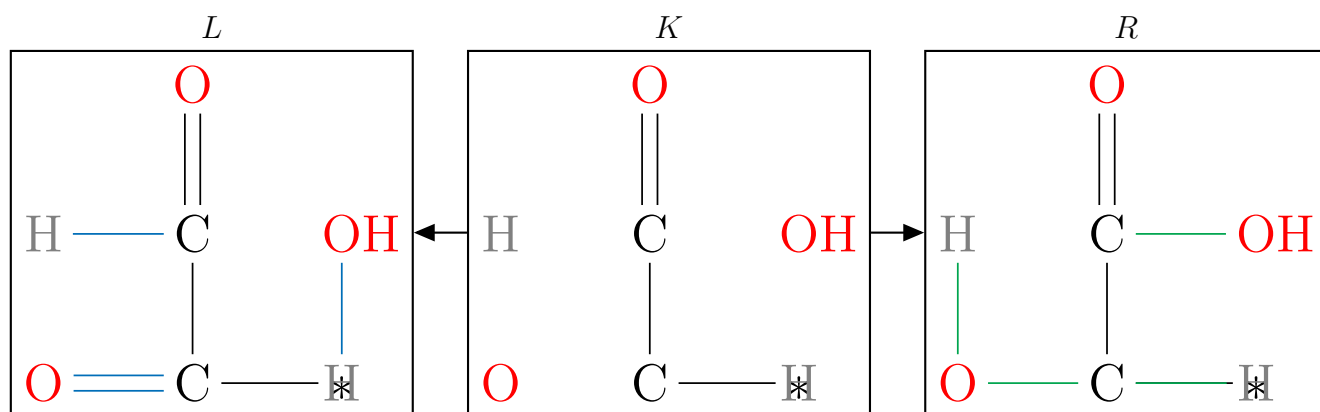
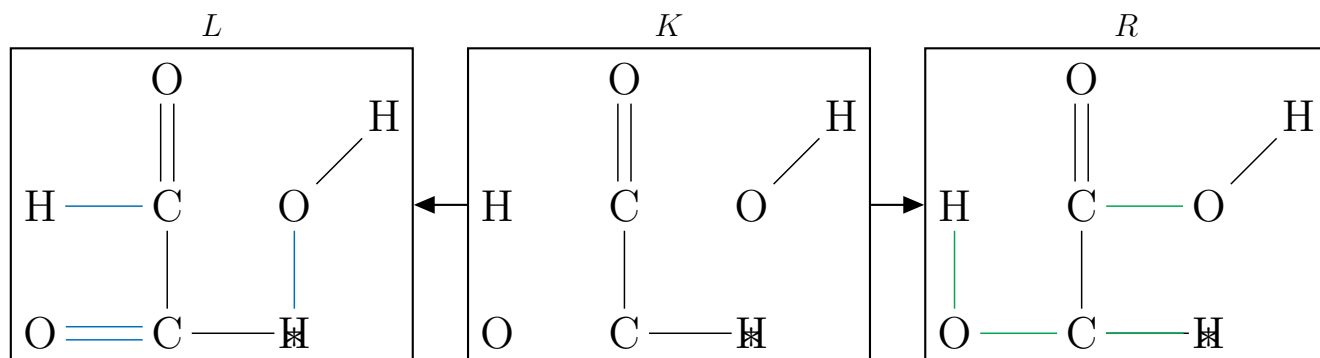
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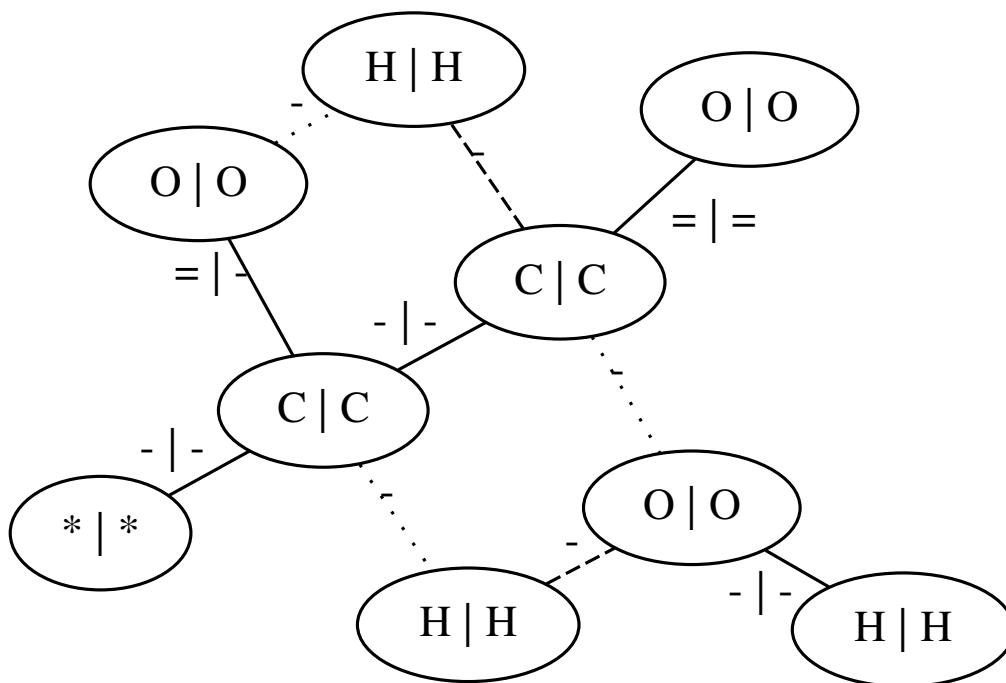
$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

0.0.9 Cannizzaro 1

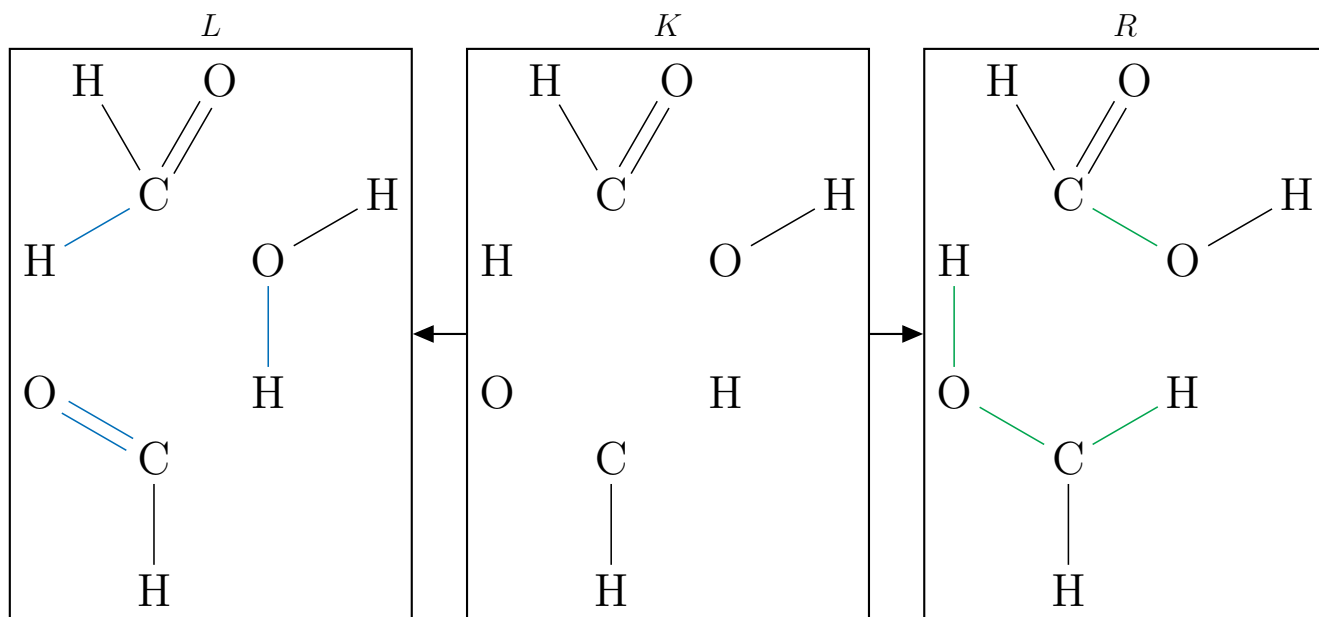




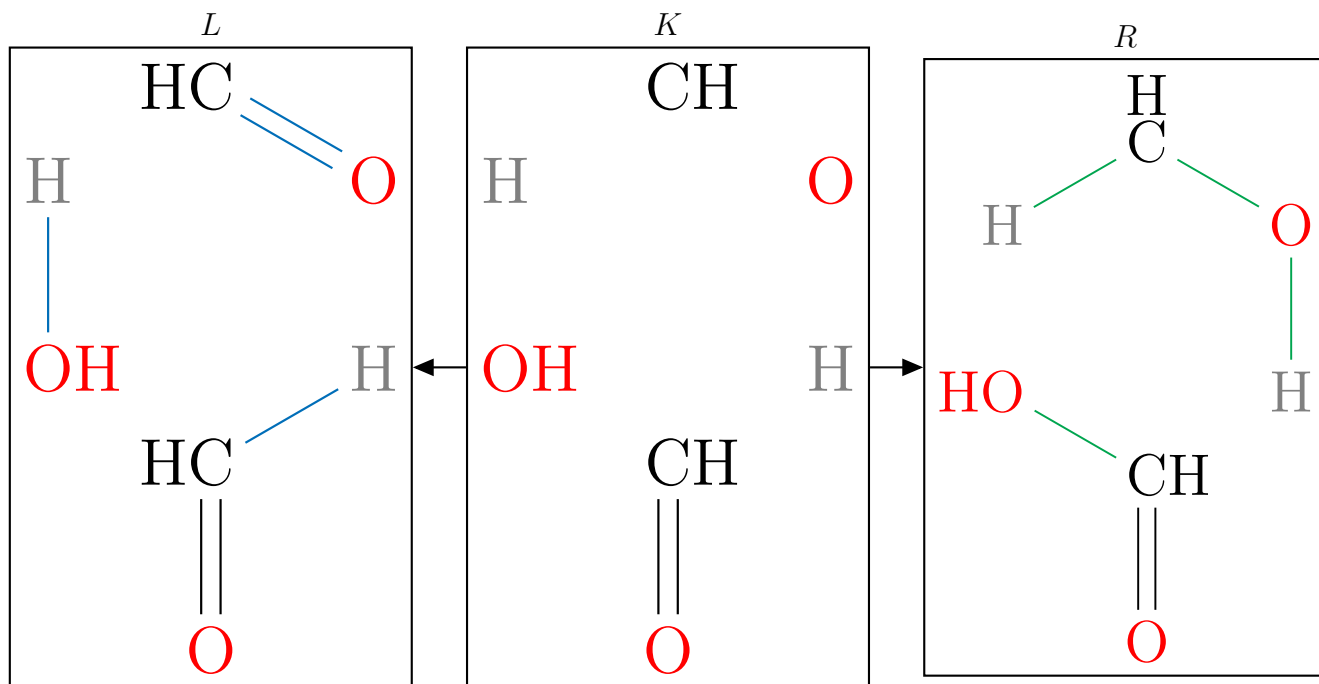
File: out/043_r_7_combined

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

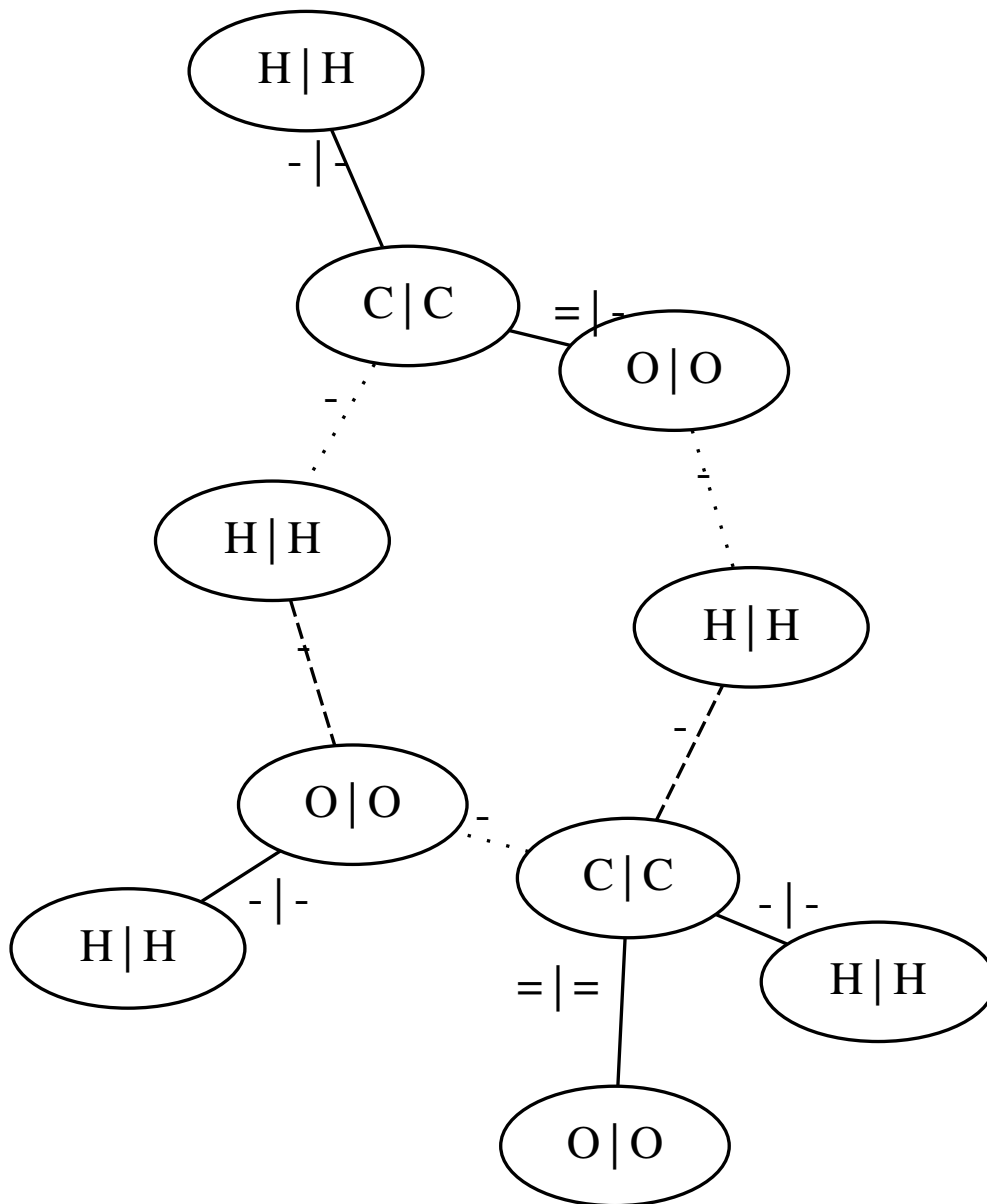
0.0.10 Cannizarro 2, HCHO (oxidation)



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



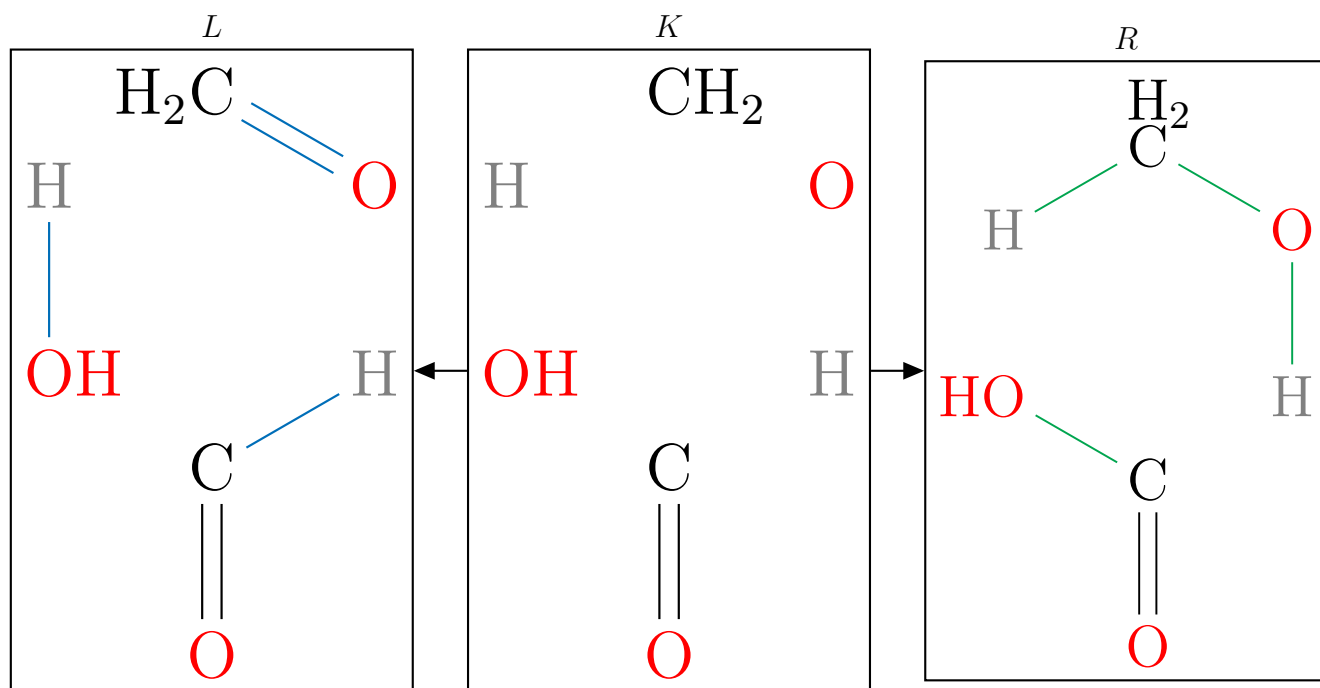
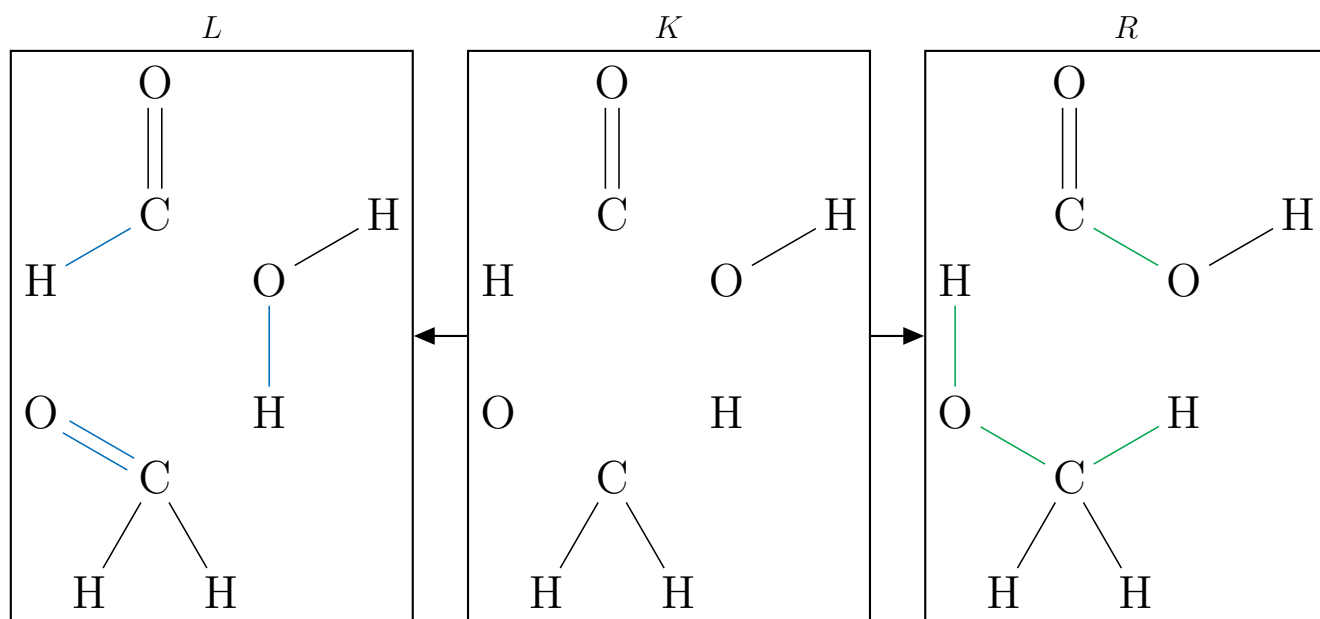
Files: out/047_r_8_11300100_{L, K, R}

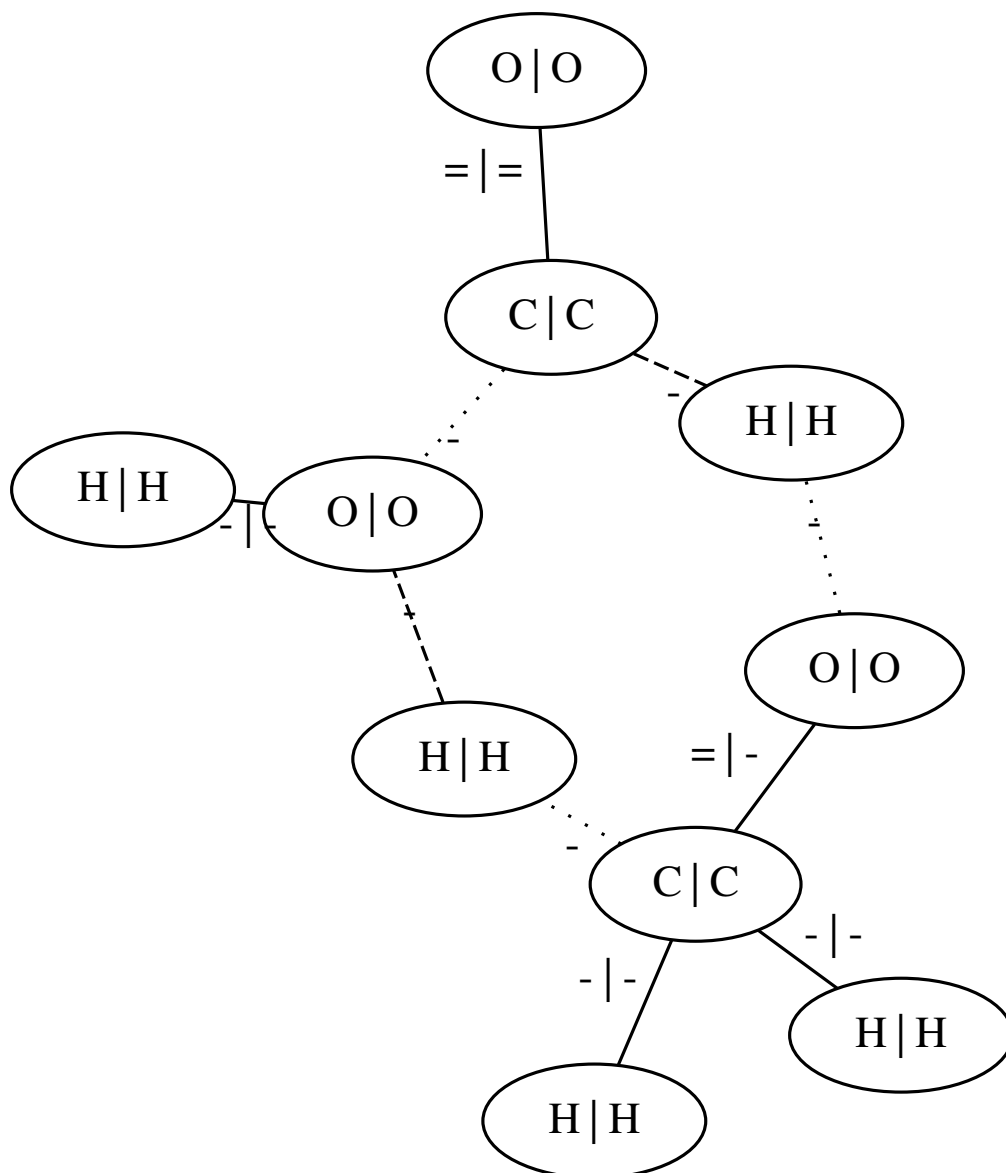


File: out/048_r_8_combined

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

0.0.11 Cannizarro 2, HCHO (reduction)

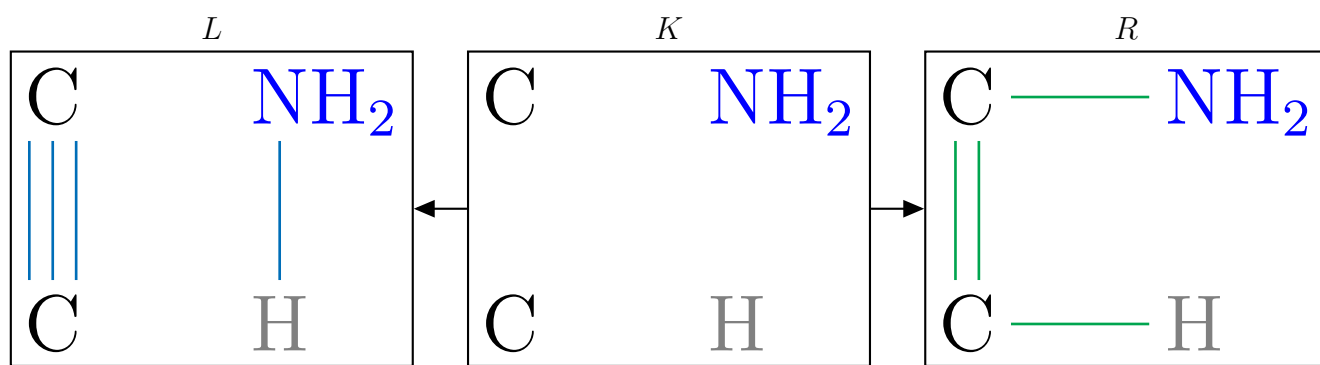
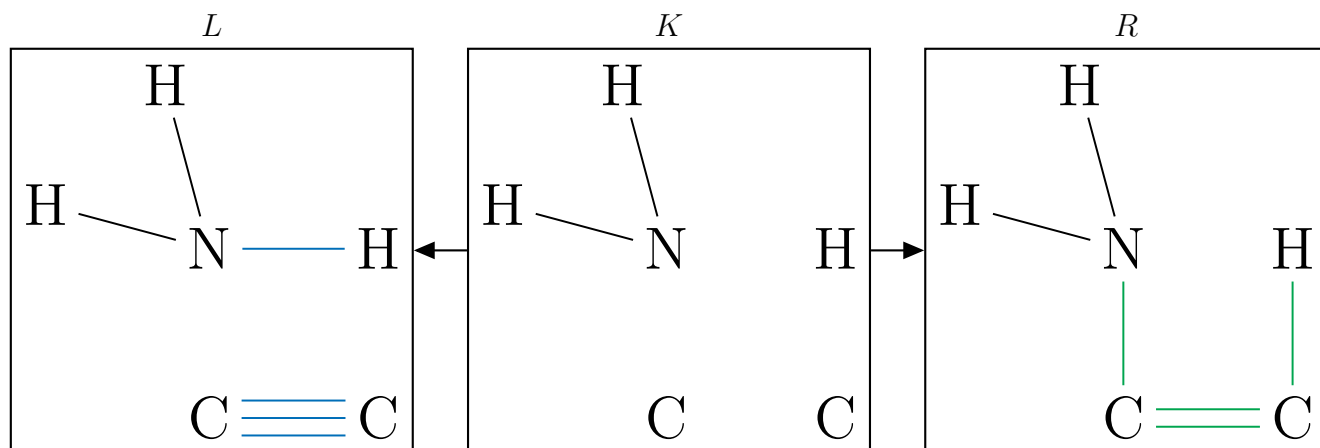


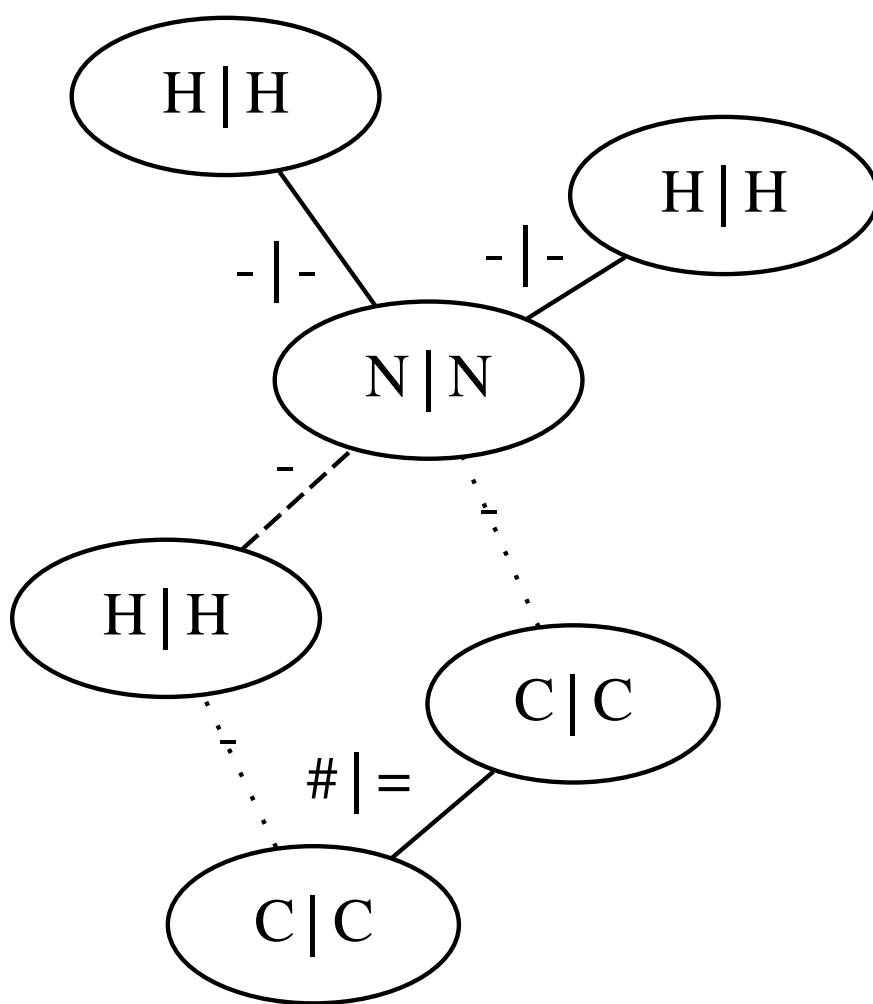


File: out/053_r_9_combined

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

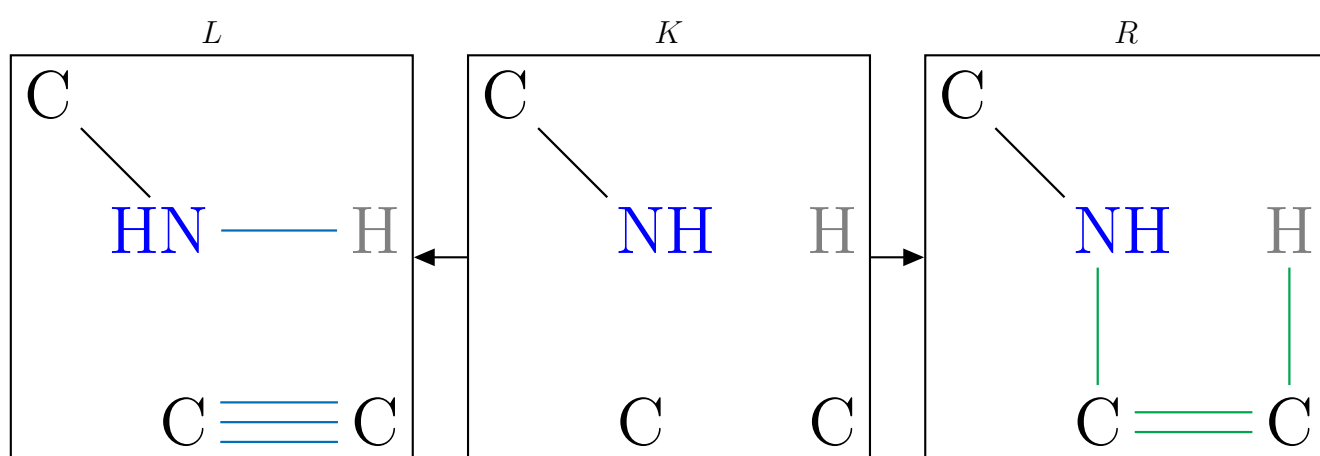
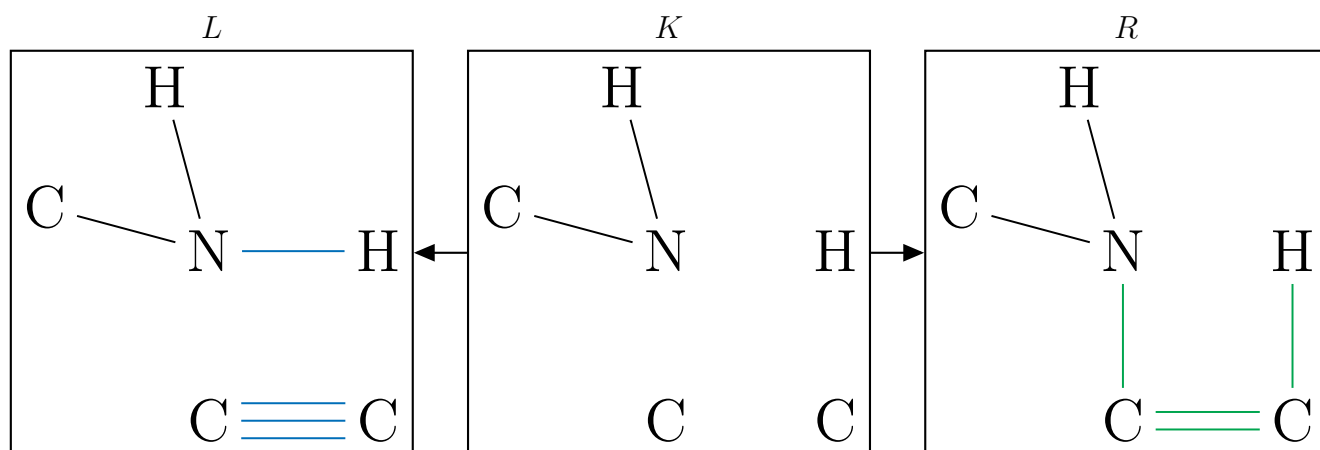
0.0.12 Alkyne Addition, N, HH

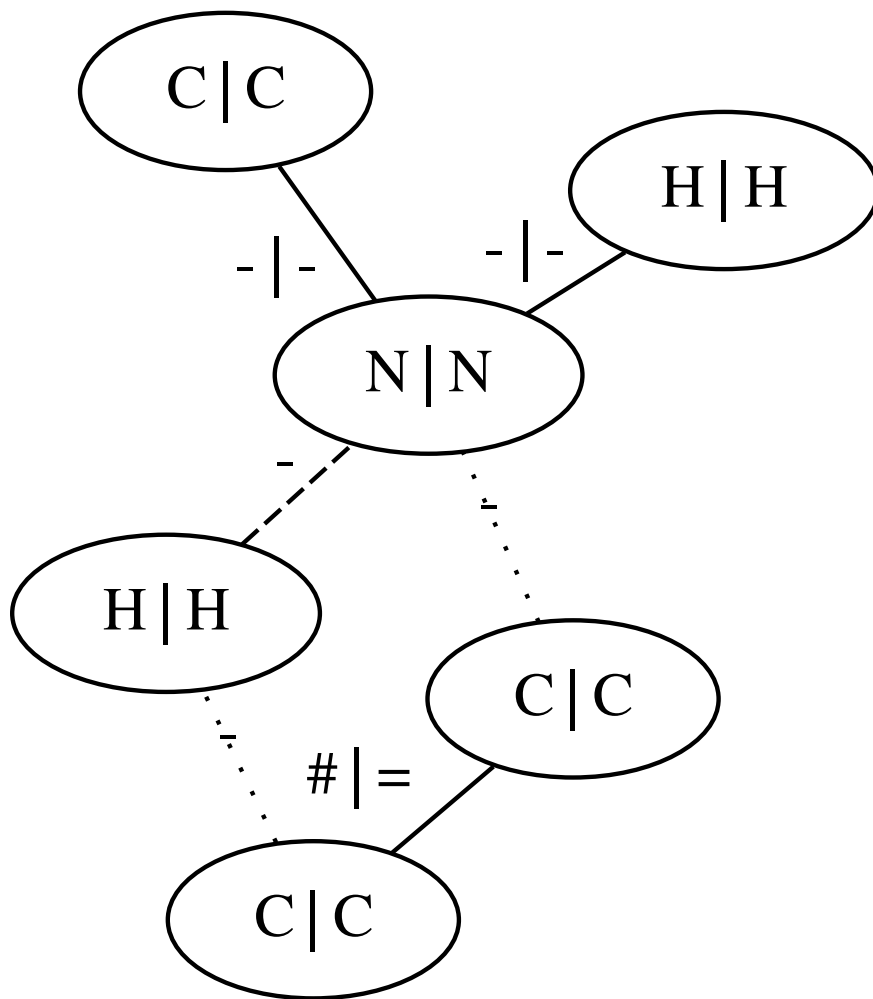




File: out/058_r_10_combined

0.0.13 Alkyne Addition, N, HC

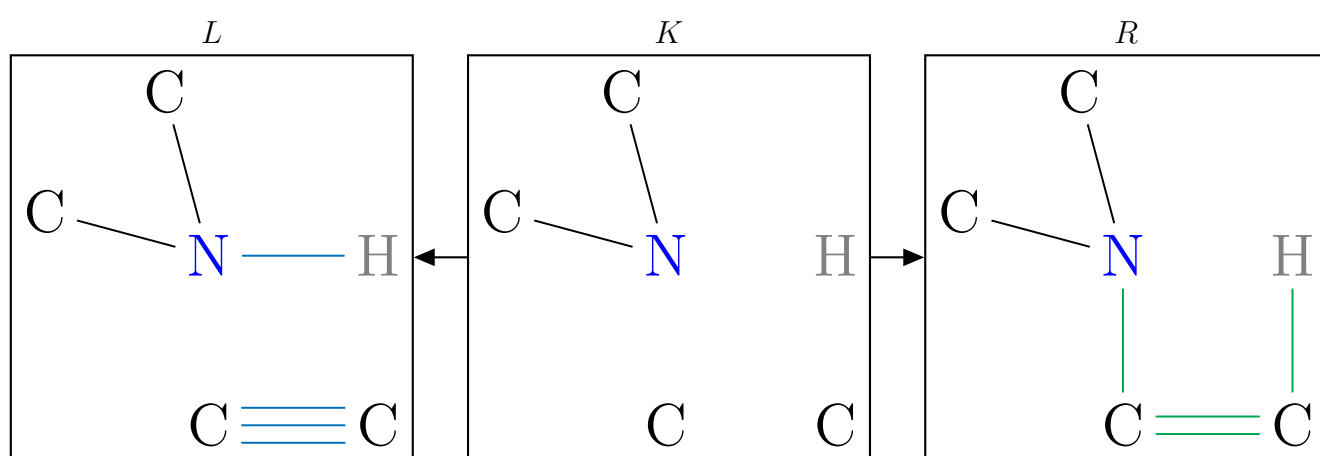
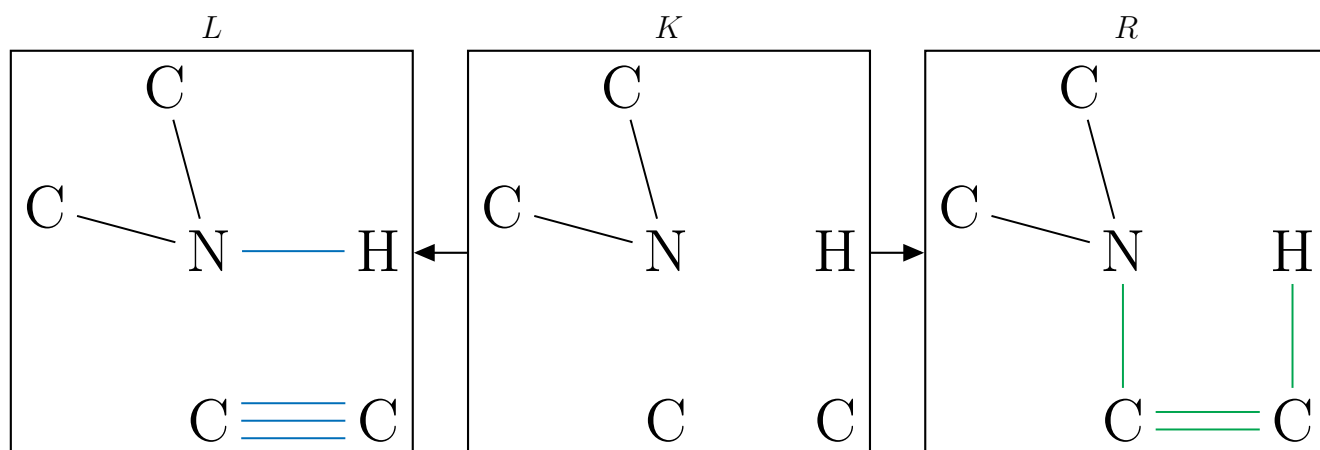


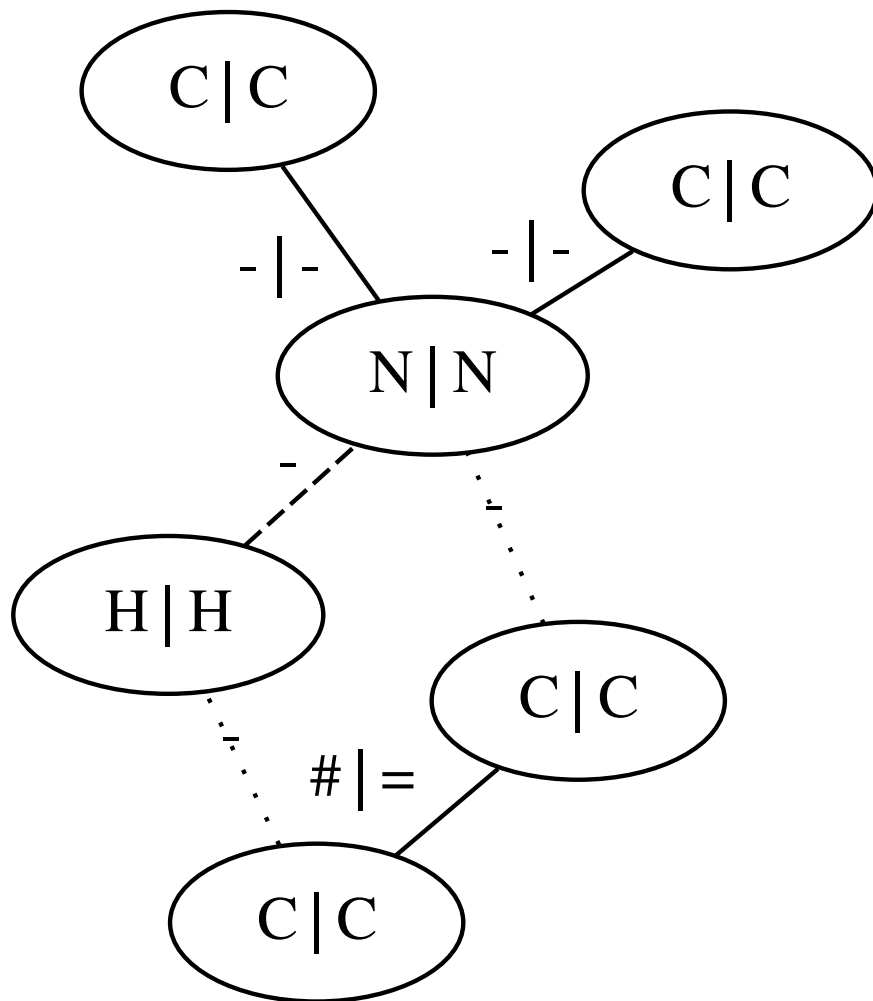


File: out/063_r_11_combined

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

0.0.14 Alkyne Addition, N, CC



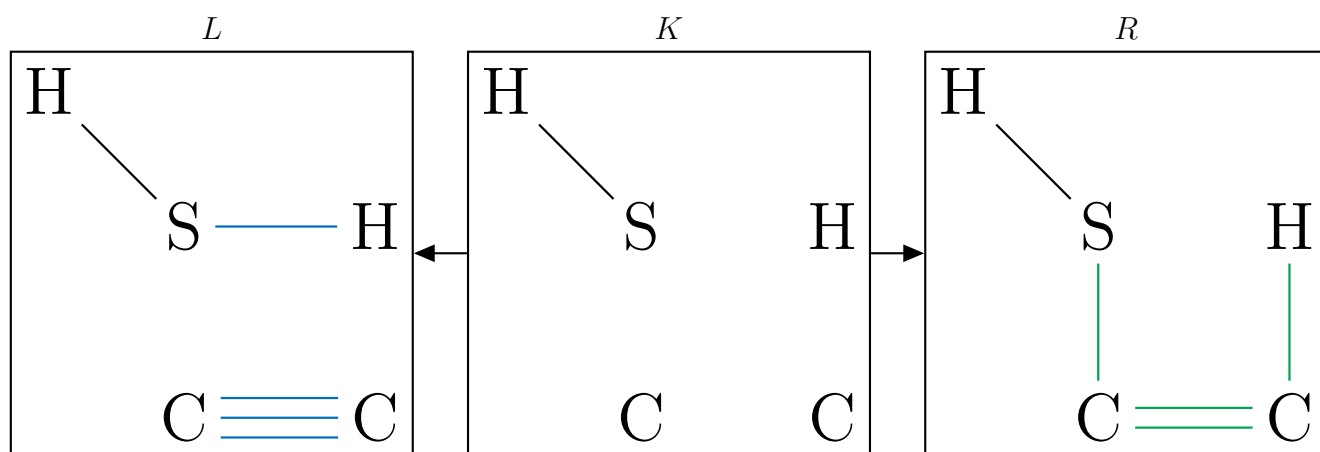


File: out/068_r_12_combined

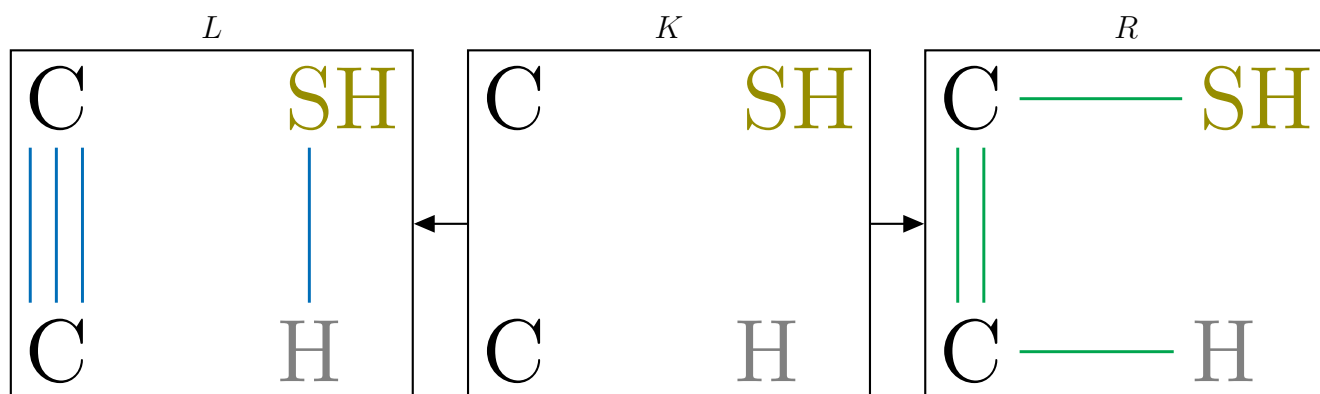
$$\begin{aligned}
 &|\{e \in \text{outEdges}(4) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{'=\'} \\
 &\}\} = 0
 \end{aligned}$$

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

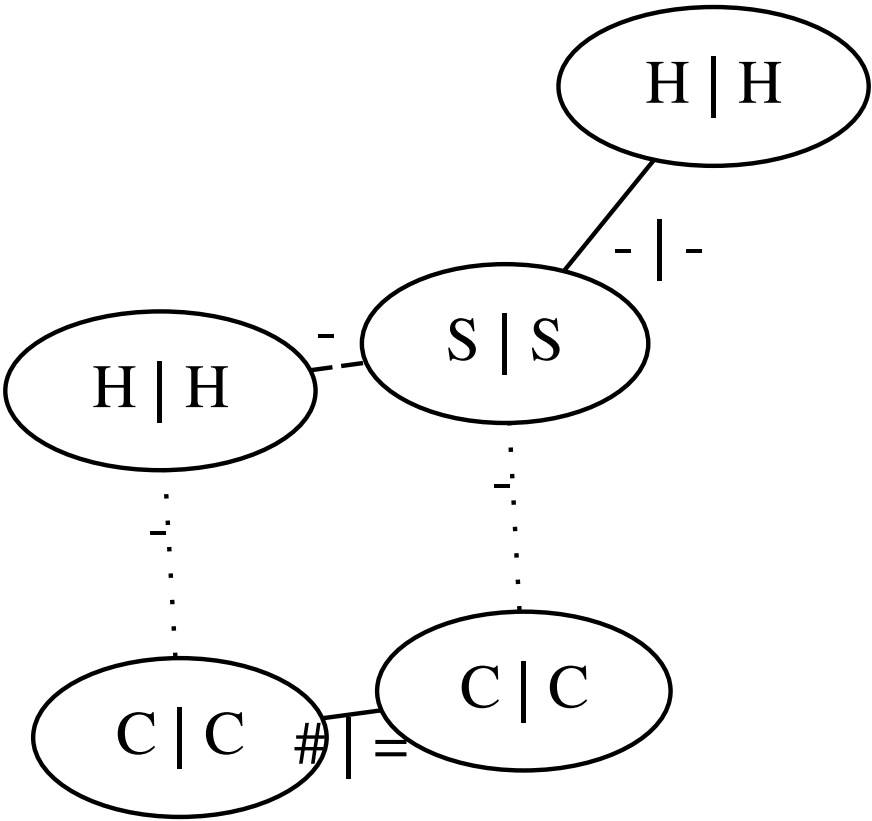
0.0.15 Alkyne Addition, S, H



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

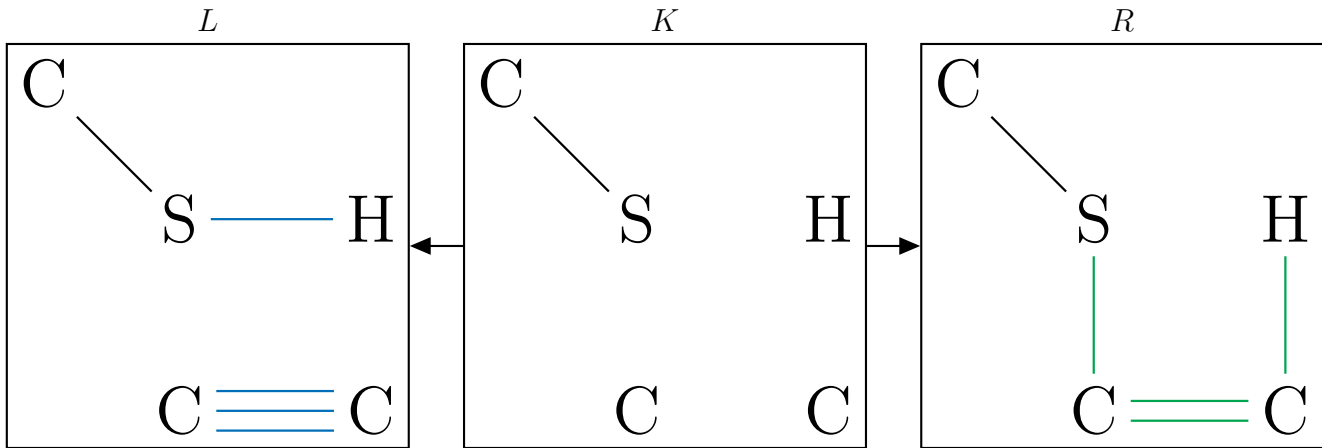


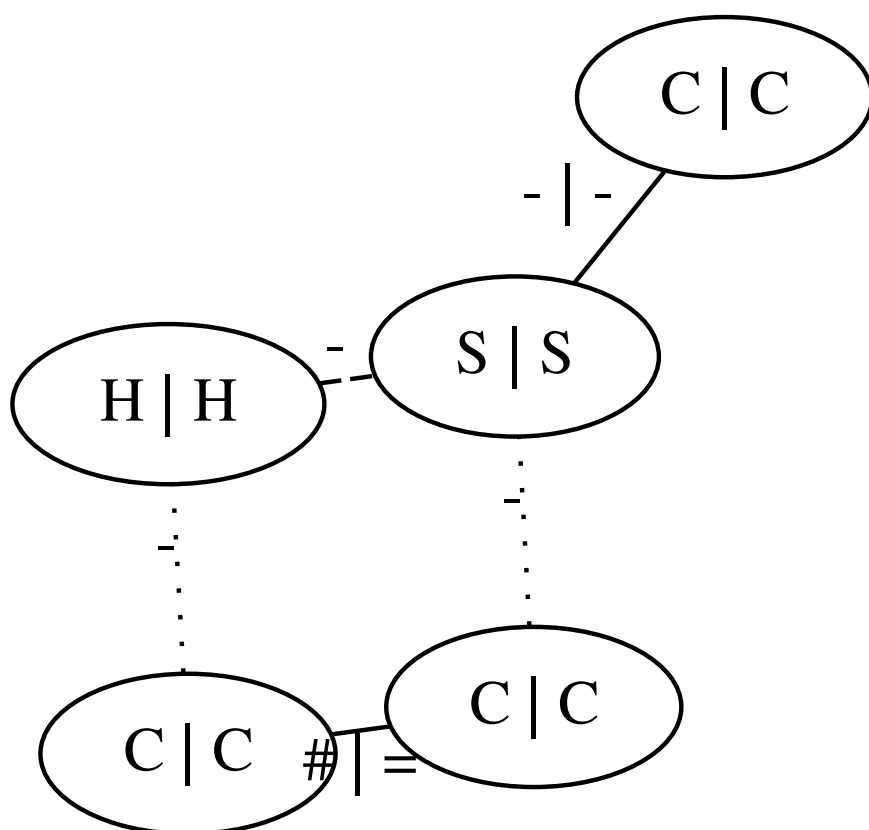
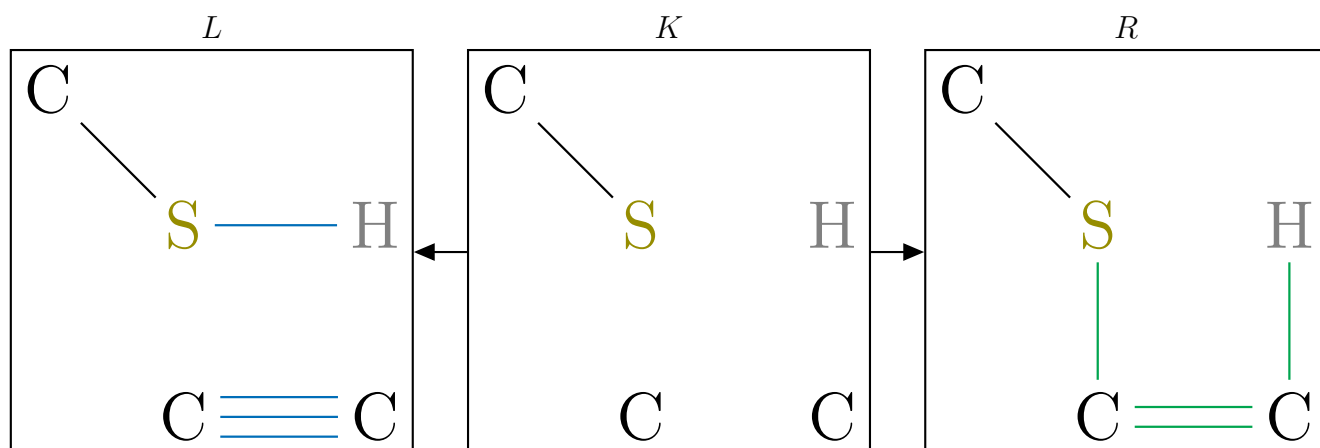
Files: out/072_r_13_11300100_{L, K, R}



File: out/073_r_13_combined

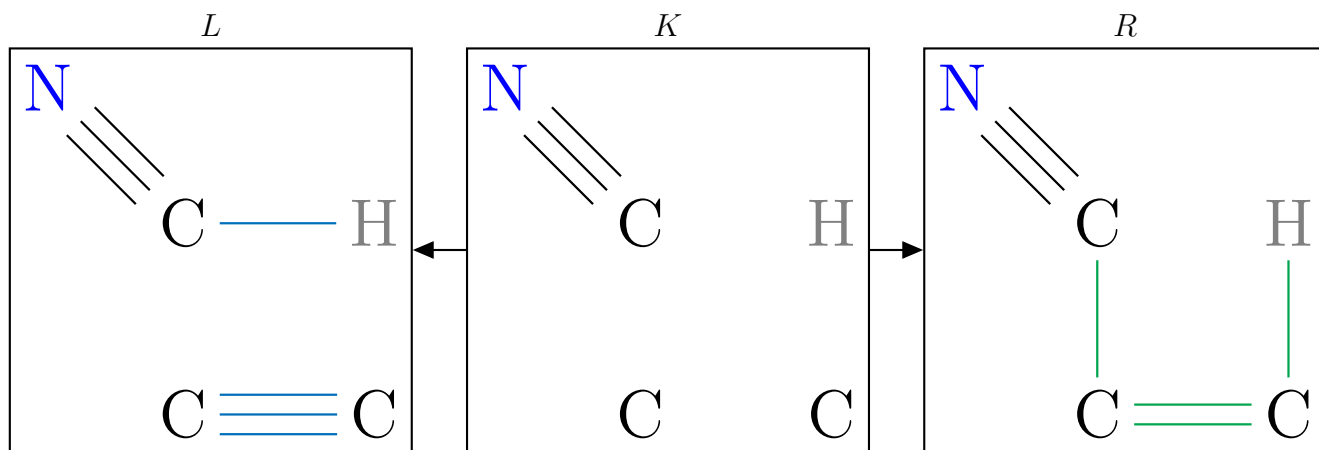
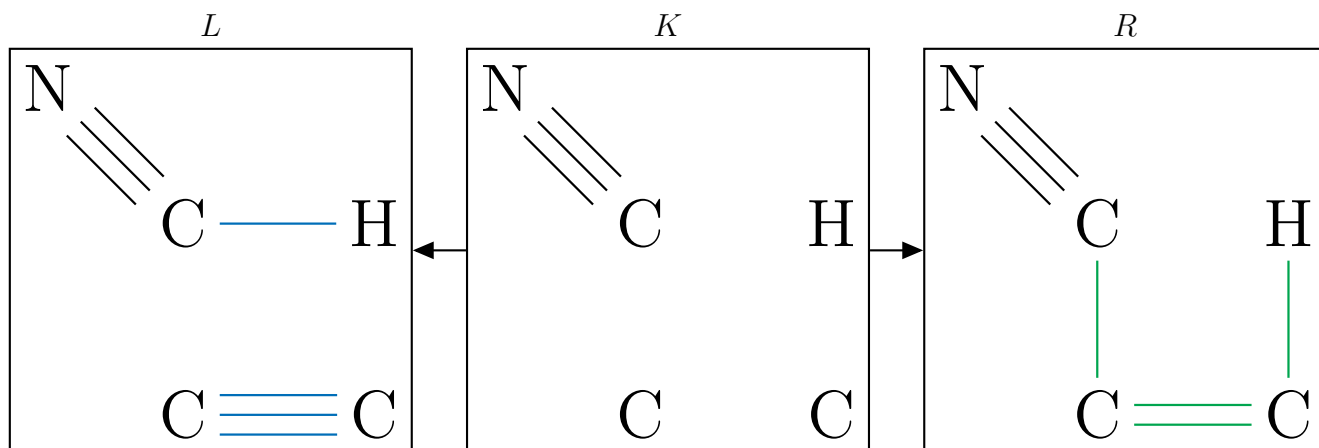
0.0.16 Alkyne Addition, S, C

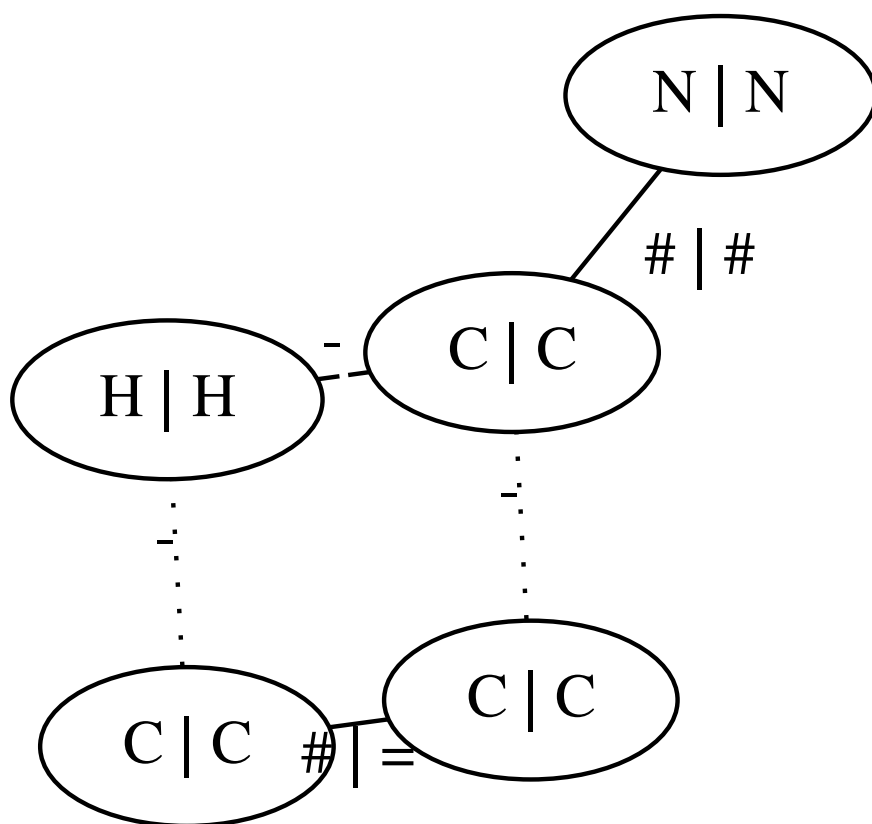




$$\begin{aligned}
 &|\{e \in \text{outEdges}(4) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{'=\'}\} \\
 &\quad \} = 0
 \end{aligned}$$

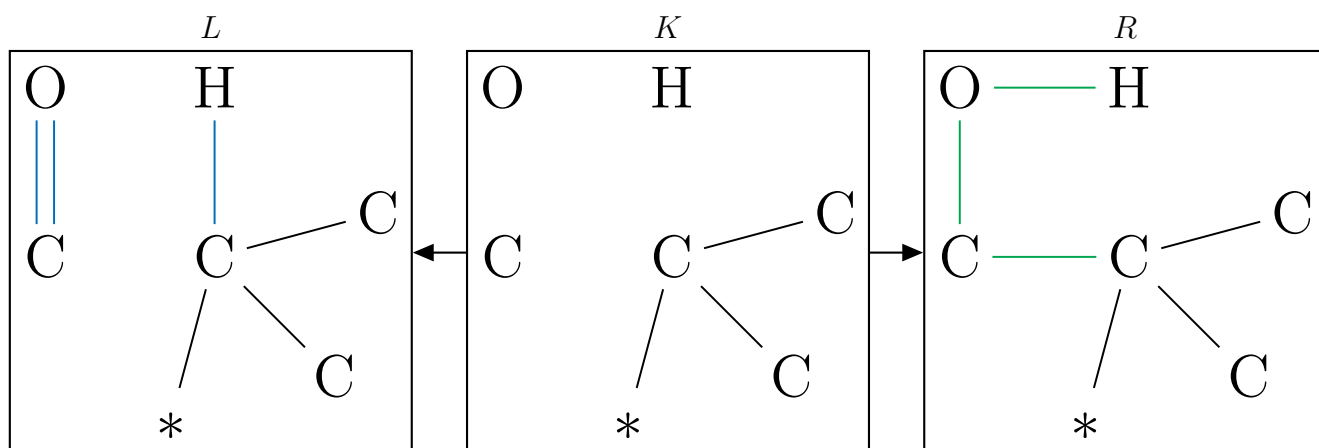
0.0.17 Alkyne Addition, C



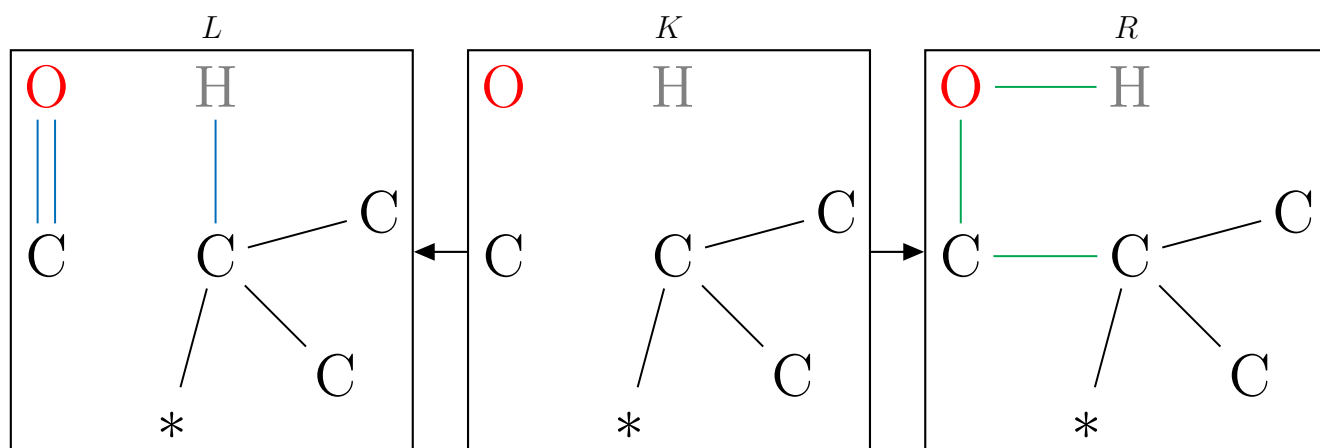


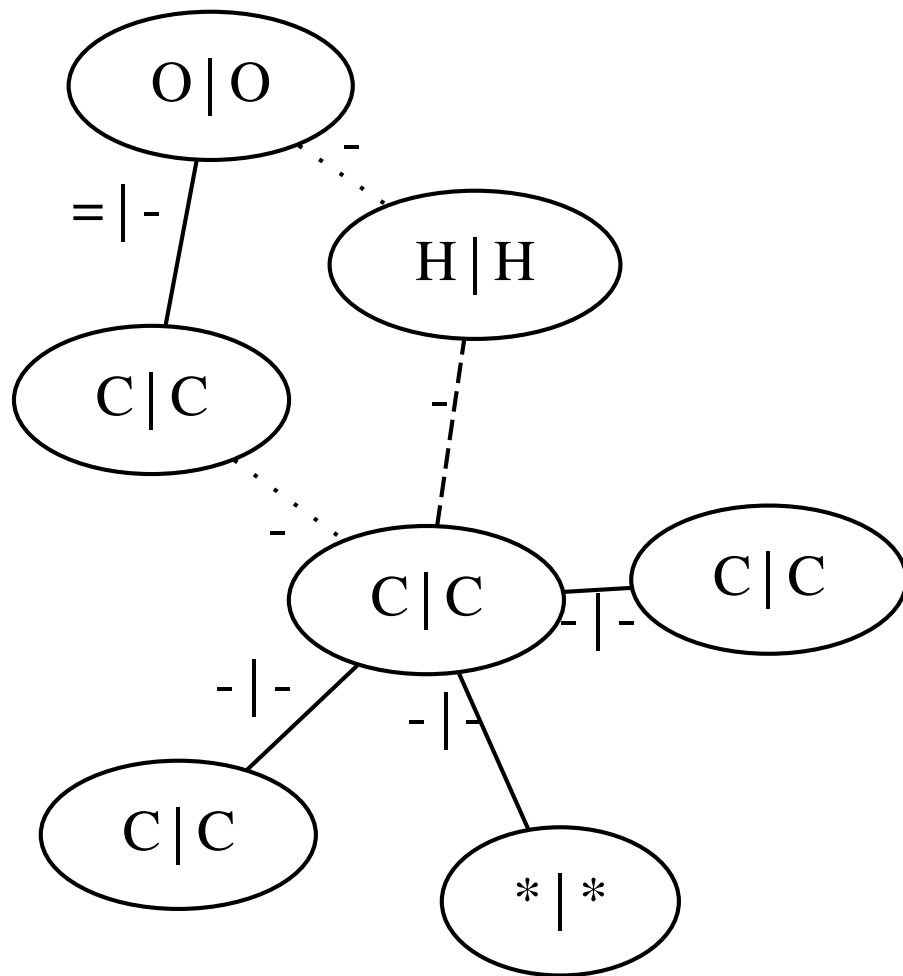
File: out/083_r_15_combined

0.0.18 Knoevenagel C



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





File: out/088_r_16_combined

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

$$|\{e \in \text{outEdges}(5) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'\#'}, \text{'='}\}$$

$$\}| = 1$$

$$|\{e \in \text{outEdges}(6) \mid$$

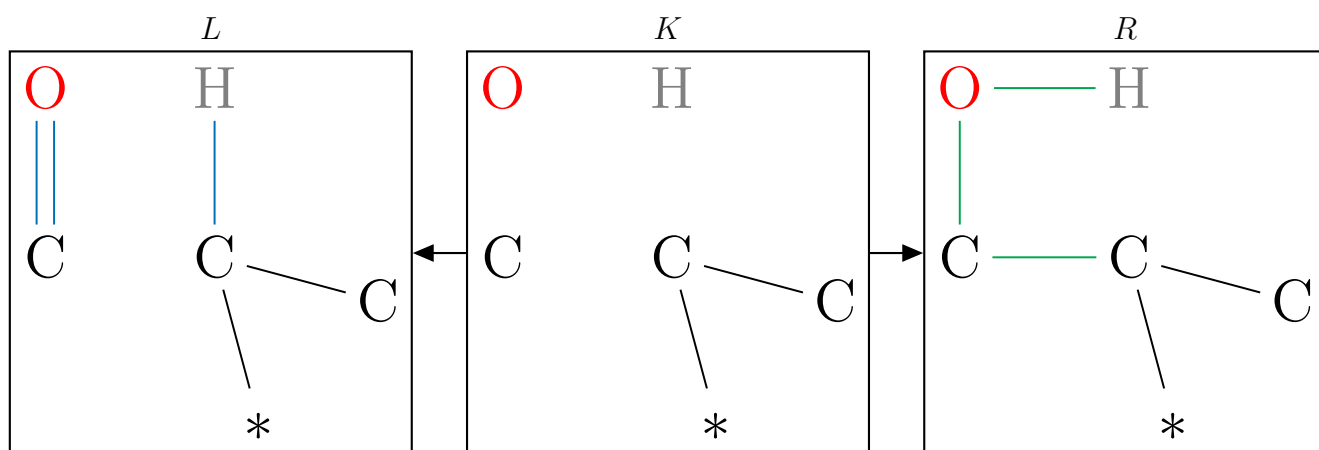
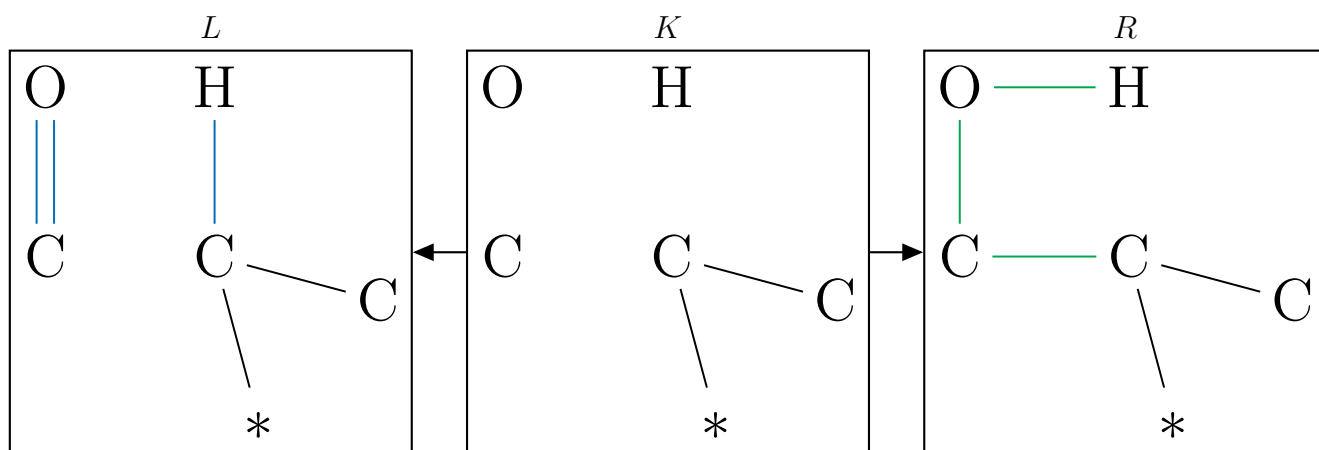
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

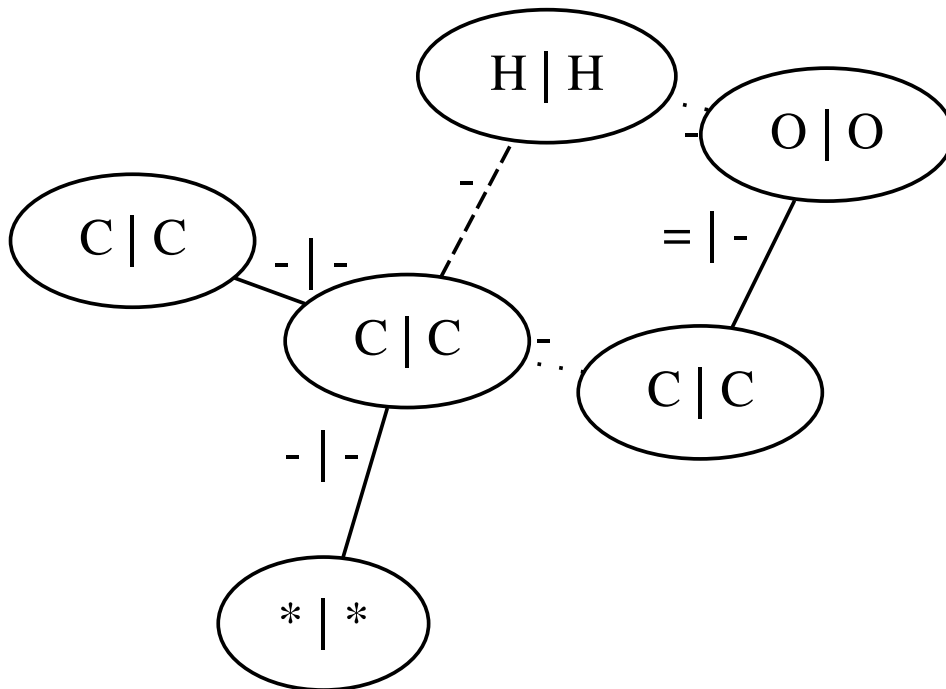
$$\wedge$$

$$\text{label}(e) \in \{\text{'\#'}, \text{'-'}, \text{'='}\}$$

$$\}| \geq 1$$

0.0.19 Knoevenagel H





File: out/093_r_17_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

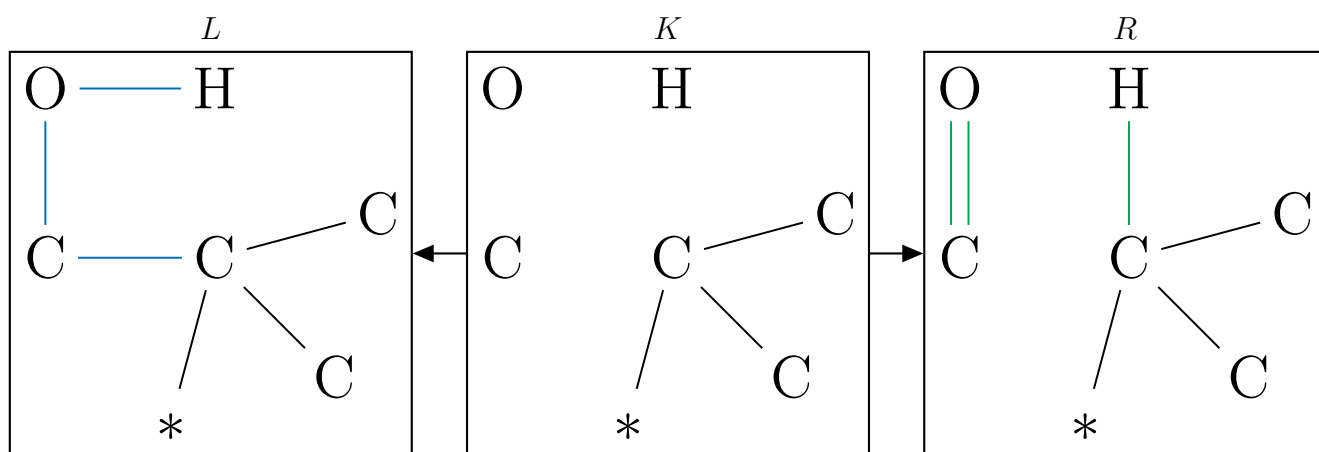
$$\wedge$$

$$\text{label}(e) \in \{\text{'\#'}, \text{'='}\}$$

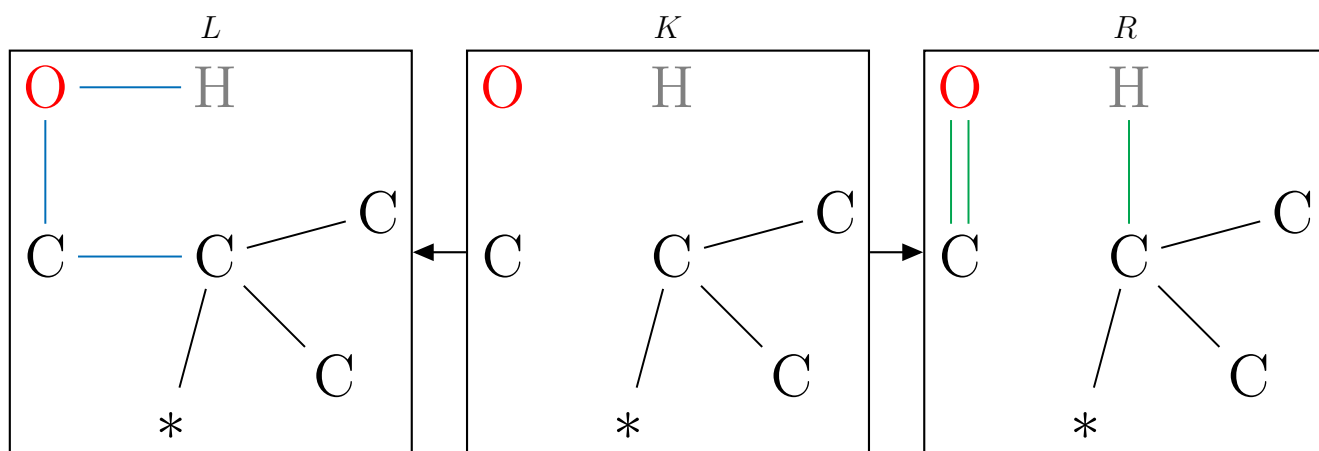
$$\}| = 1$$

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

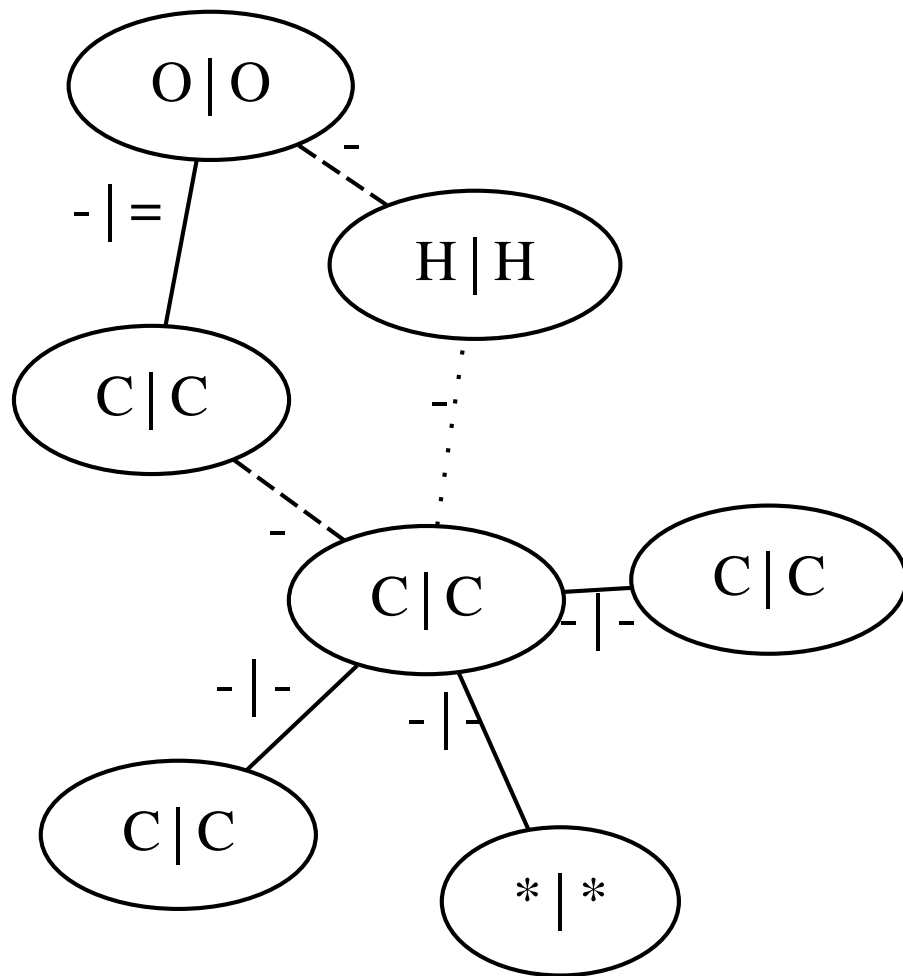
0.0.20 Knoevenagel C (inverse)



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



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



File: out/098_r_18_combined

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

$$|\{e \in \text{outEdges}(5) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'\#'}, \text{'='}\}$$

$$\}| = 1$$

$$|\{e \in \text{outEdges}(6) \mid$$

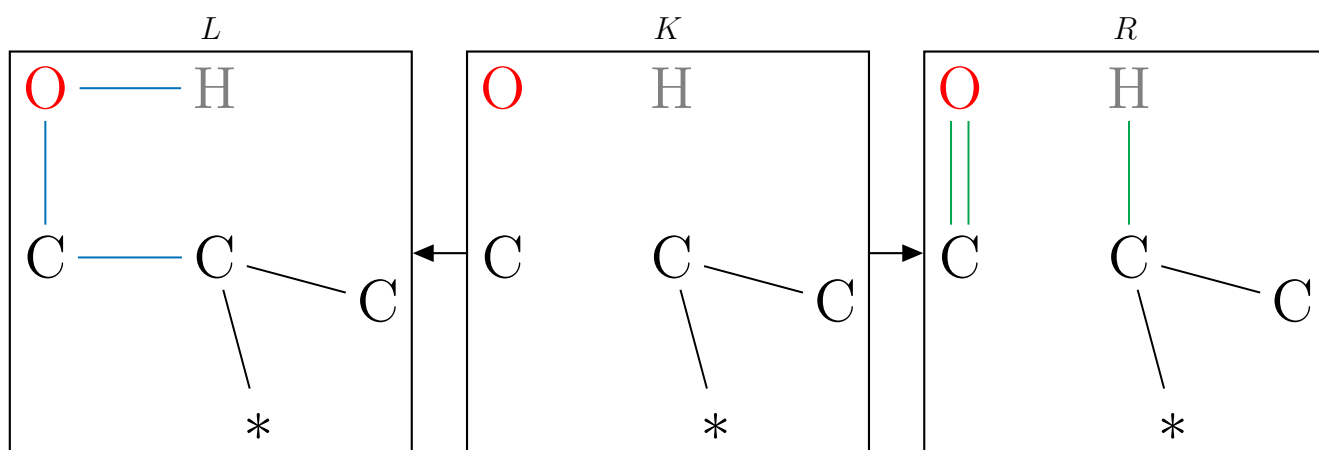
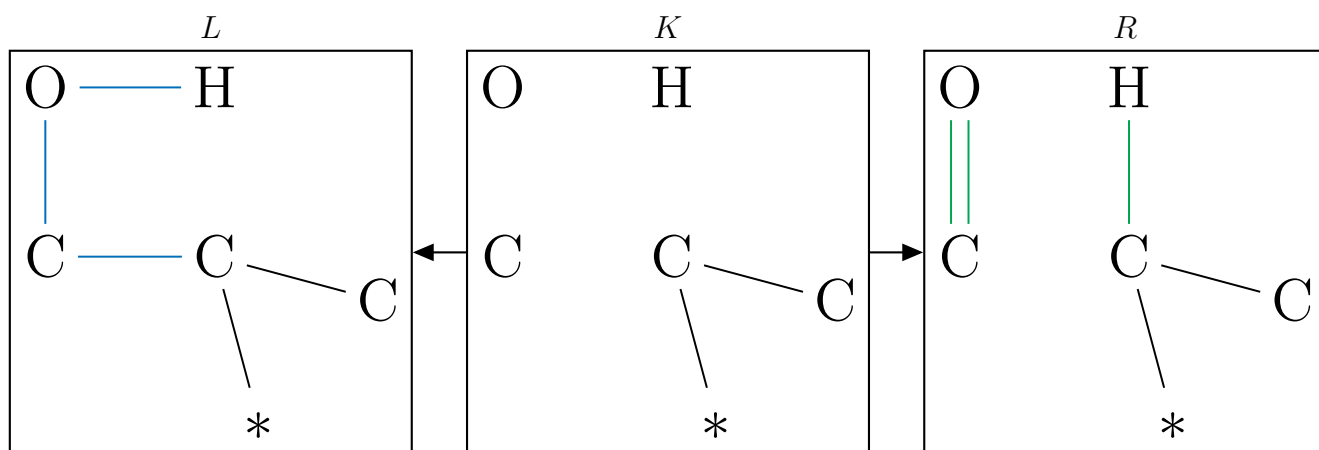
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

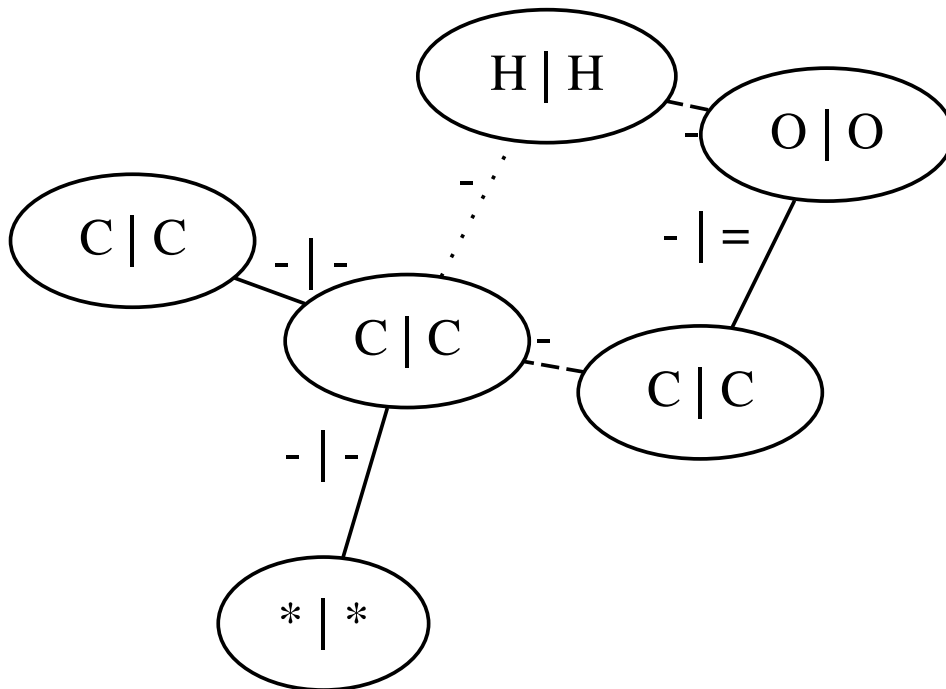
$$\wedge$$

$$\text{label}(e) \in \{\text{'\#'}, \text{'-'}, \text{'='}\}$$

$$\}| \geq 1$$

0.0.21 Knoevenagel H (inv)





File: out/103_r_19_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

$$\text{label}(\text{target}(e)) \in \{'N', '0'\}$$

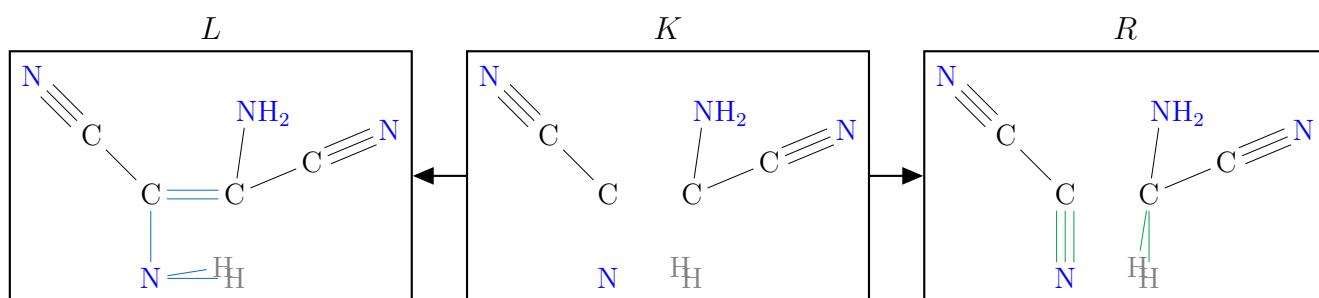
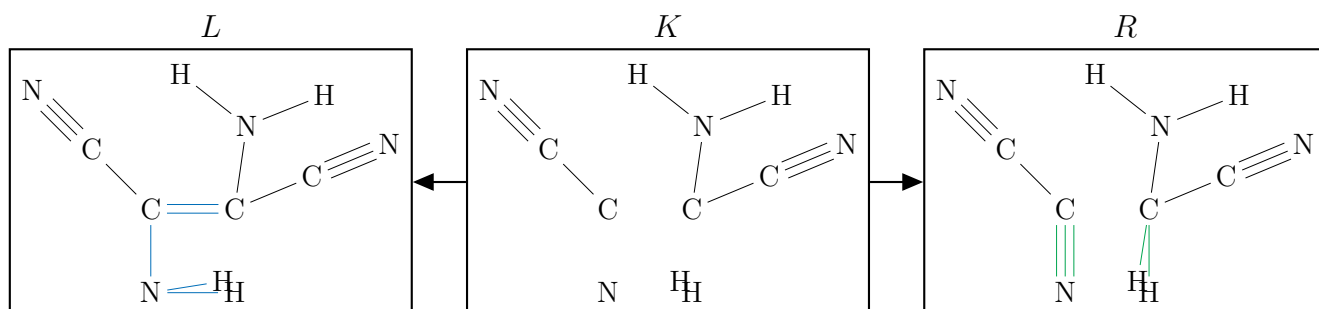
$$\wedge$$

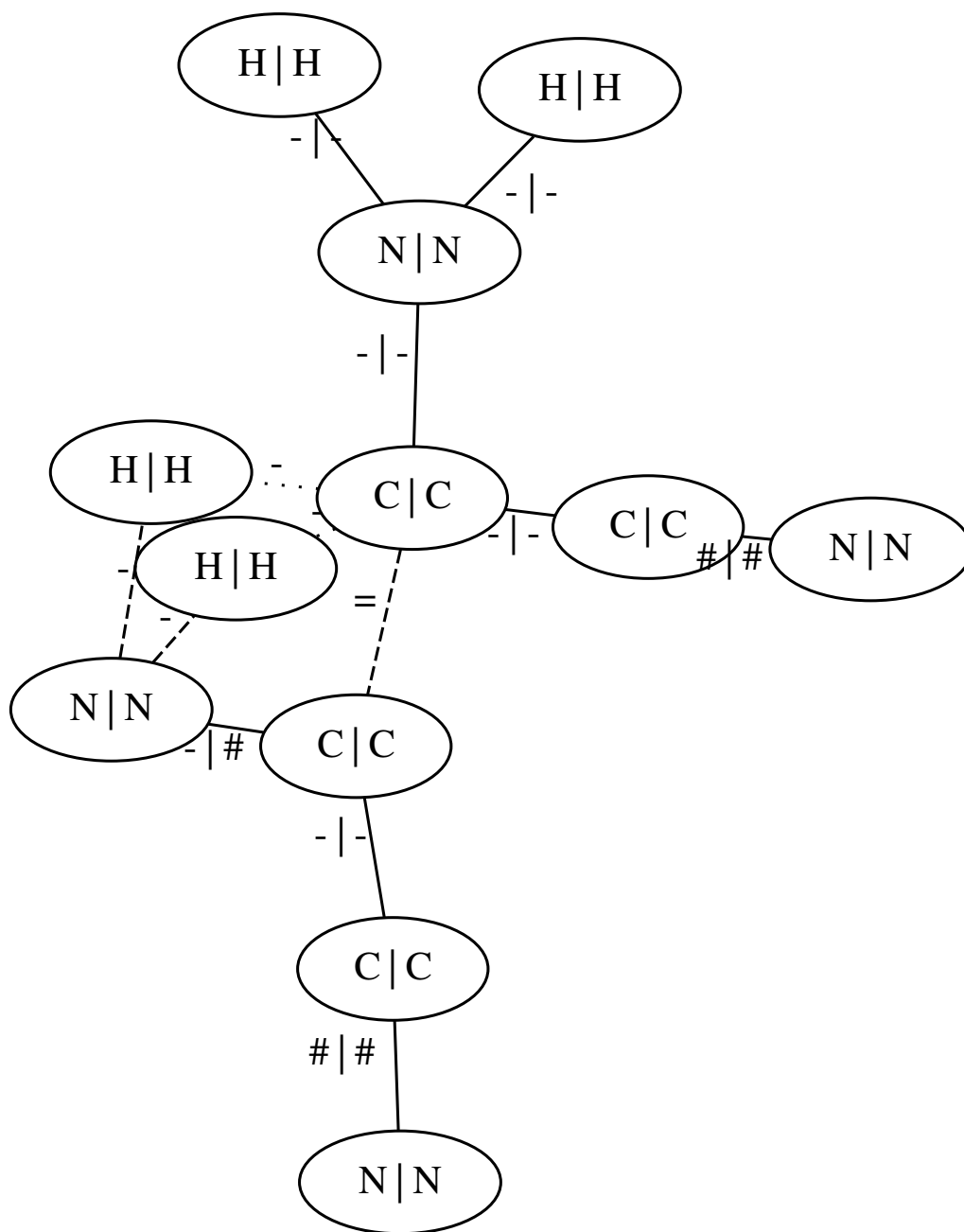
$$\text{label}(e) \in \{'\#', '='\}$$

$$| = 1$$

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

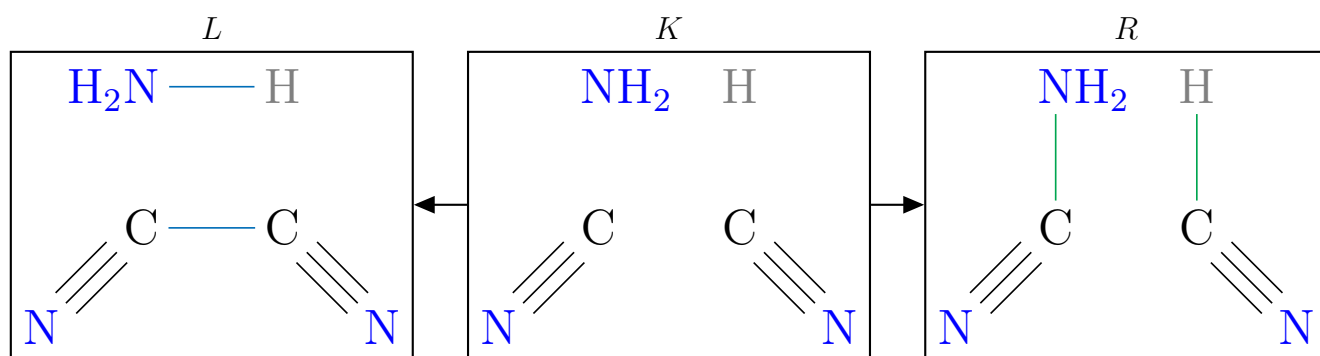
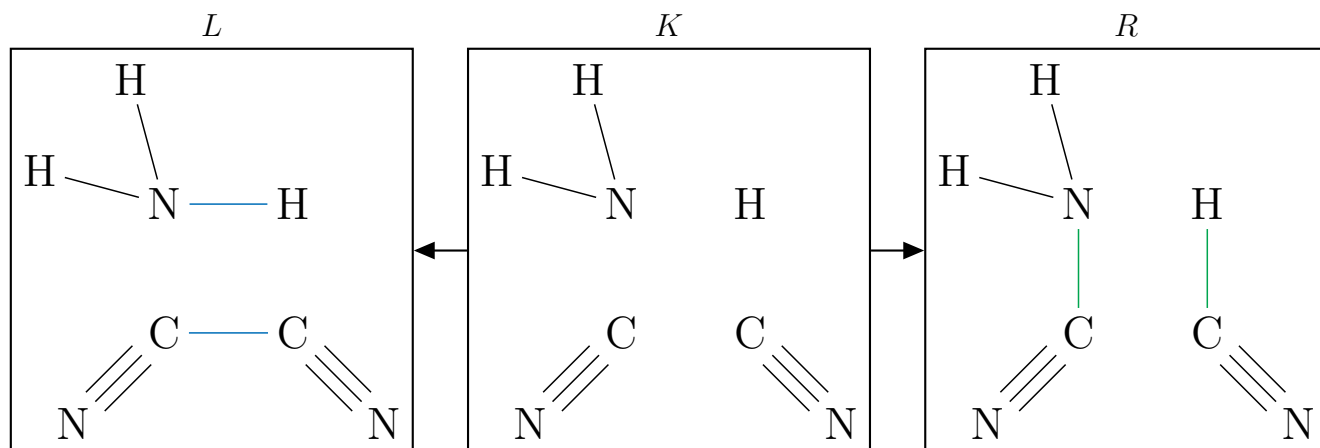
0.0.22 DAMN Scission

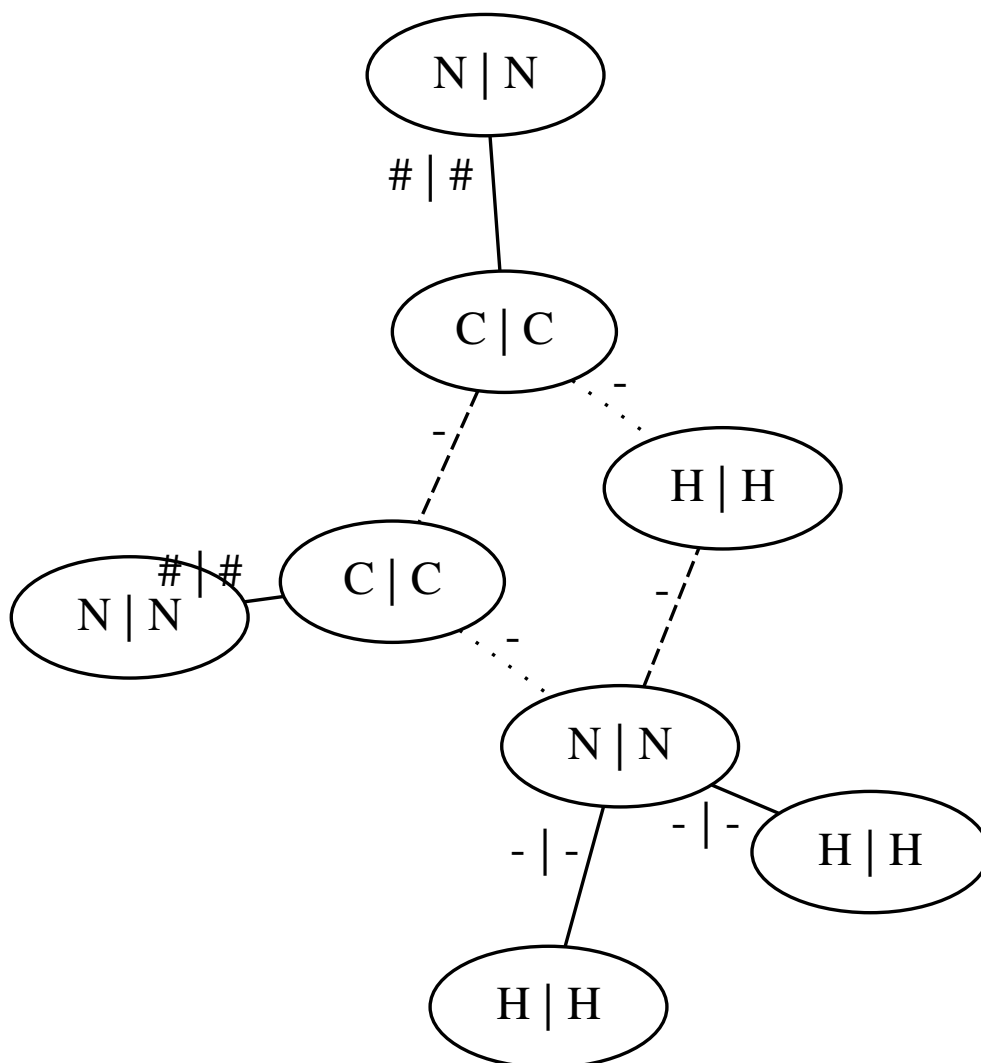




File: out/108_r_20_combined

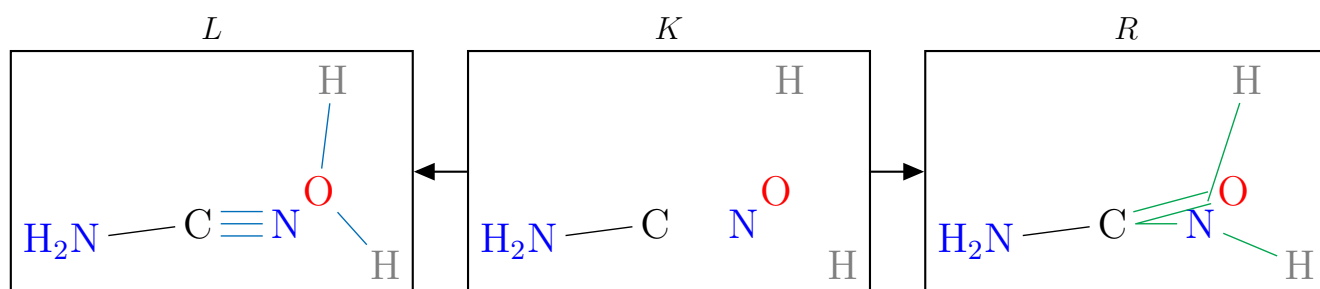
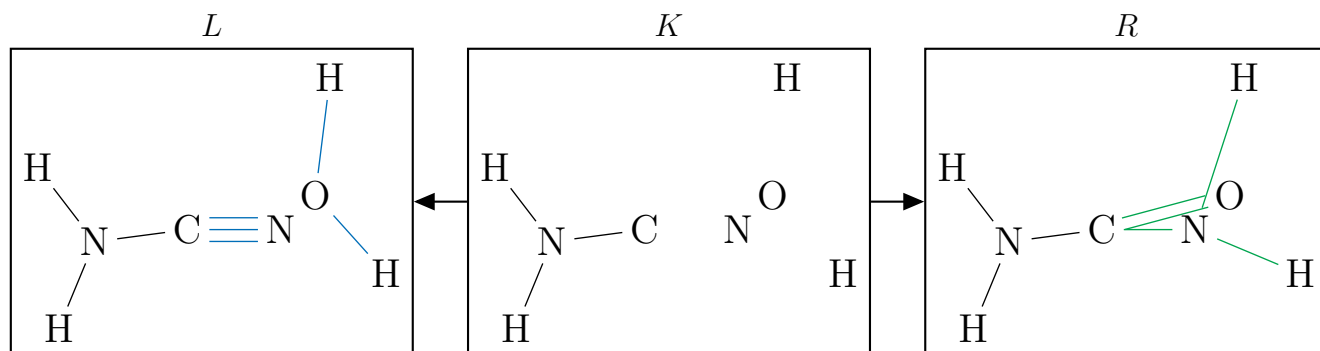
0.0.23 Cyanogen Ammonolysis

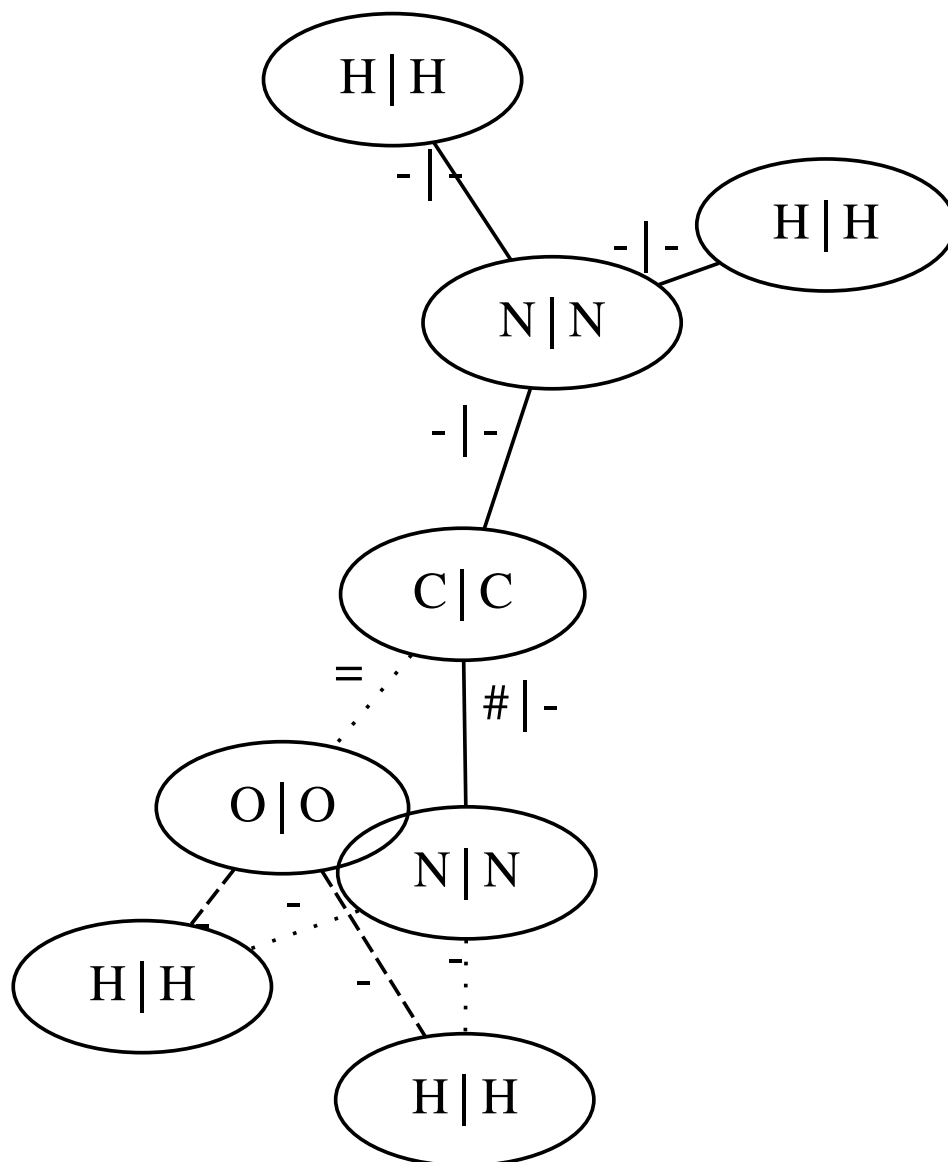




File: out/113_r_21_combined

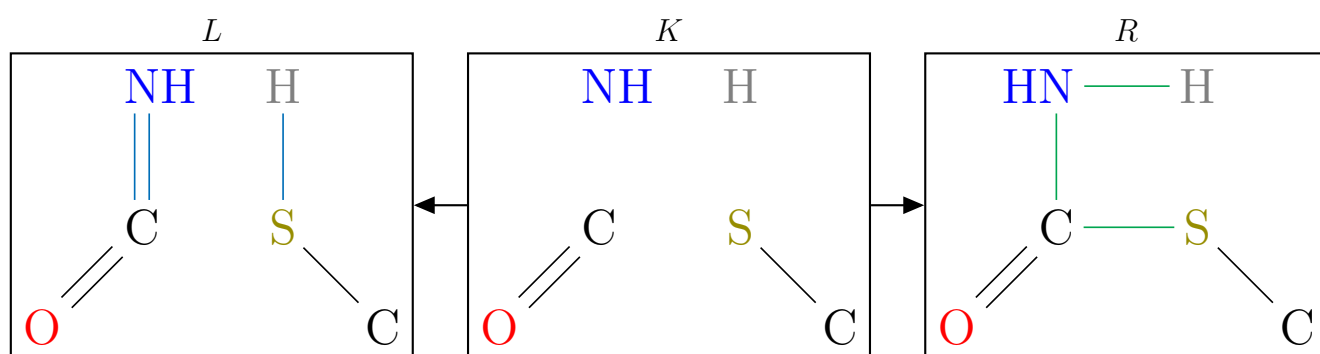
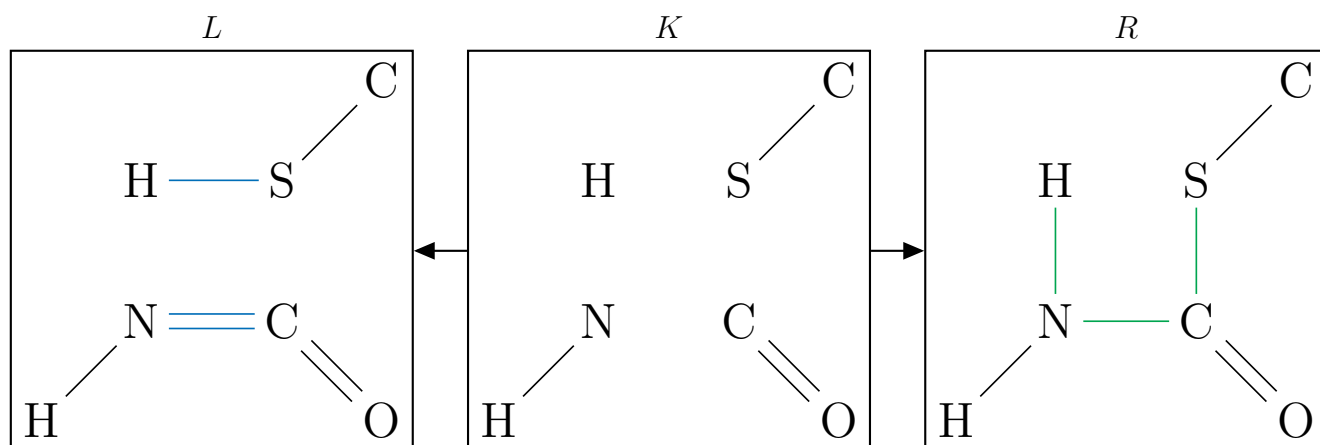
0.0.24 Cyanamide Hydration

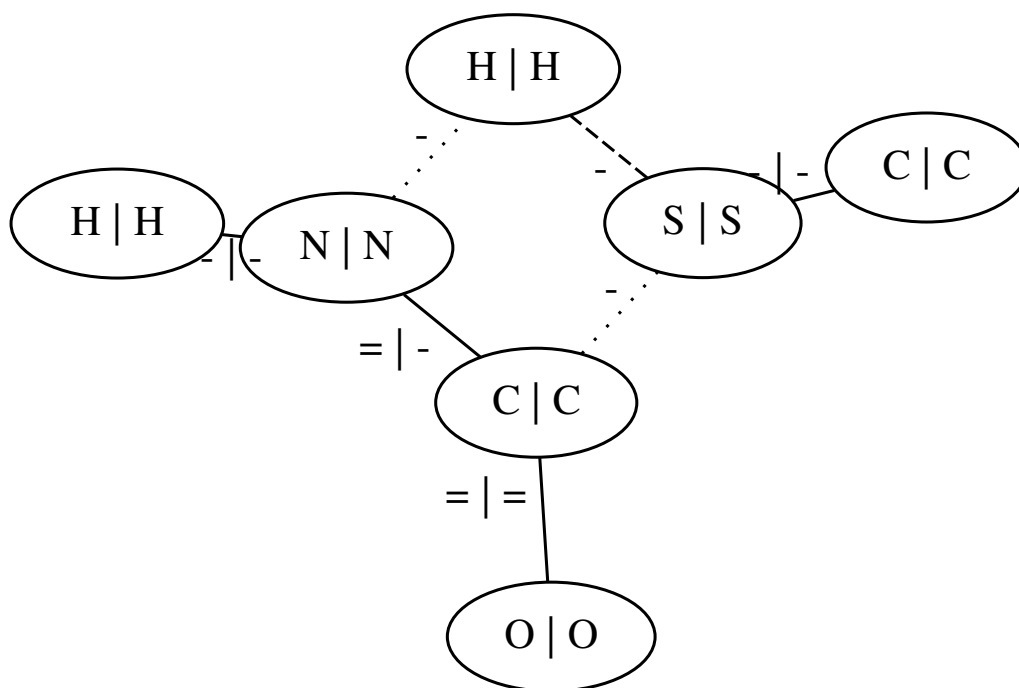




File: out/118_r_22_combined

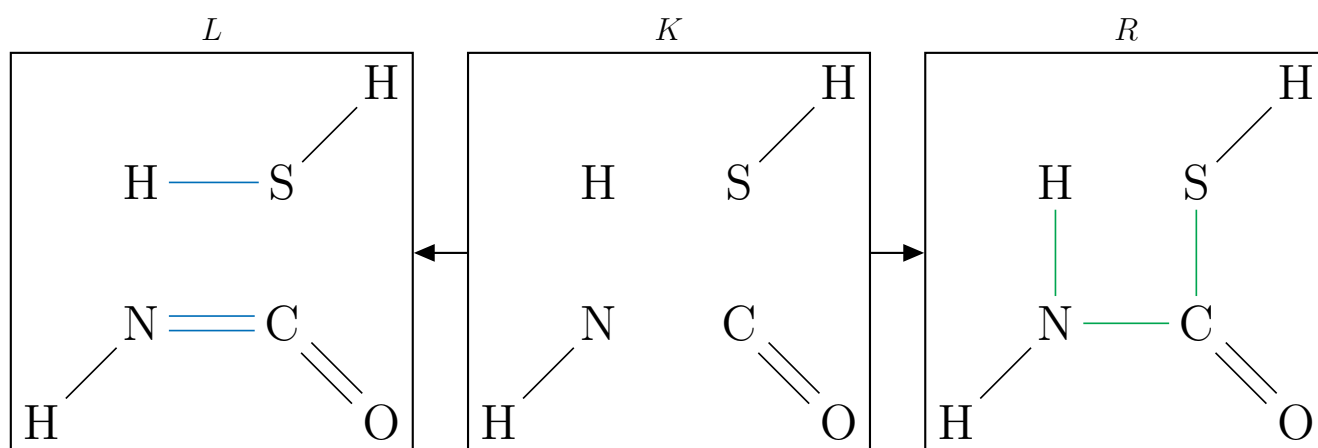
0.0.25 Carbamylation, SC



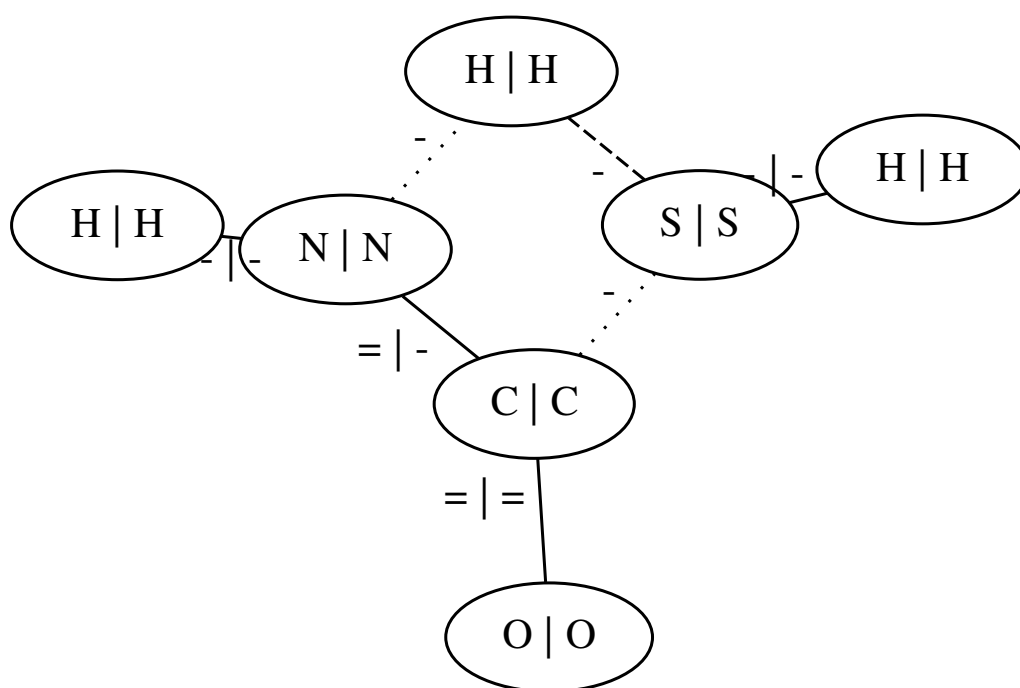
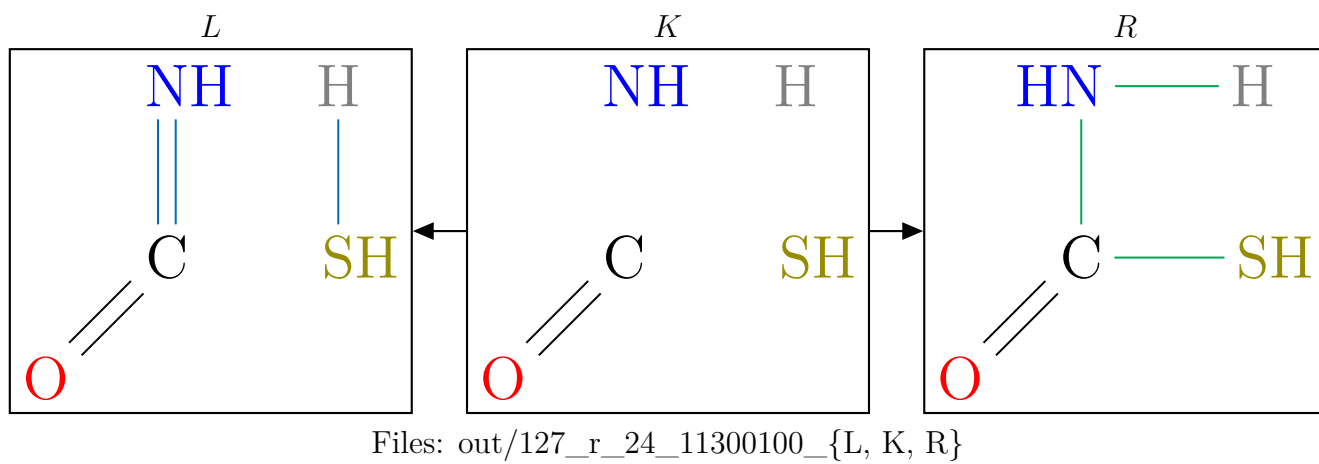


File: out/123_r_23_combined

0.0.26 Carbamylation, SH

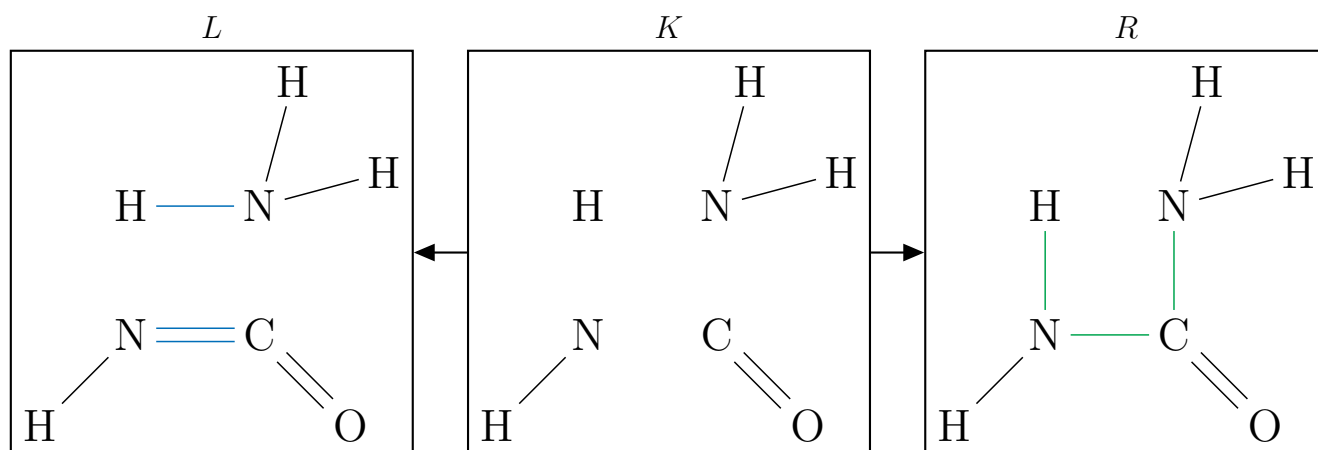


Files: out/126_r_24_10300000_{L, K, R}

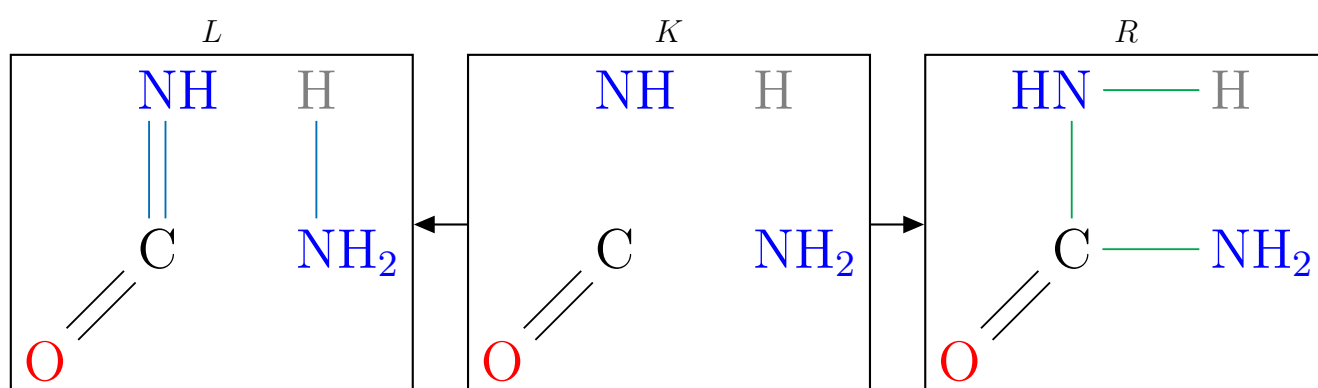


File: out/128_r_24_combined

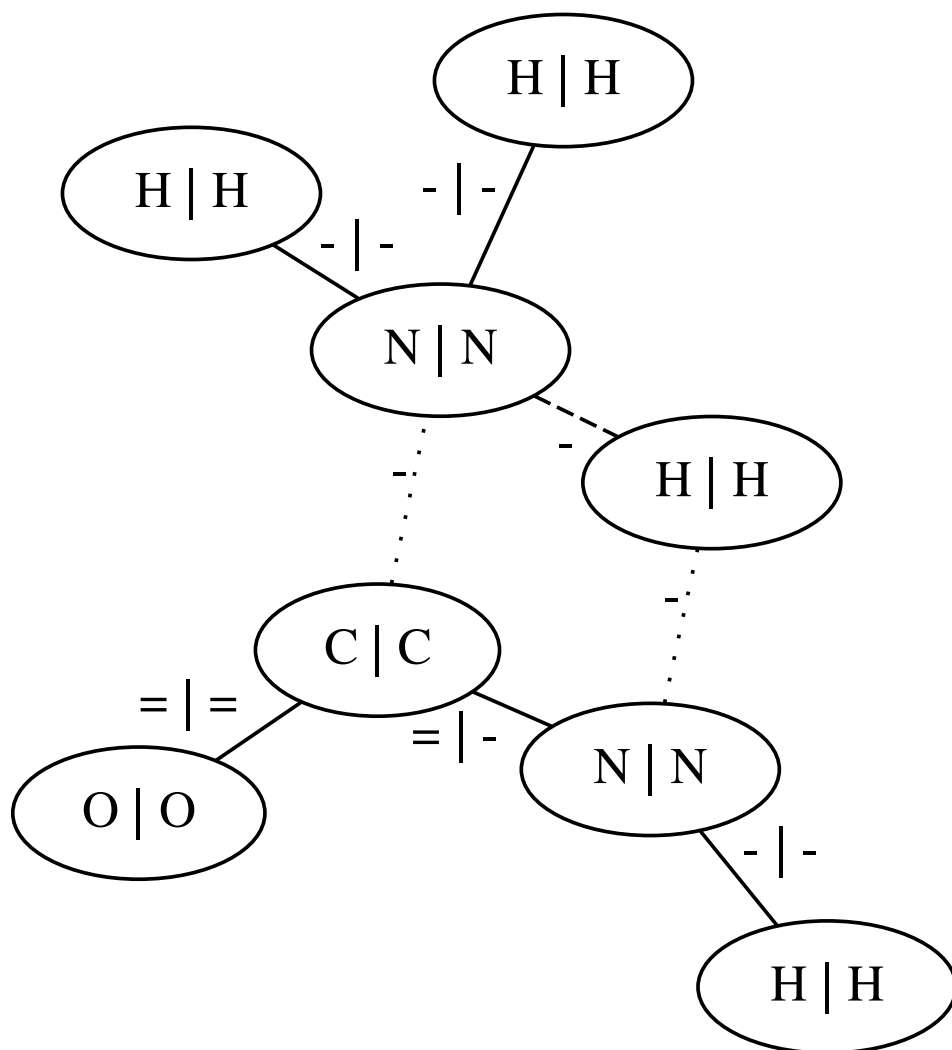
0.0.27 Carbamylation, N, HH



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

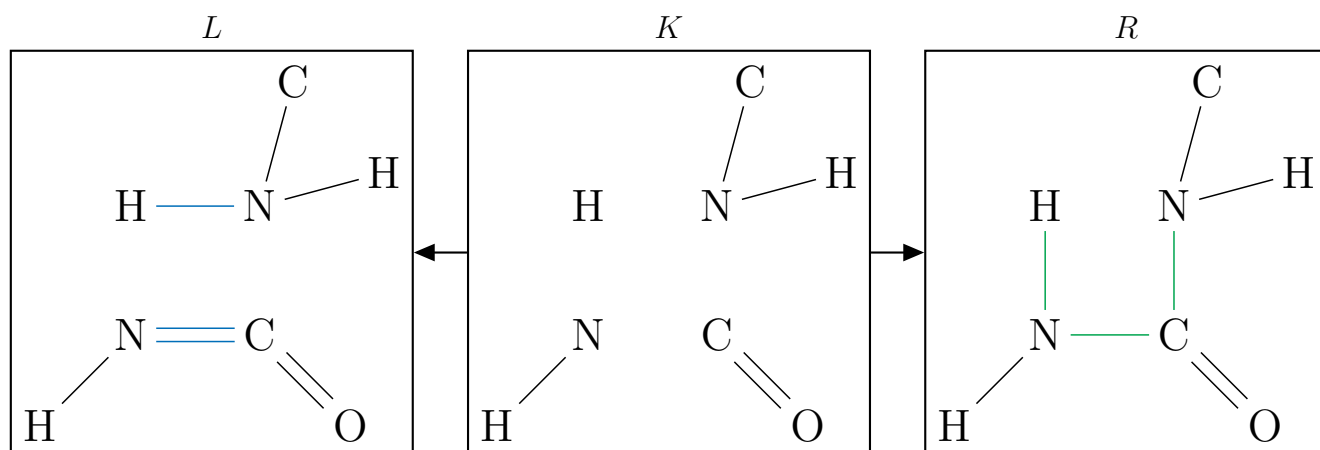


Files: out/132_r_25_11300100_{L, K, R}

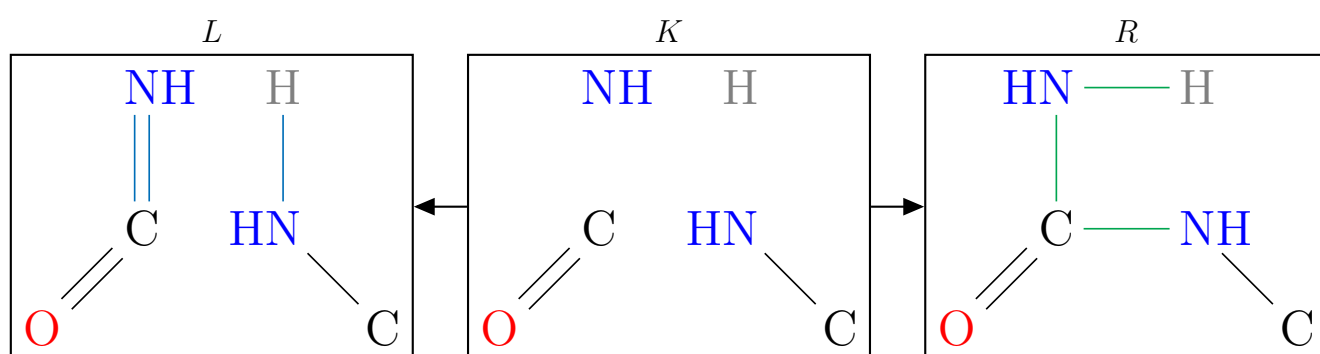


File: out/133_r_25_combined

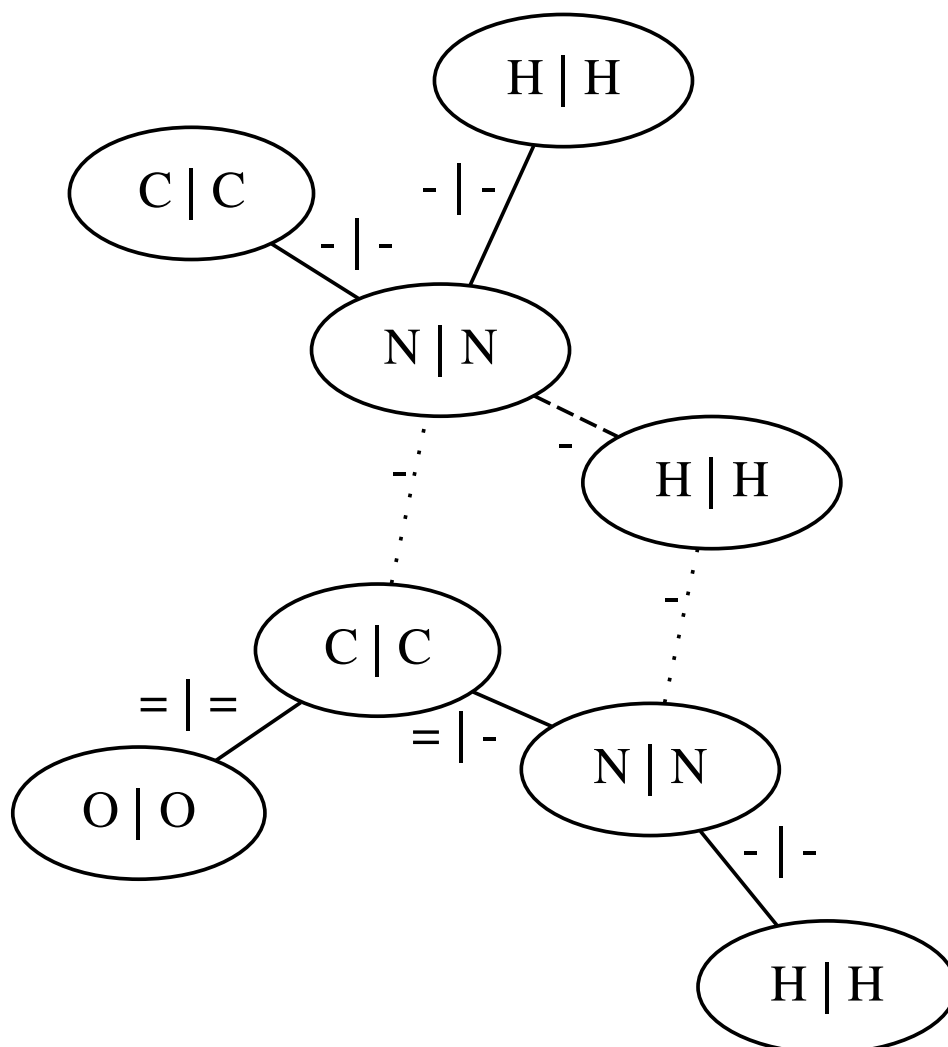
0.0.28 Carbamylation, N, HC



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



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



File: out/138_r_26_combined

$$|\{e \in \text{outEdges}(5) \mid$$

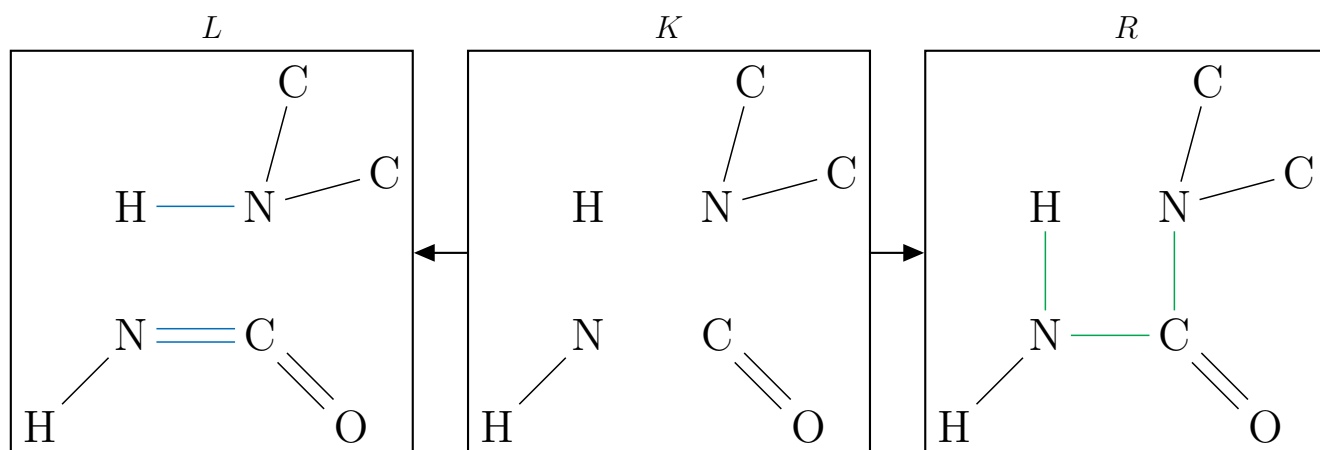
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

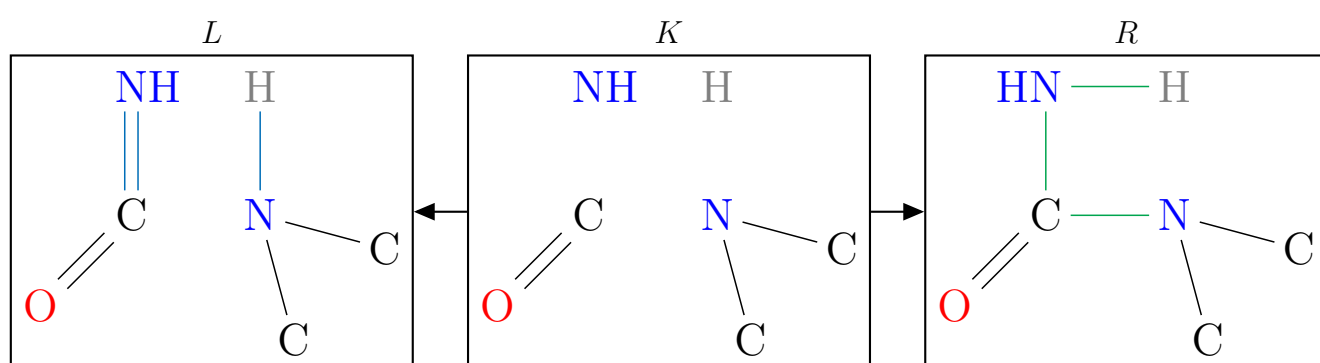
$$\text{label}(e) \in \{'=\'}\}$$

$$\} = 0$$

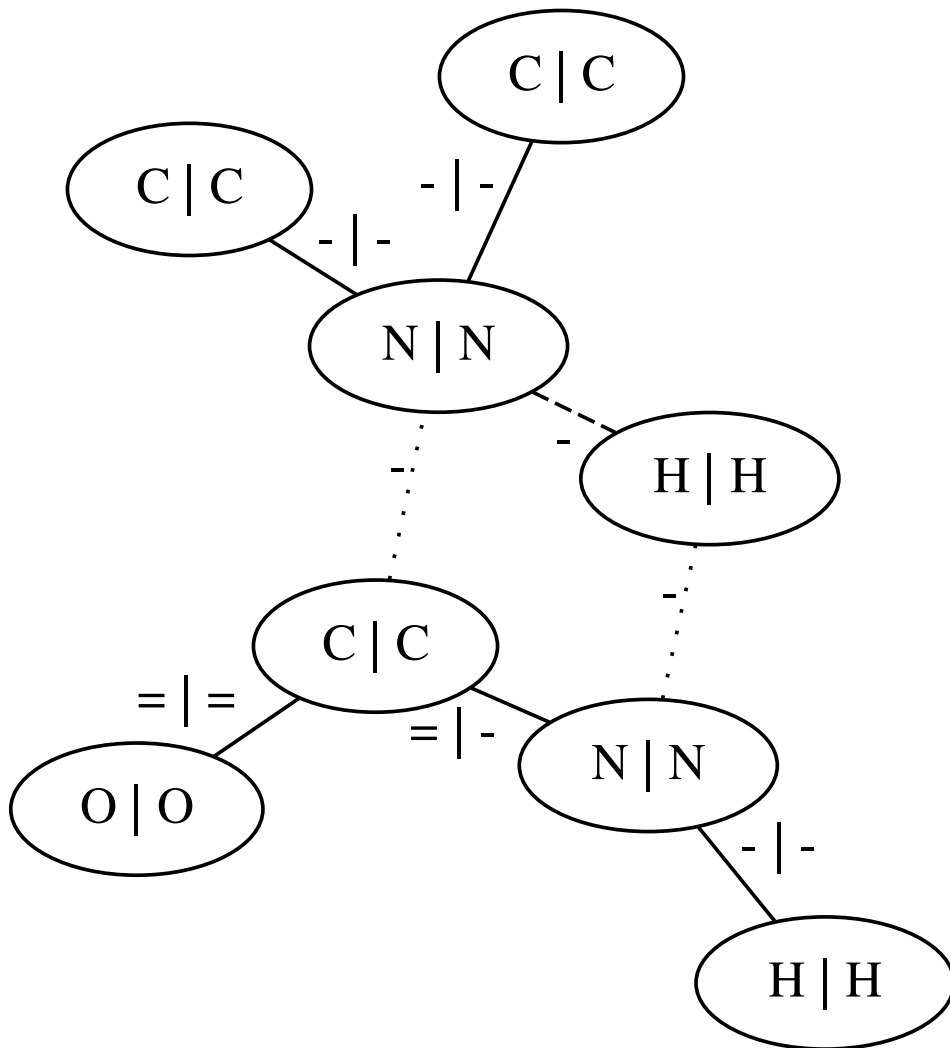
0.0.29 Carbamylation, N, CC



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



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



File: out/143_r_27_combined

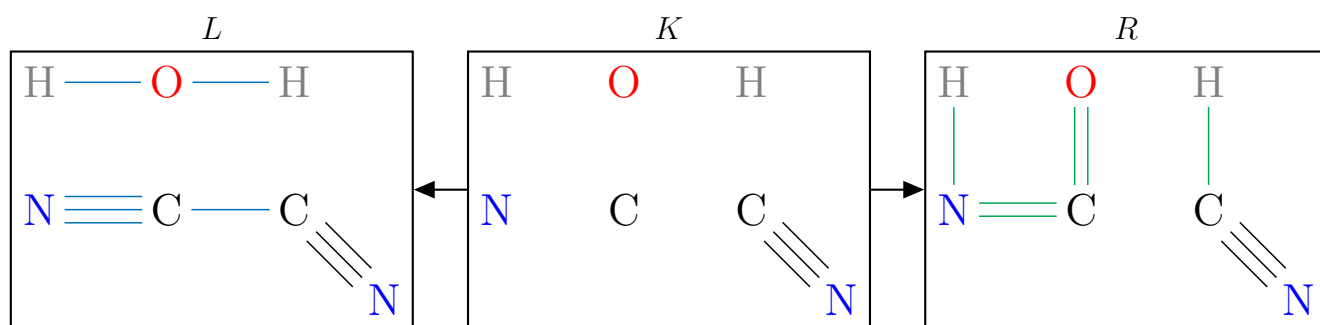
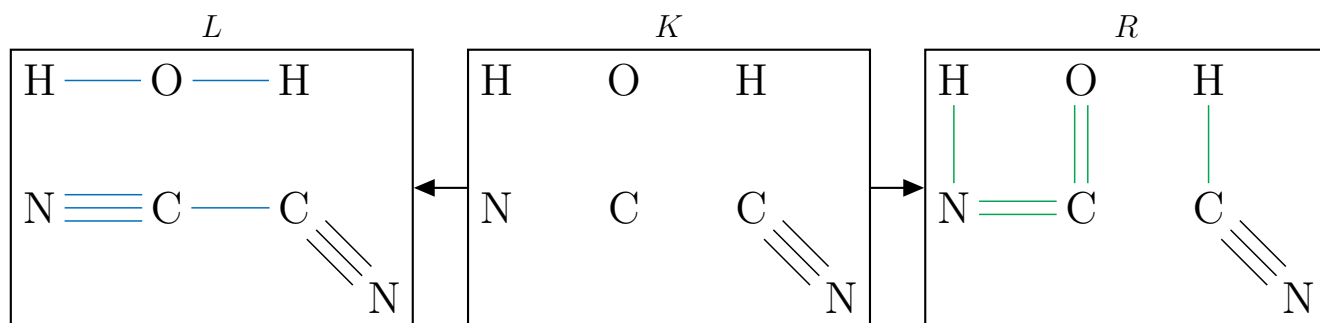
```

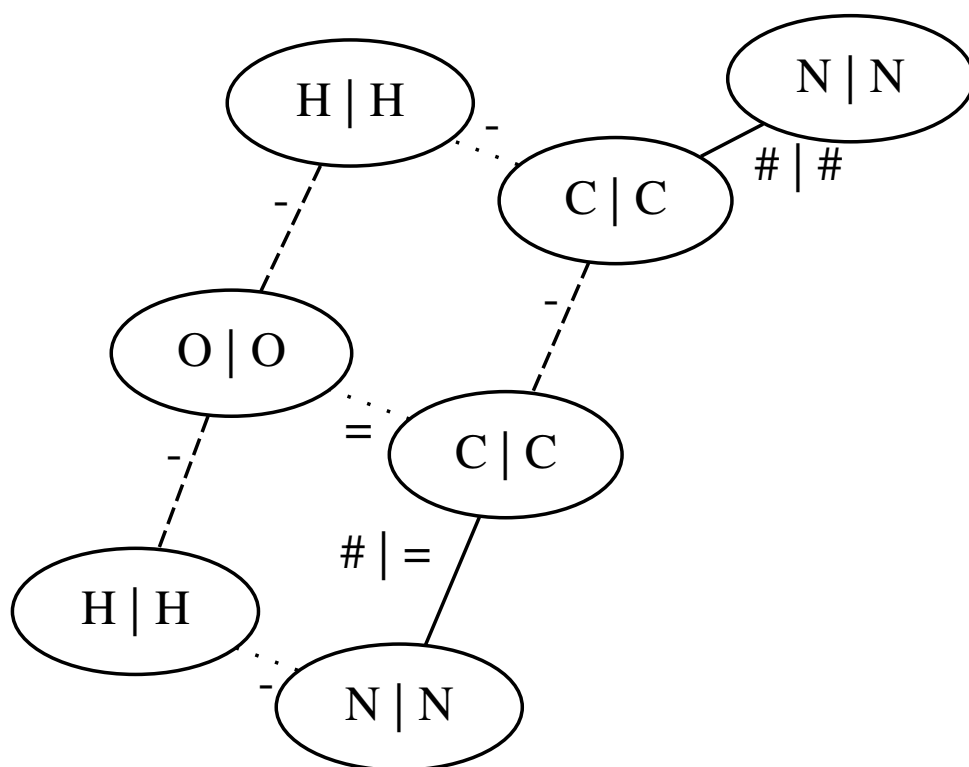
|{e ∈ outEdges(4) |
  label(target(e)) ∈ {'0'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

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

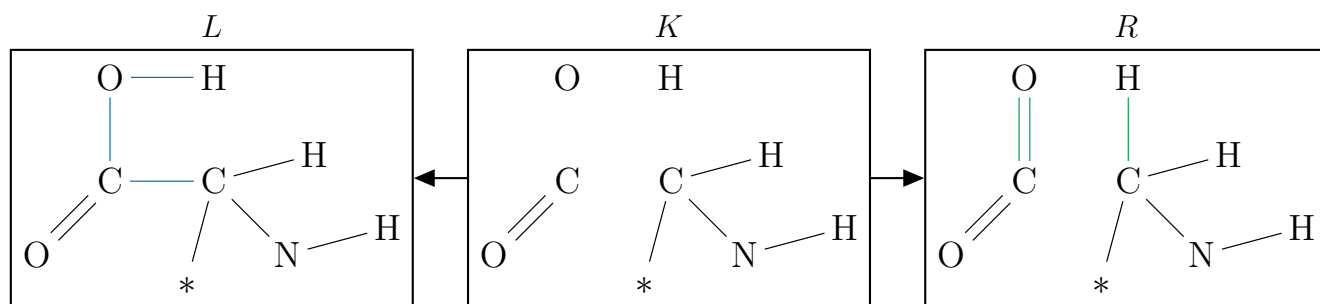
0.0.30 Cyanate from cyanogen



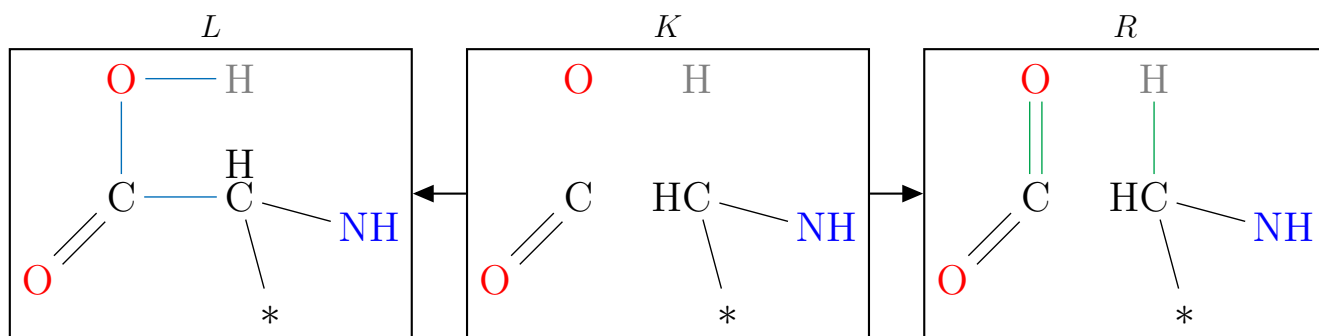


File: out/148_r_28_combined

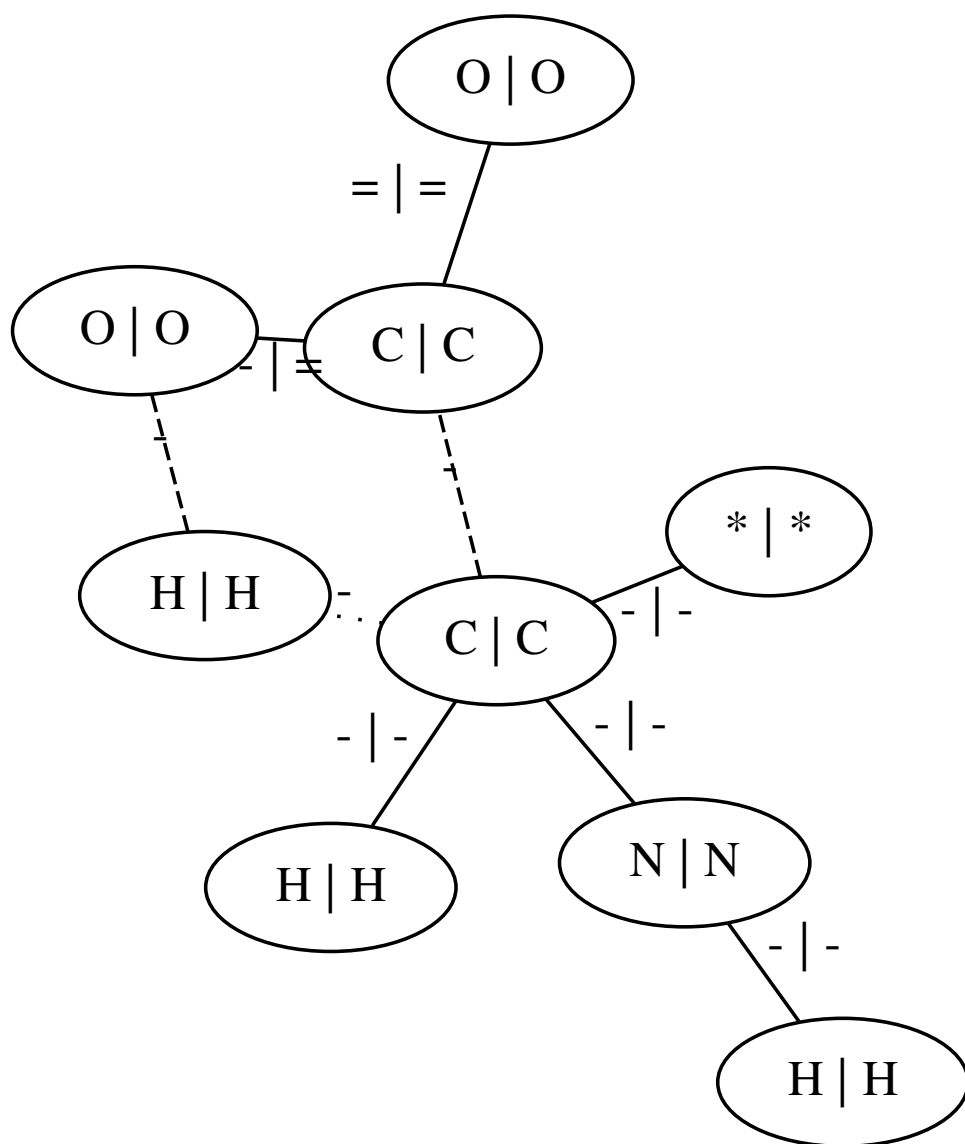
0.0.31 Ketone-Catalyzed Decarboxylation



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

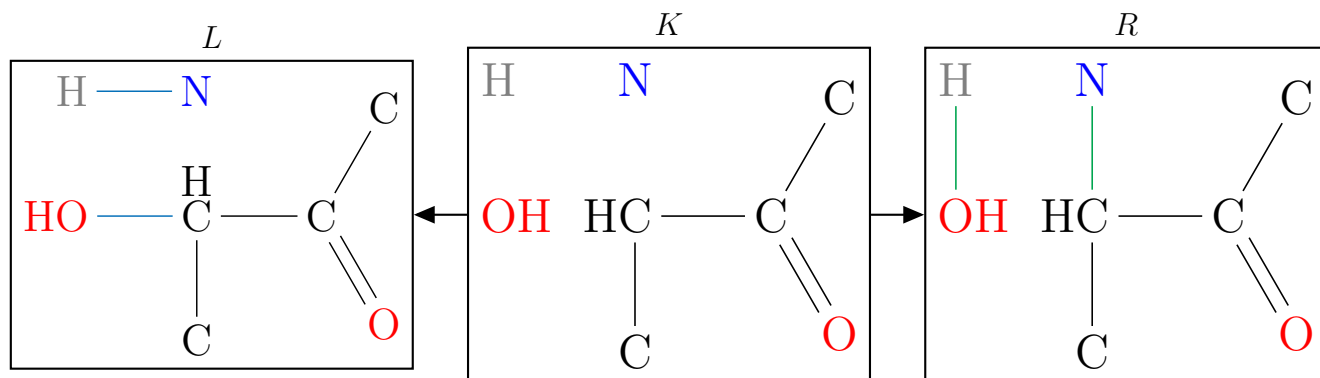
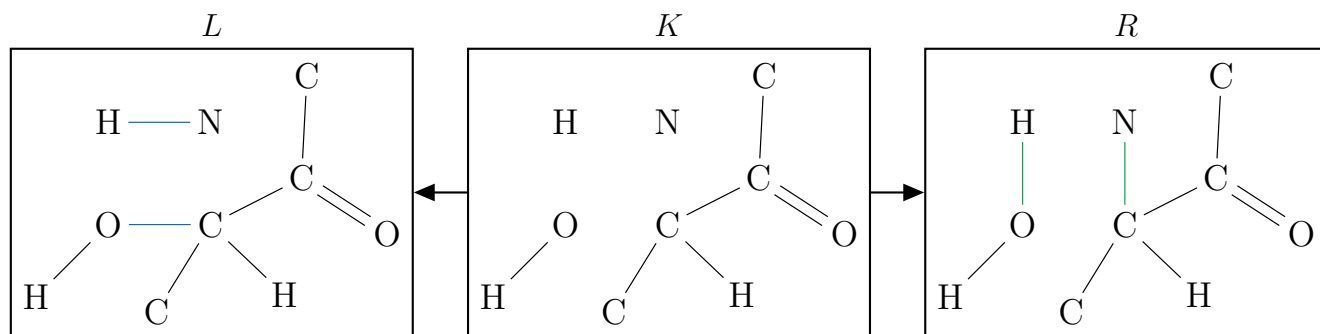


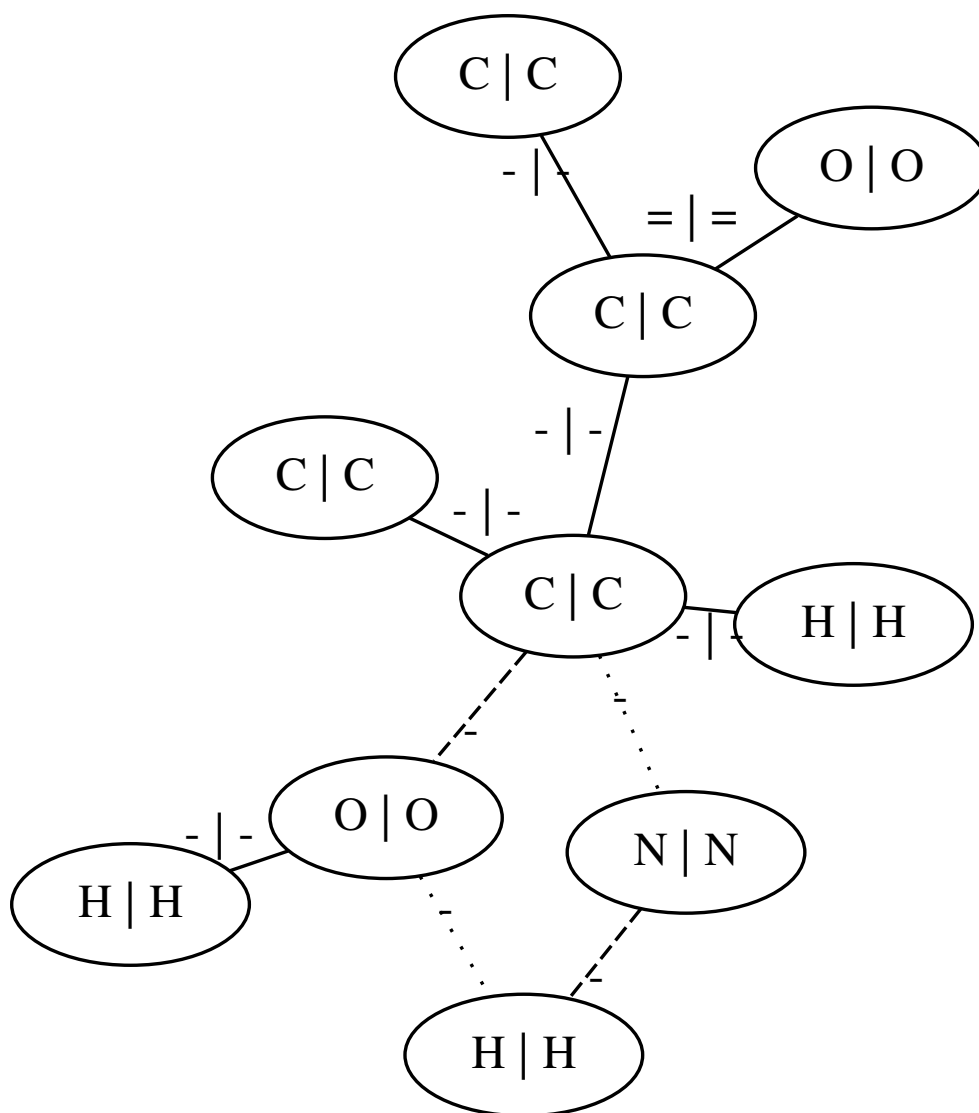
Files: out/152_r_29_11300100_{L, K, R}



File: out/153_r_29_combined

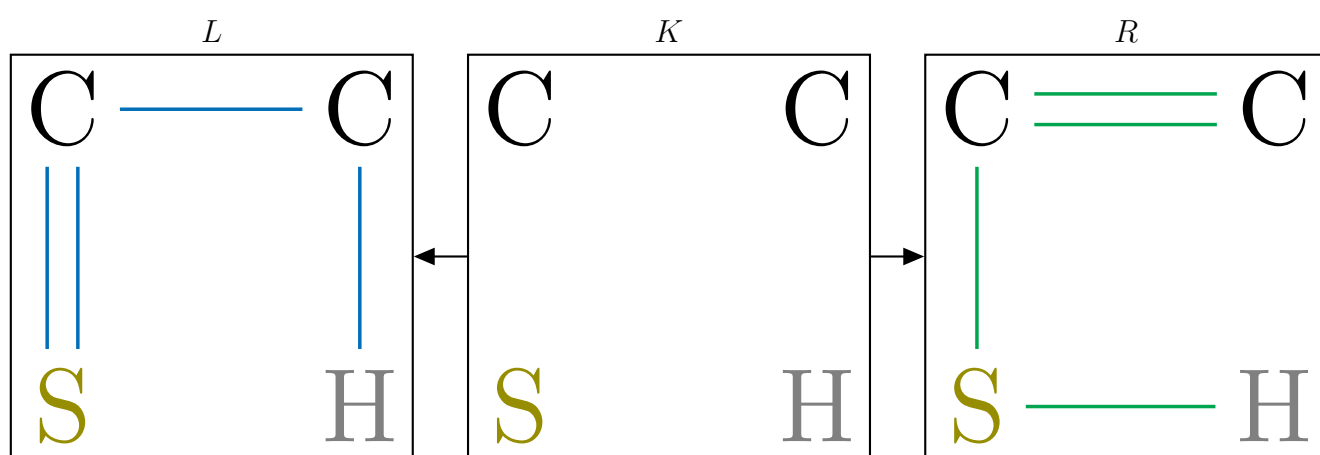
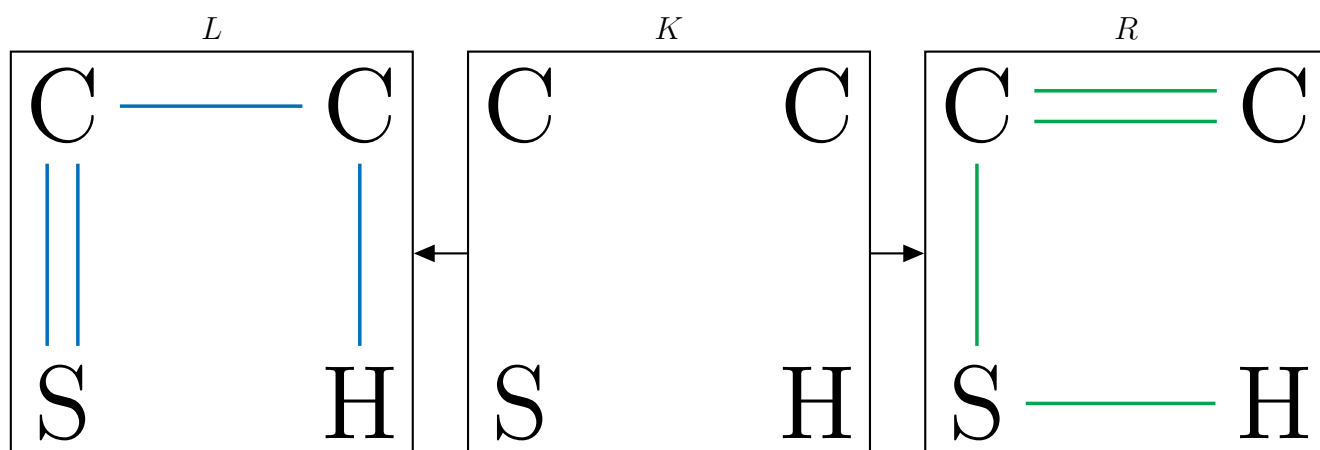
0.0.32 Amadori Rearrangement

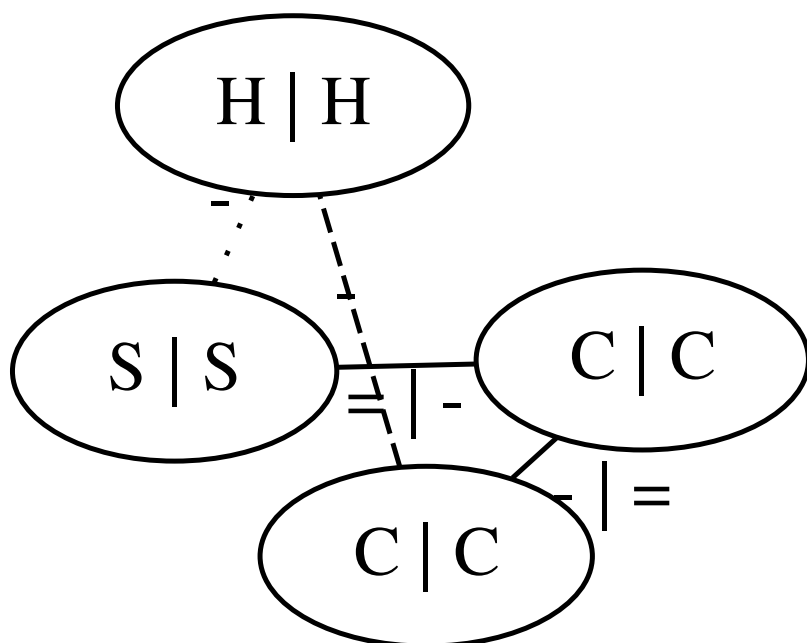




File: out/158_r_30_combined

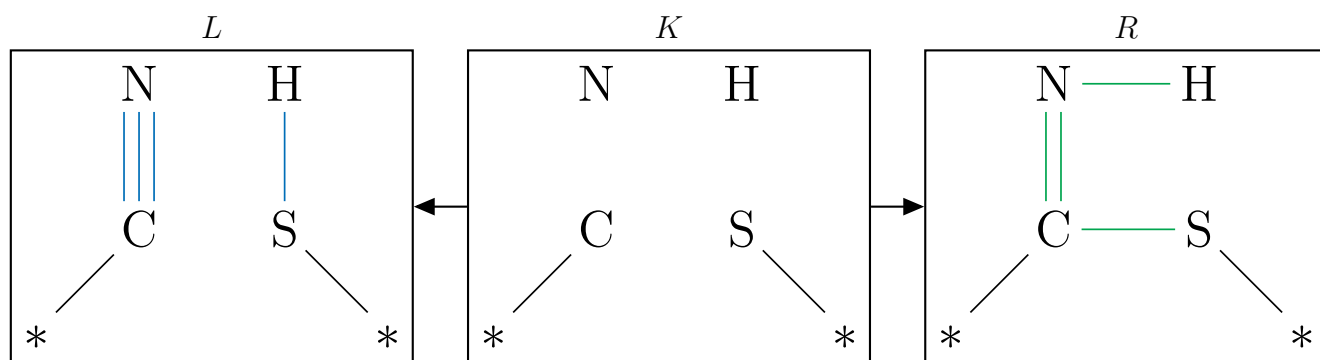
0.0.33 Thial -> Thiene



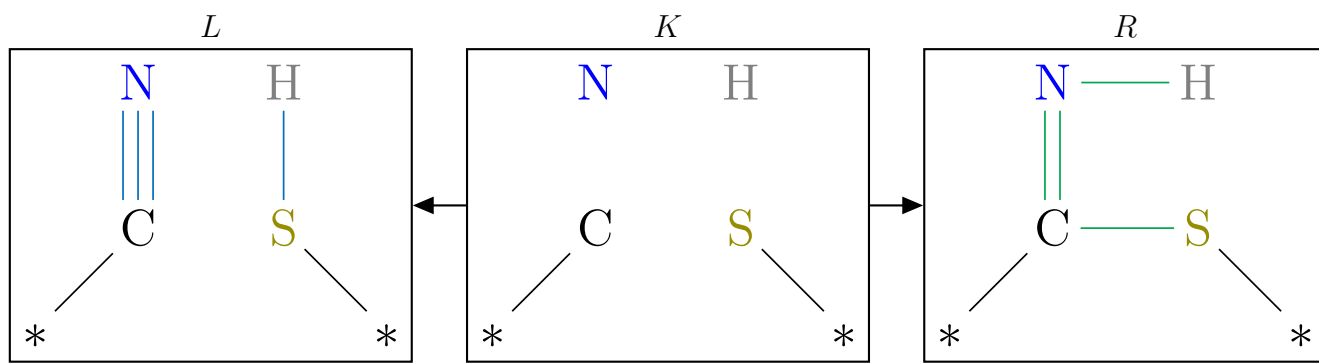


File: out/163_r_31_combined

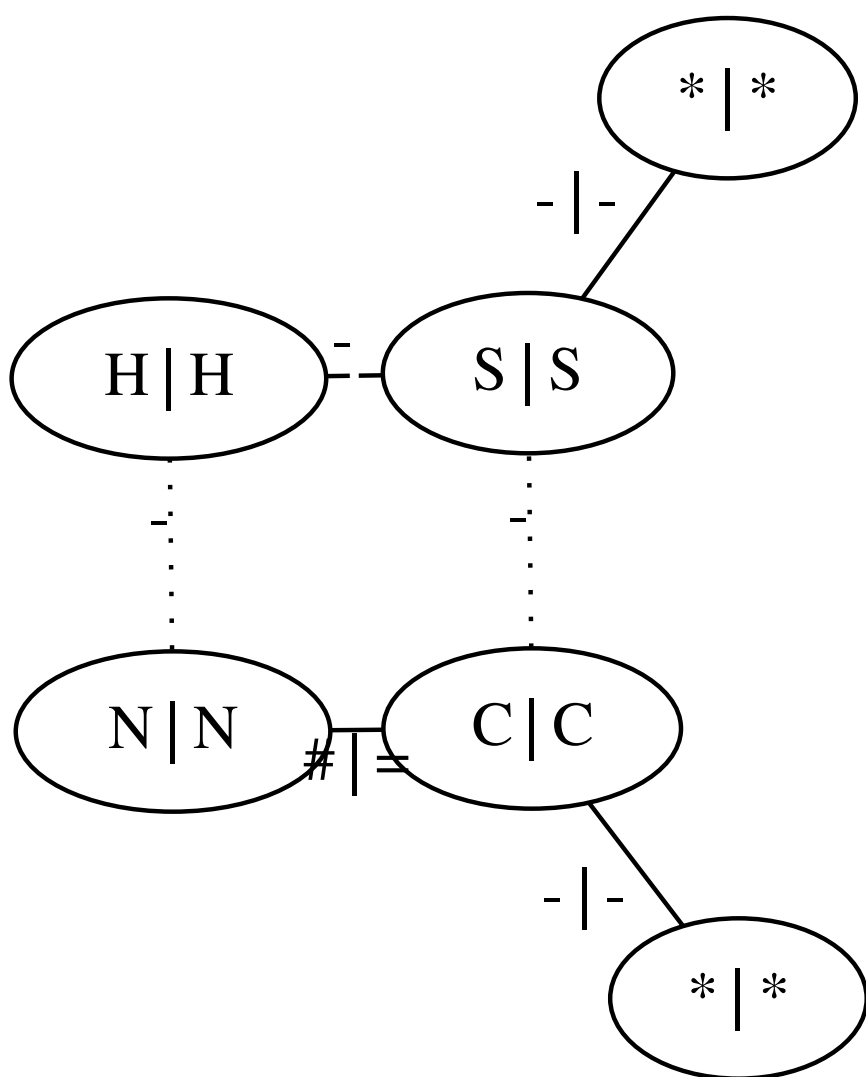
0.0.34 Sulfide to Nitrile Addition



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

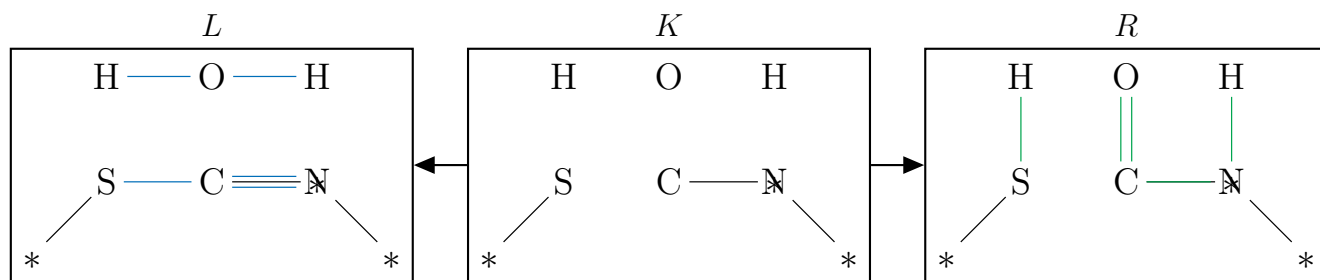


Files: out/167_r_32_11300100_{L, K, R}

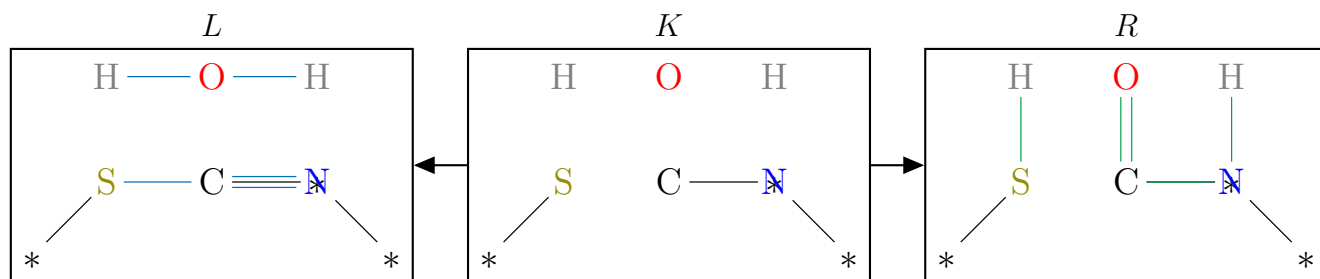


File: out/168_r_32_combined

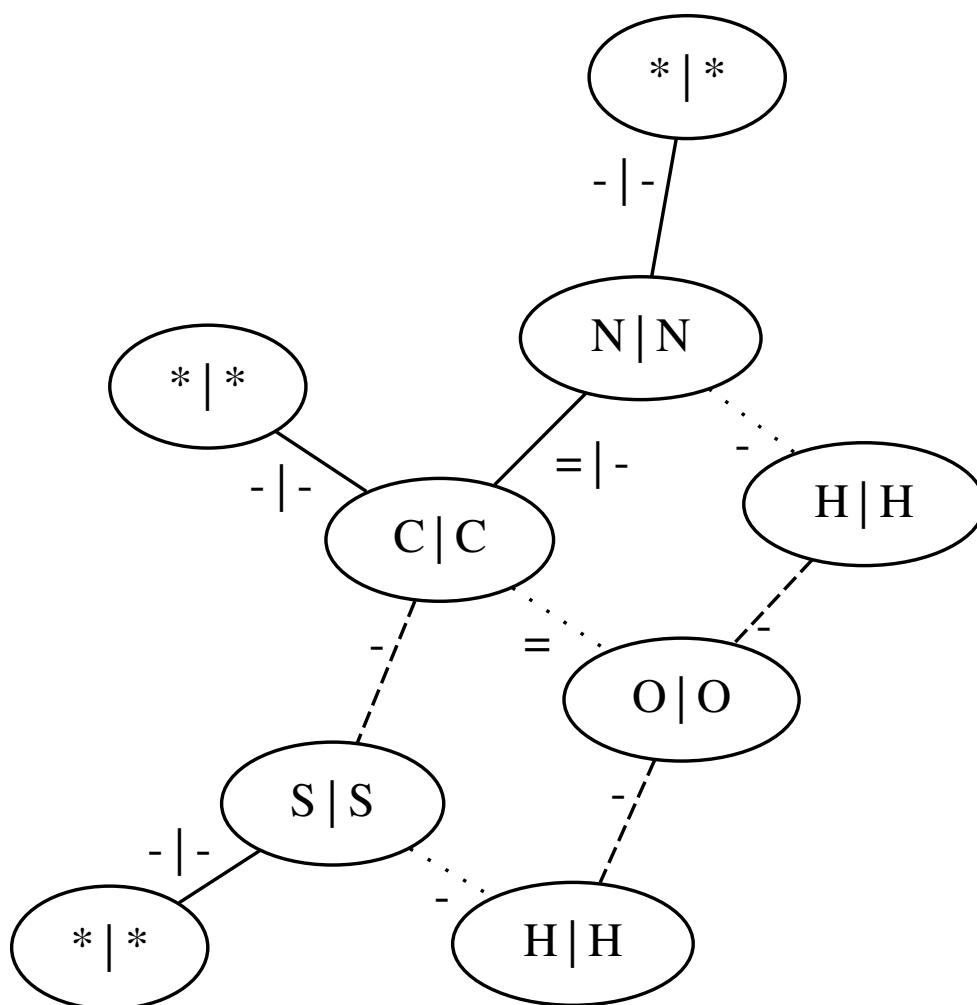
0.0.35 Thioamidine to Amide Hydrolysis



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

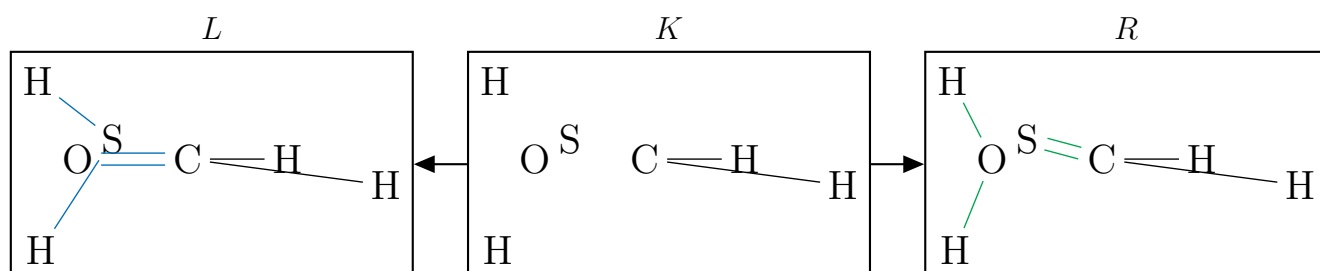


Files: out/172_r_33_11300100_{L, K, R}

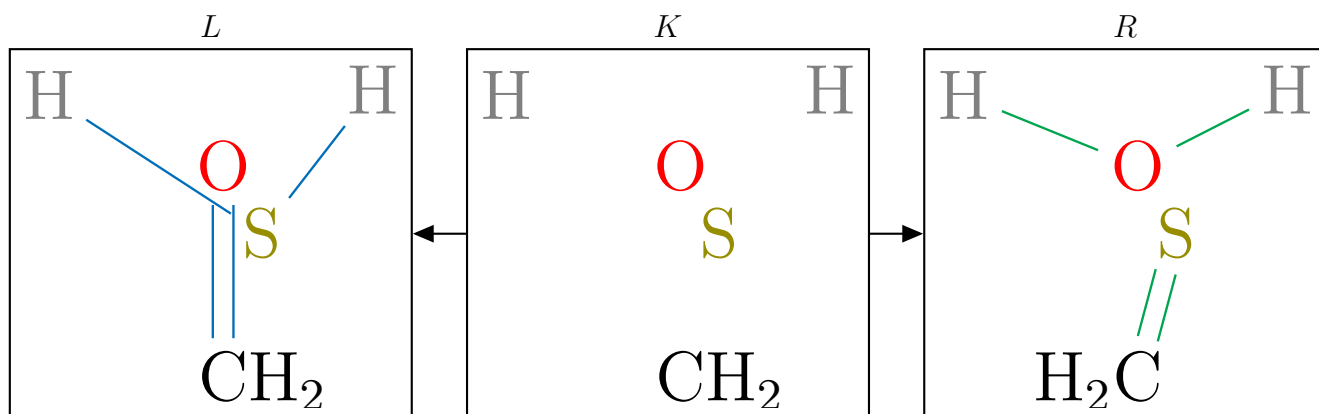


File: out/173_r_33_combined

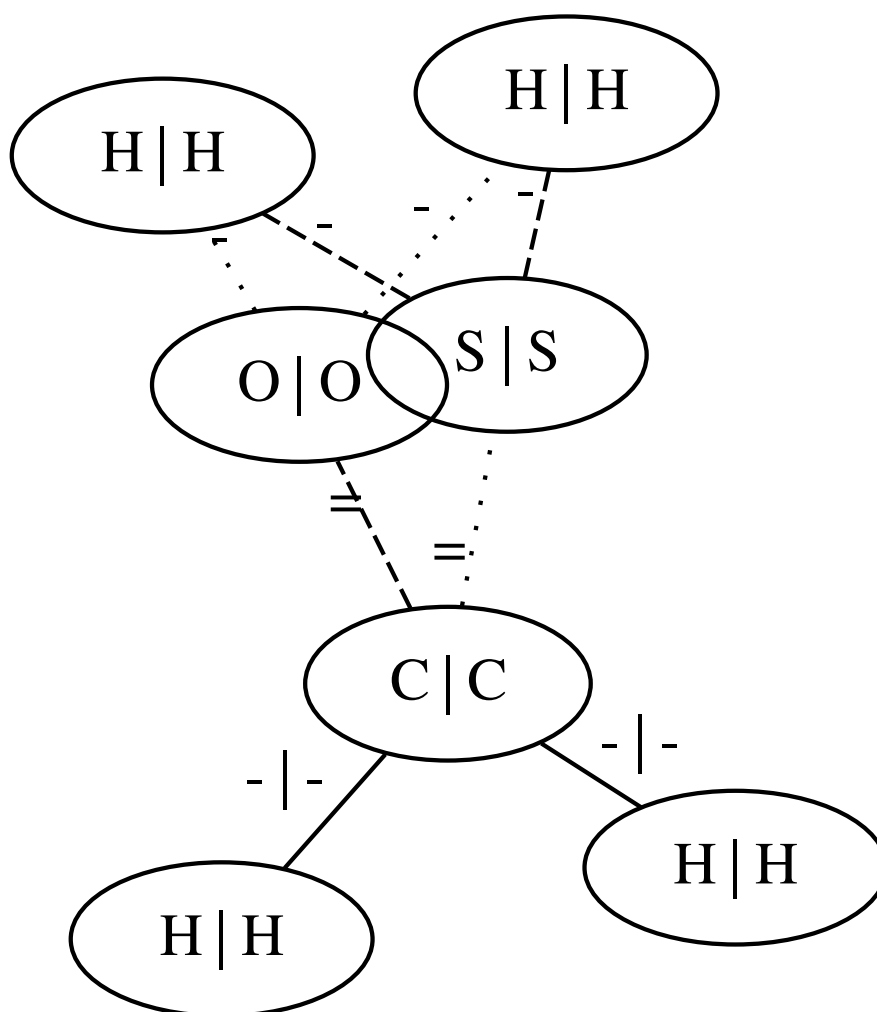
0.0.36 Ketone/Aldehyde to Thioketone/Thial, HH



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

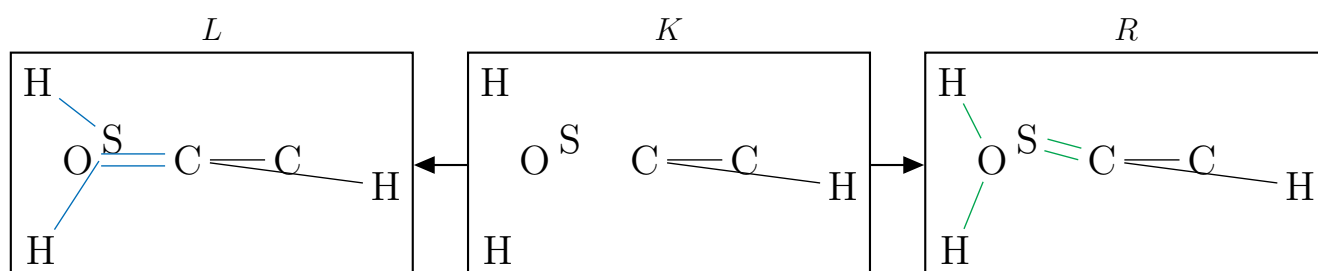


Files: out/177_r_34_11300100_{L, K, R}

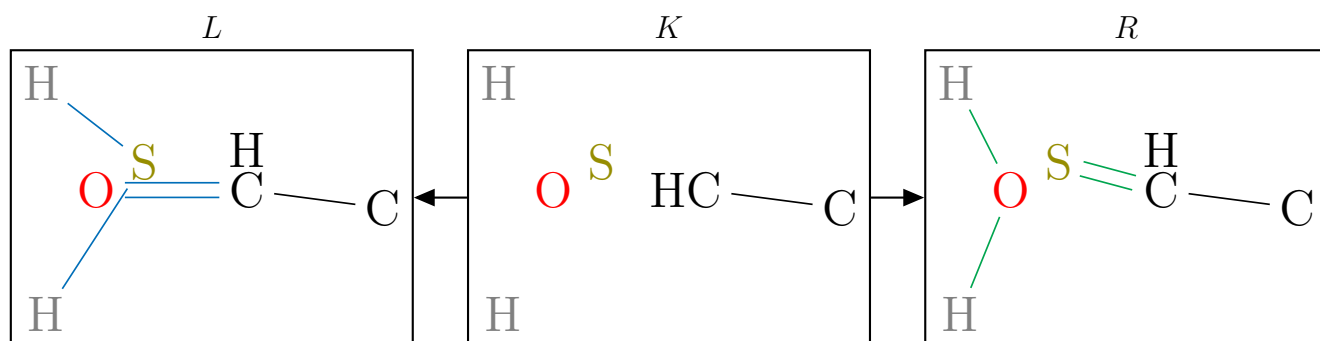


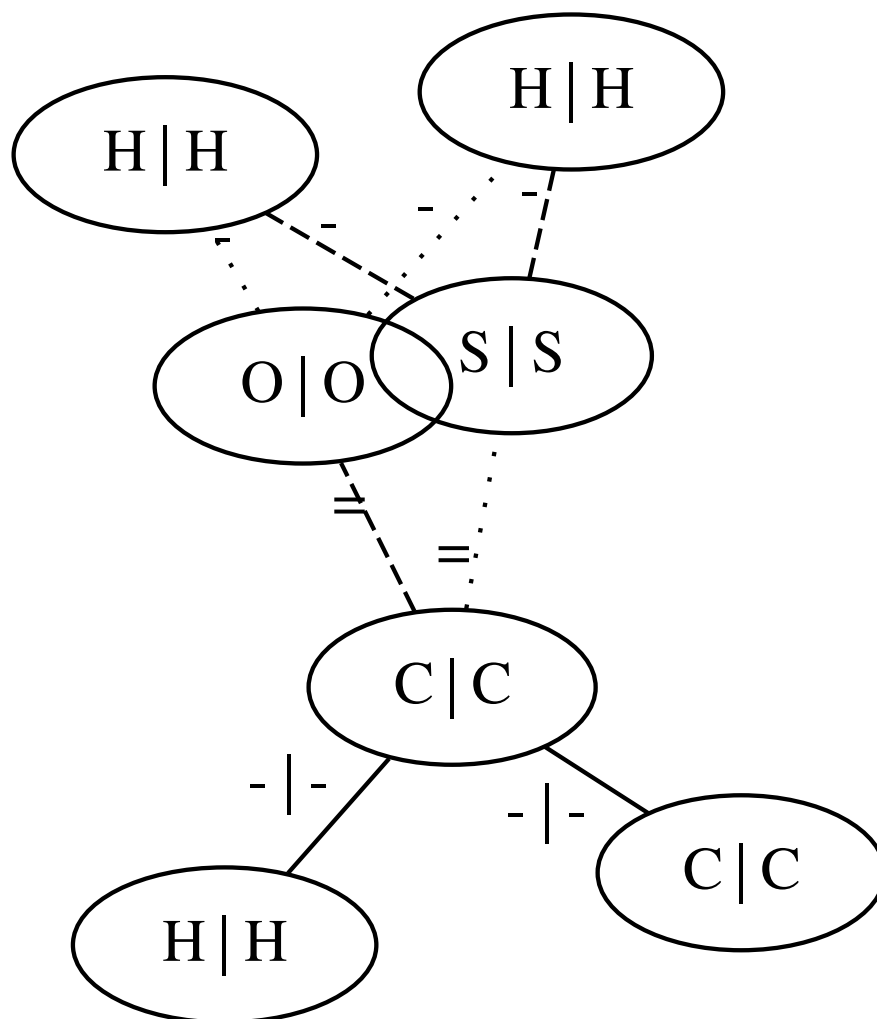
File: out/178_r_34_combined

0.0.37 Ketone/Aldehyde to Thioketone/Thial, HC



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





File: out/183_r_35_combined

$$|\{e \in \text{outEdges}(1) \mid$$

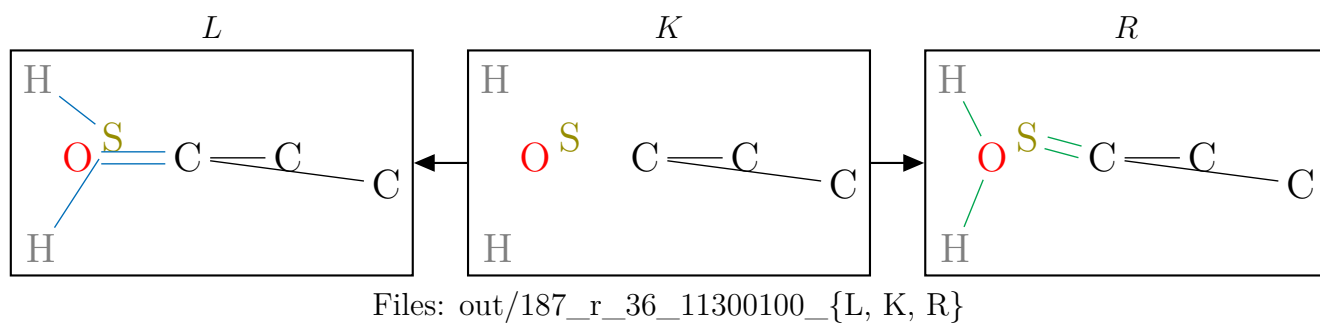
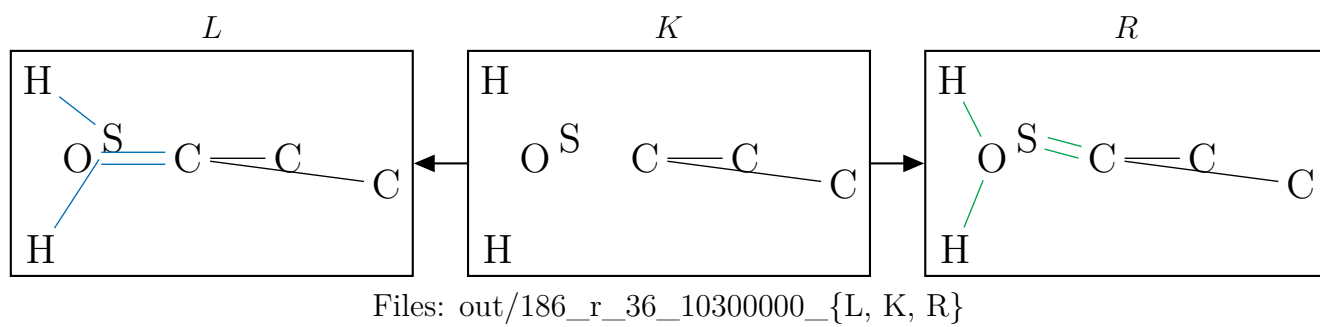
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

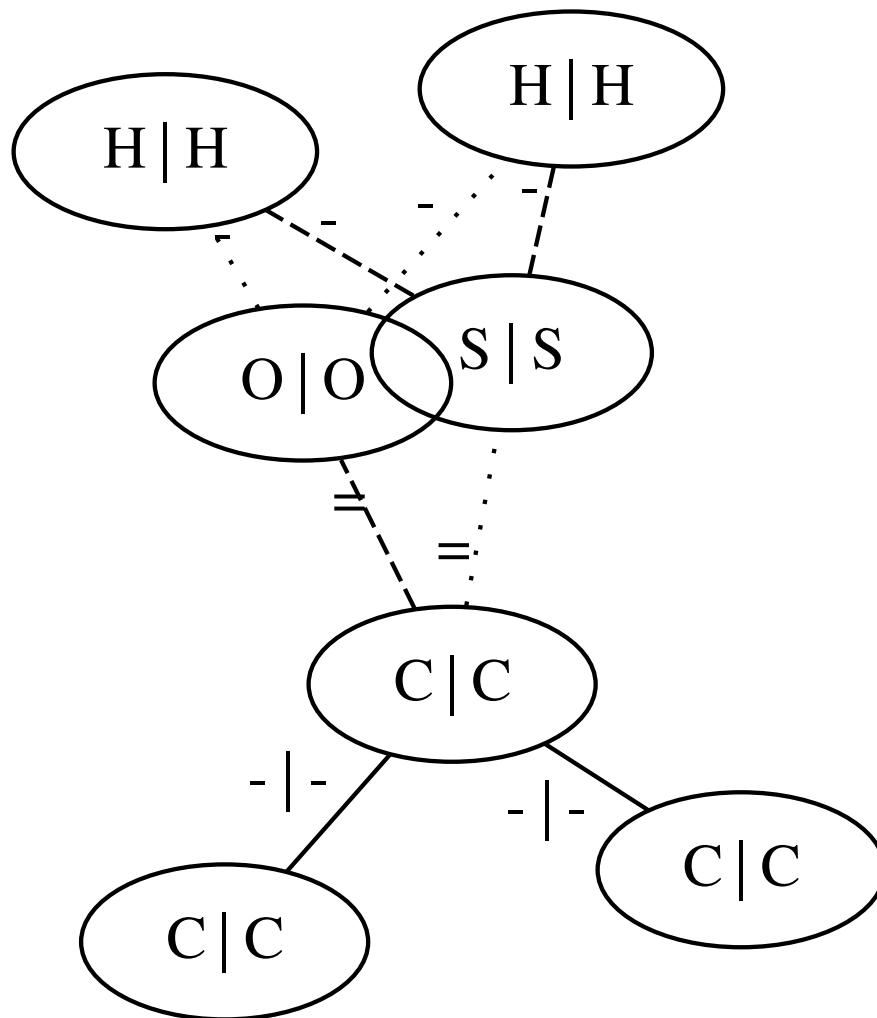
$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\} = 0$$

0.0.38 Ketone/Aldehyde to Thioketone/Thial, CC





File: out/188_r_36_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

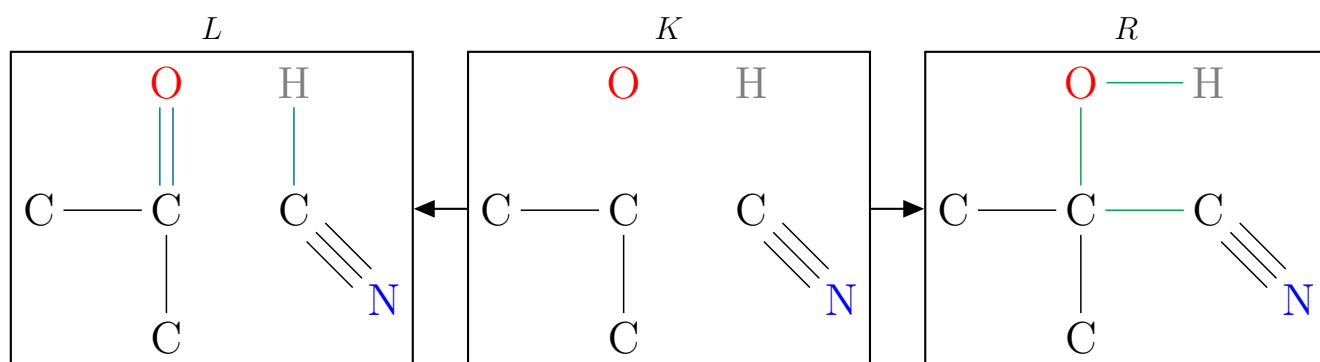
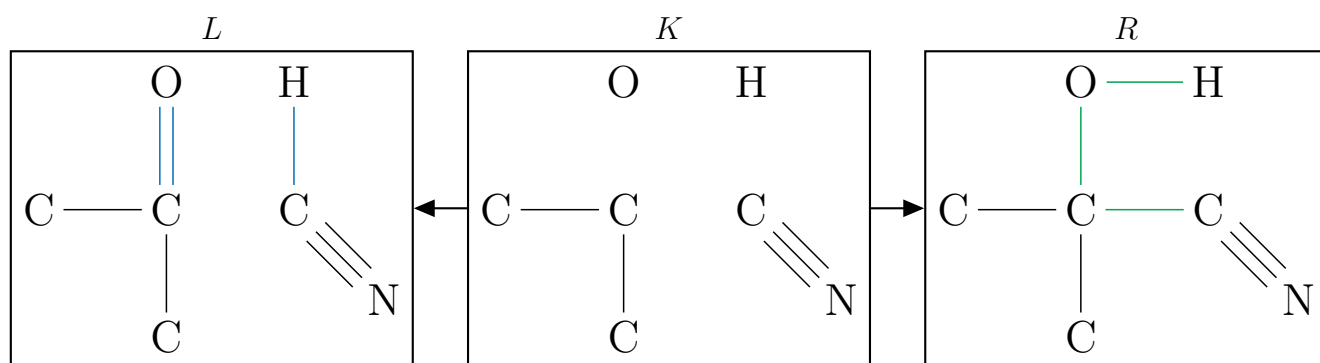
$$\wedge$$

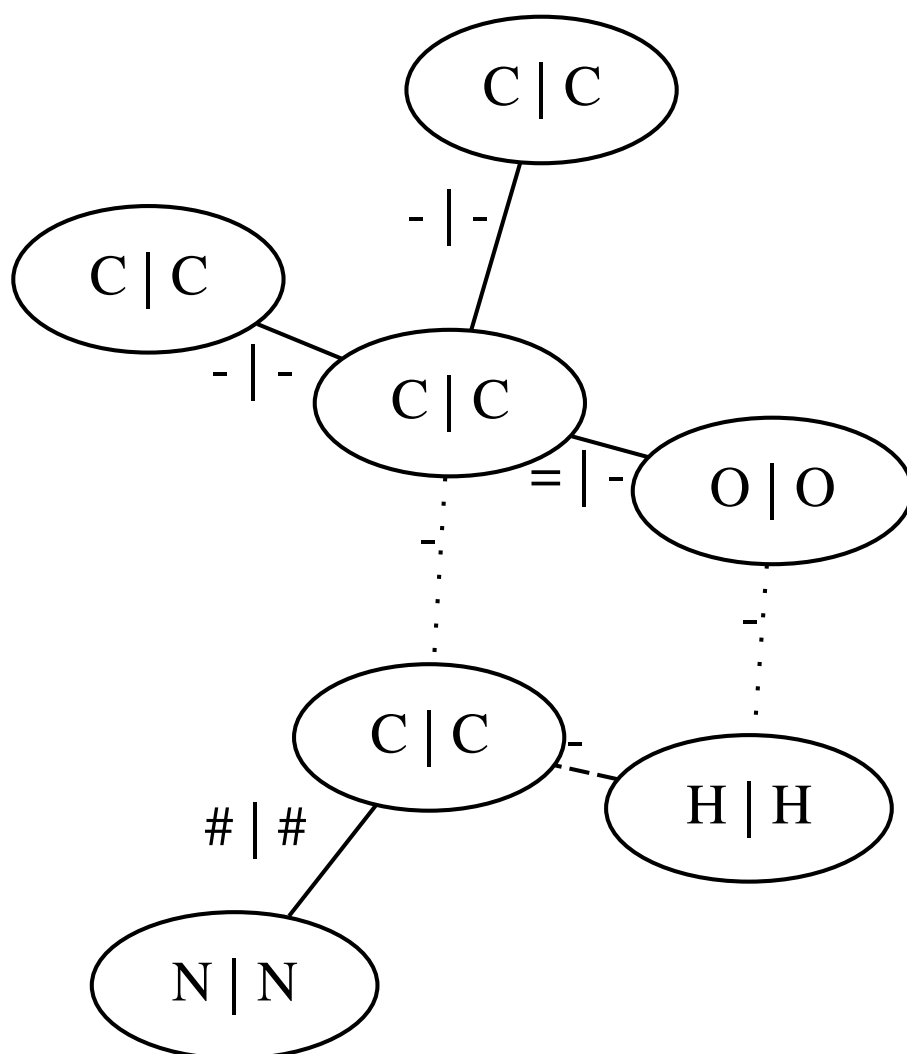
$$\text{label}(e) \in \{'=\'}\}$$

$$\} = 0$$

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

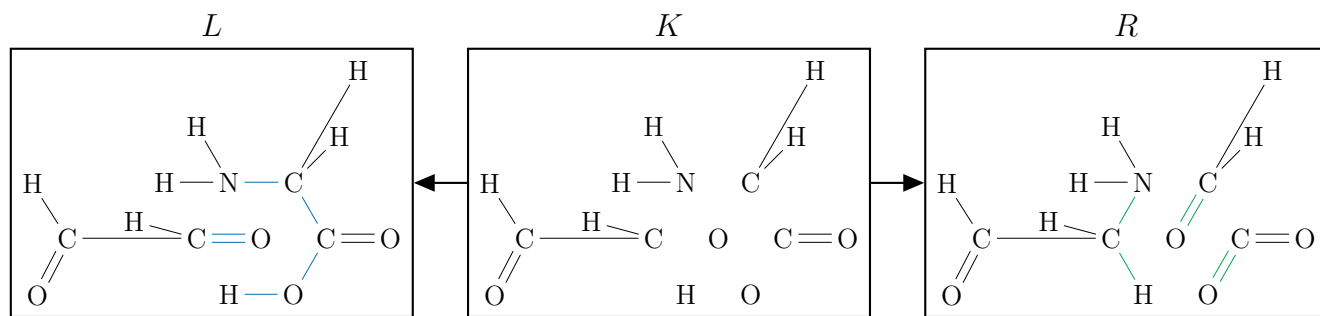
0.0.39 HCN to Ketone



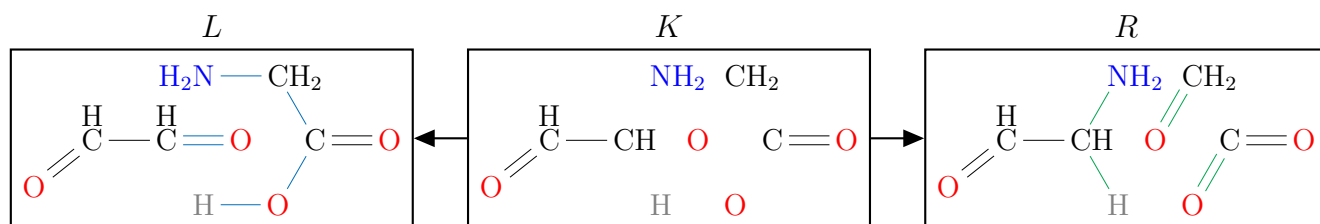


File: out/193_r_37_combined

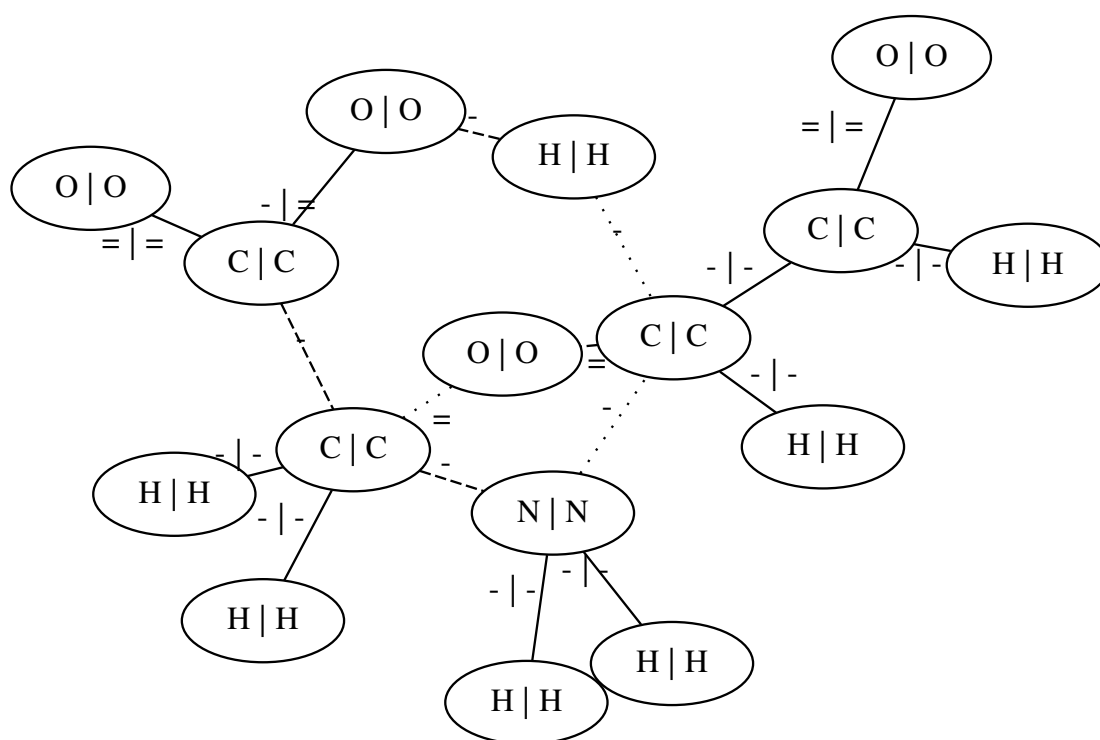
0.0.40 Strecker Degradation Dicarbonyl, H, H, H, H



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

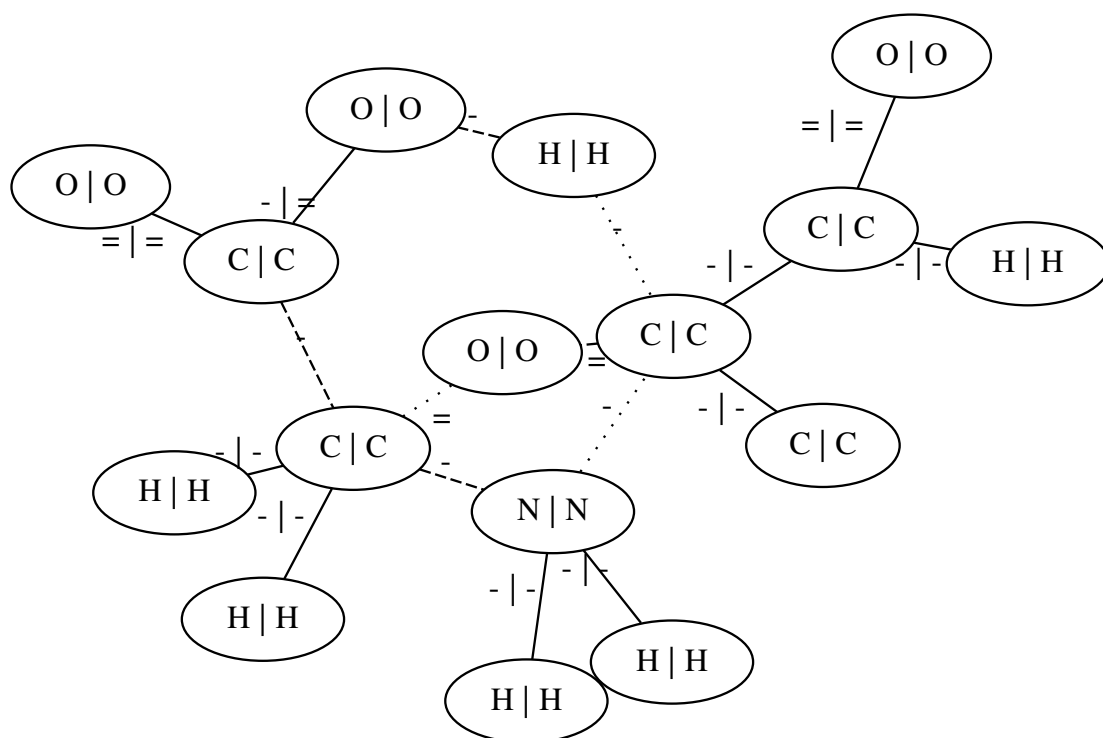
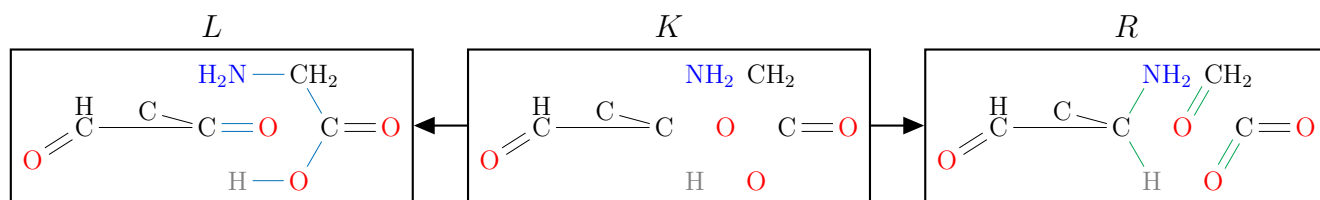
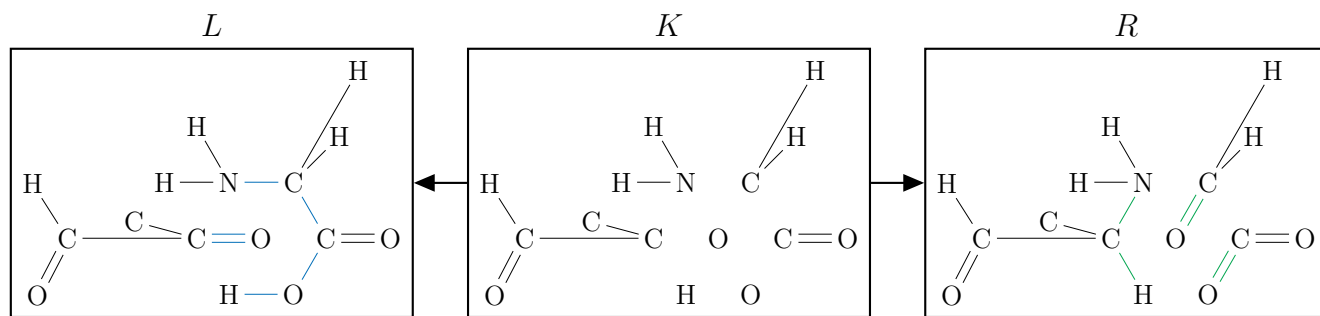


Files: out/197_r_38_11300100_{L, K, R}



File: out/198_r_38_combined

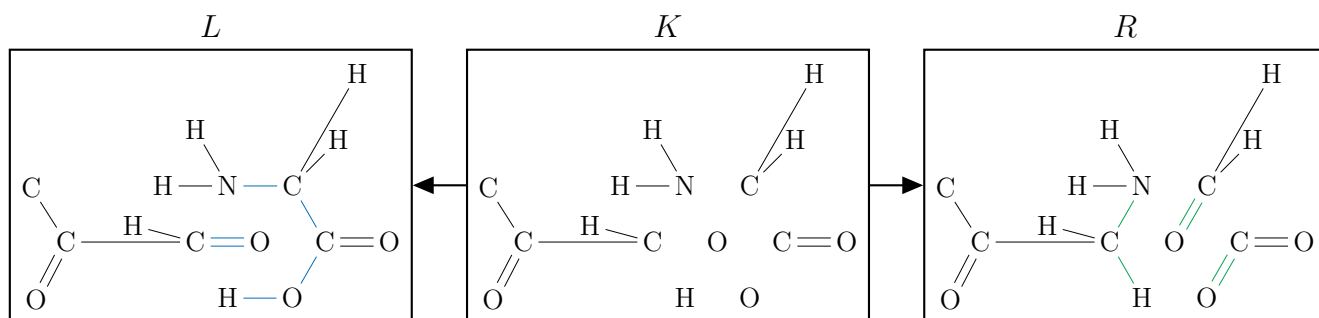
0.0.41 Strecker Degradation Dicarbonyl, H, H, H, C



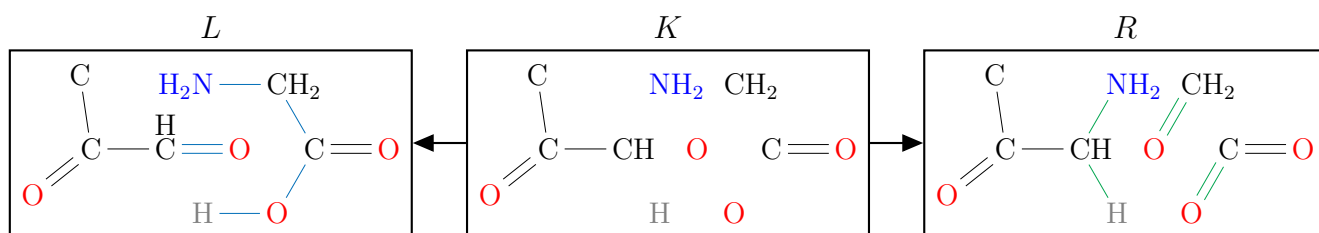
File: out/203_r_39_combined

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

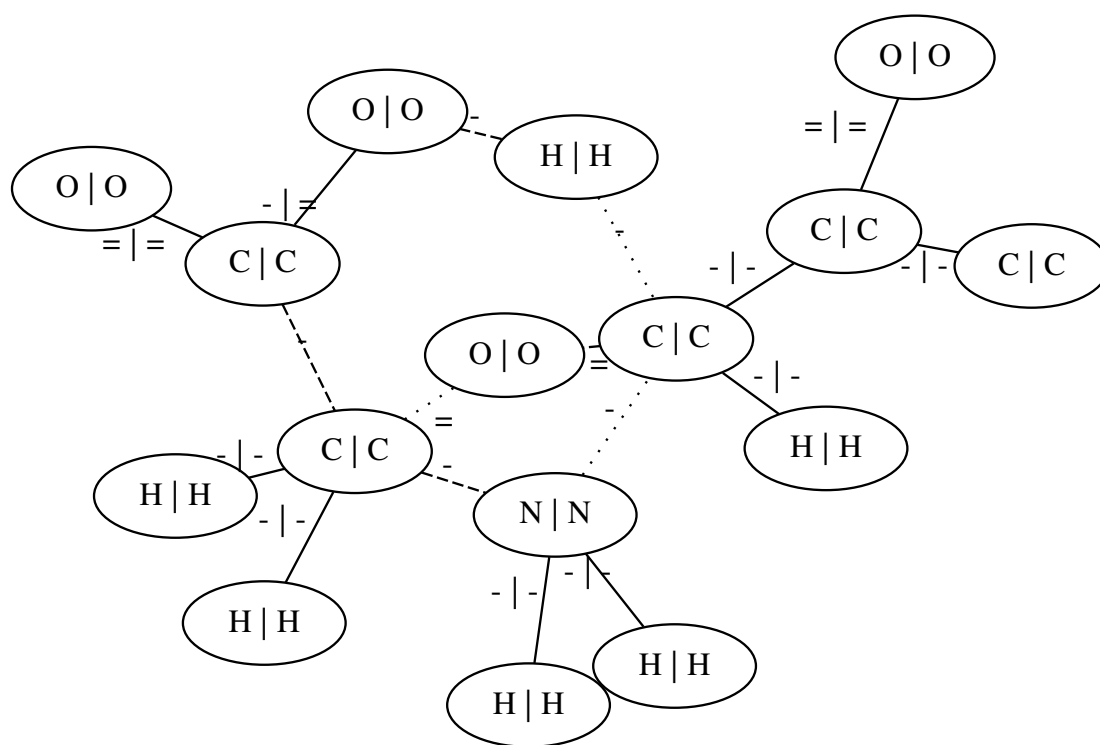
0.0.42 Strecker Degradation Dicarbonyl, H, H, C, H



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



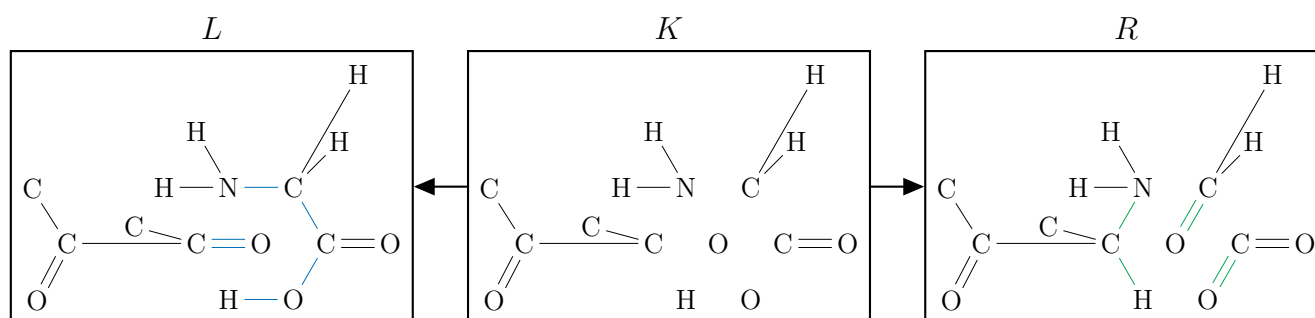
Files: out/207_r_40_11300100_{L, K, R}



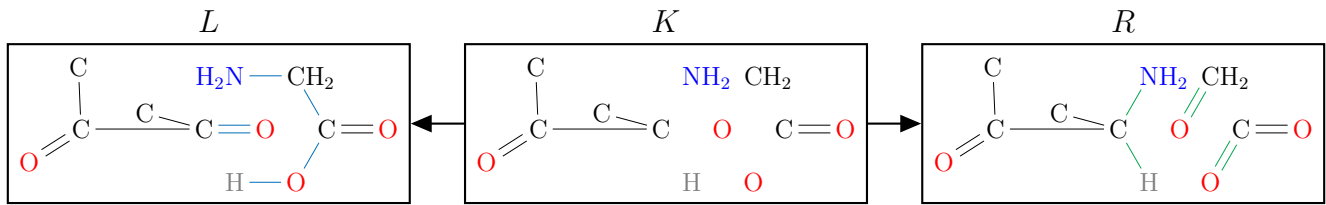
File: out/208_r_40_combined

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

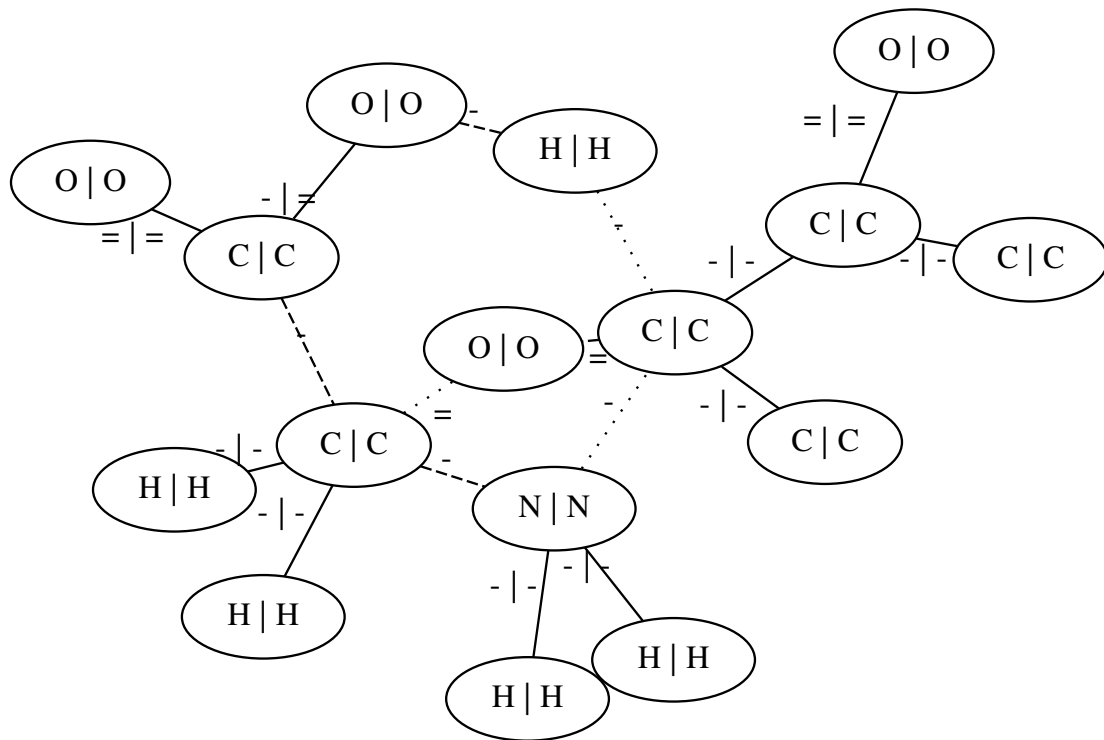
0.0.43 Strecker Degradation Dicarbonyl, H, H, C, C



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 ∈ outEdges(10) |
  label(target(e)) ∈ {'O'}
  ∧
  label(e) ∈ {'='}
}| = 0

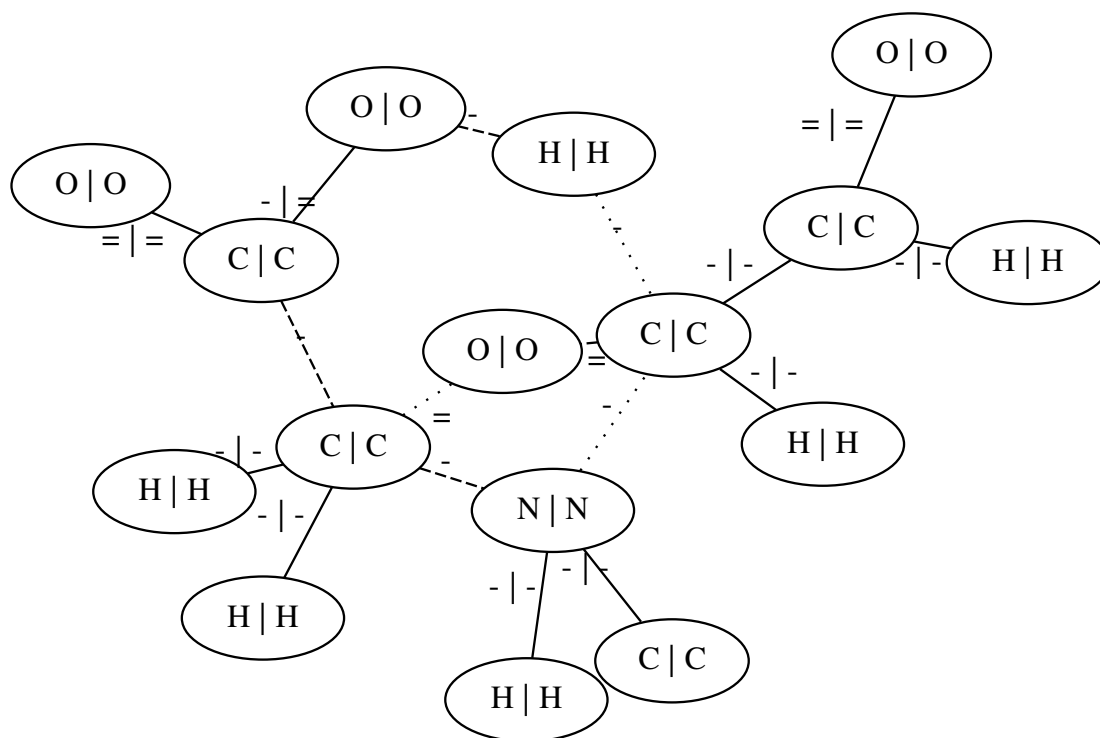
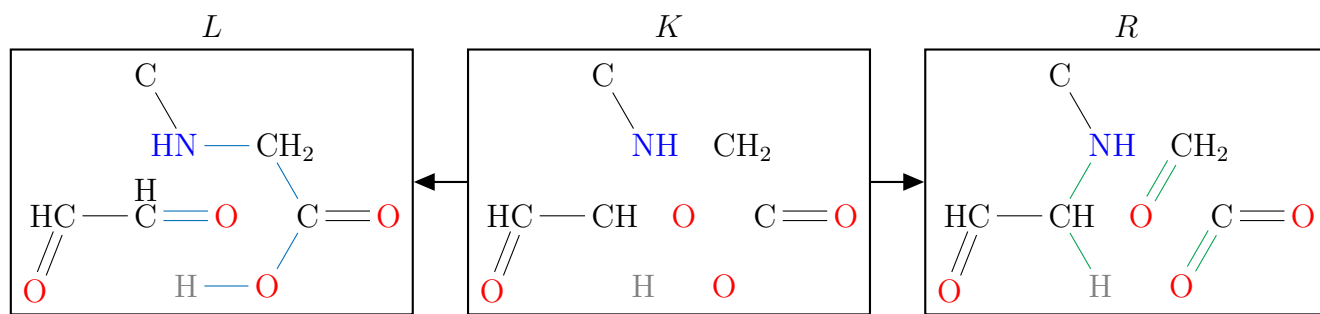
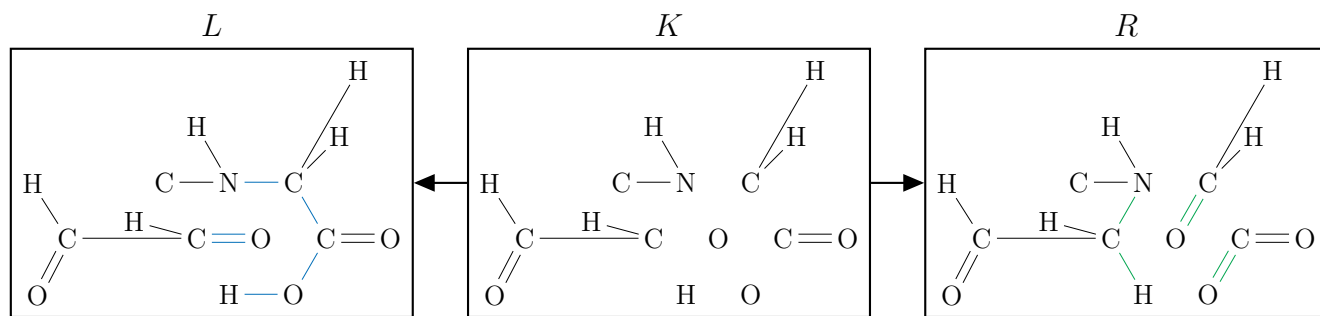
```

```

|{e ∈ outEdges(15) |
  label(target(e)) ∈ {'O'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

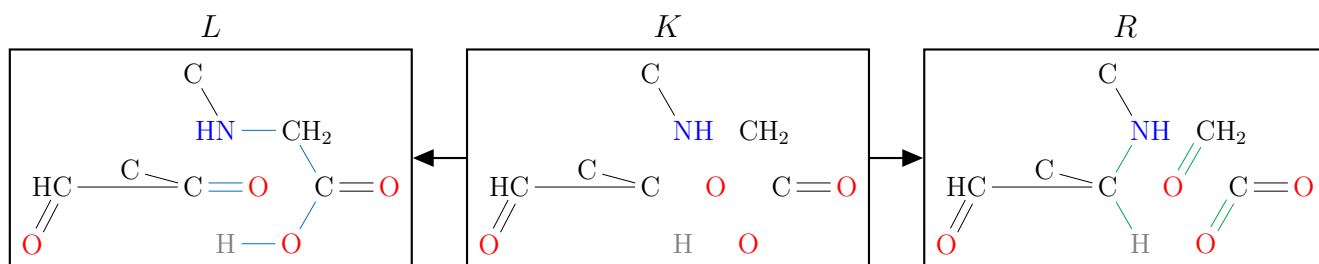
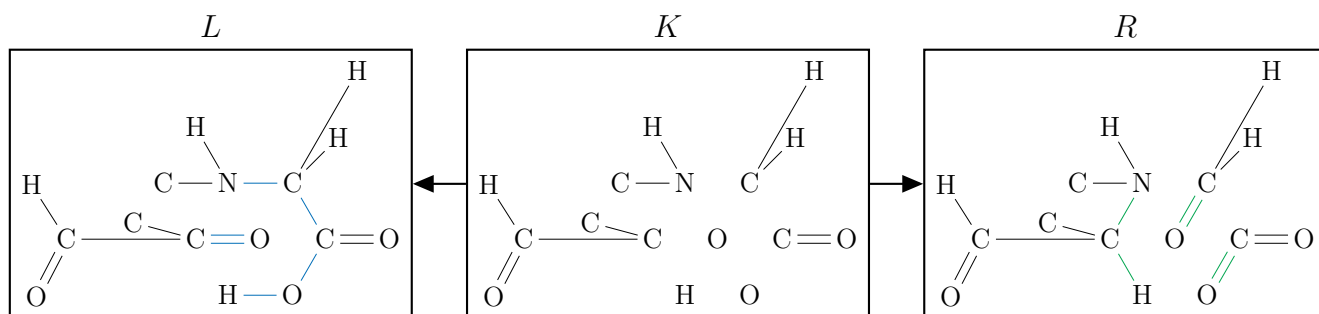
0.0.44 Strecker Degradation Dicarbonyl, H, C, H, H

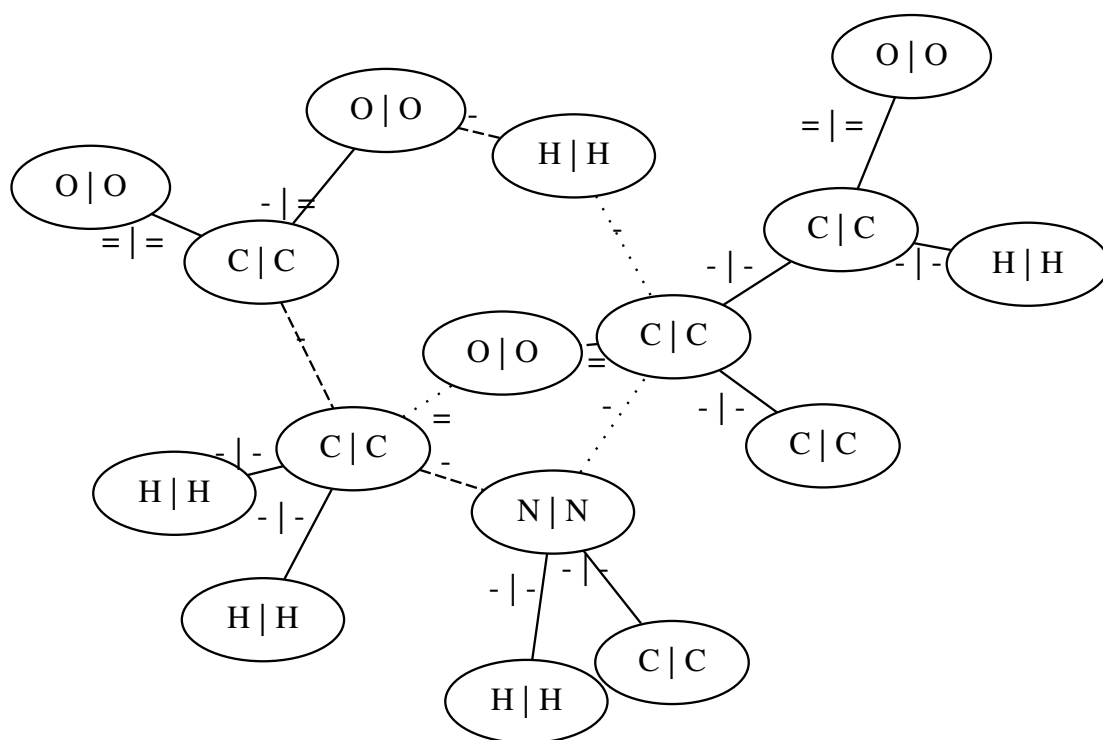


File: out/218_r_42_combined

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

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





File: out/223_r_43_combined

$$|\{e \in \text{outEdges}(9) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid$$

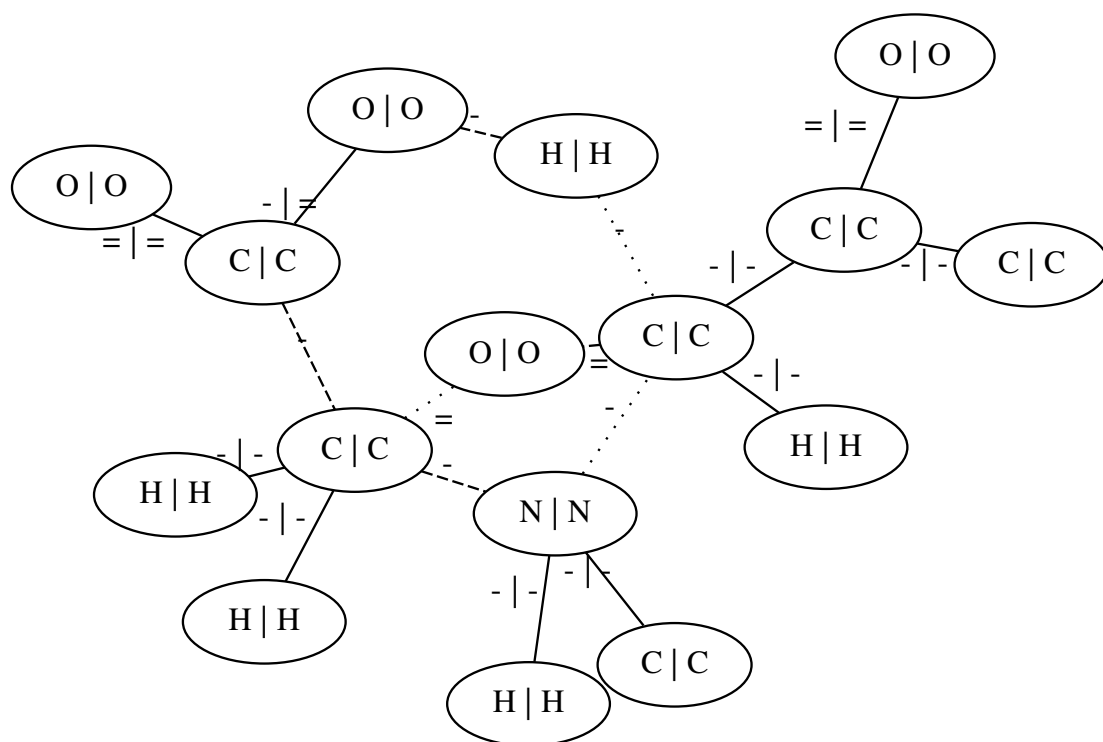
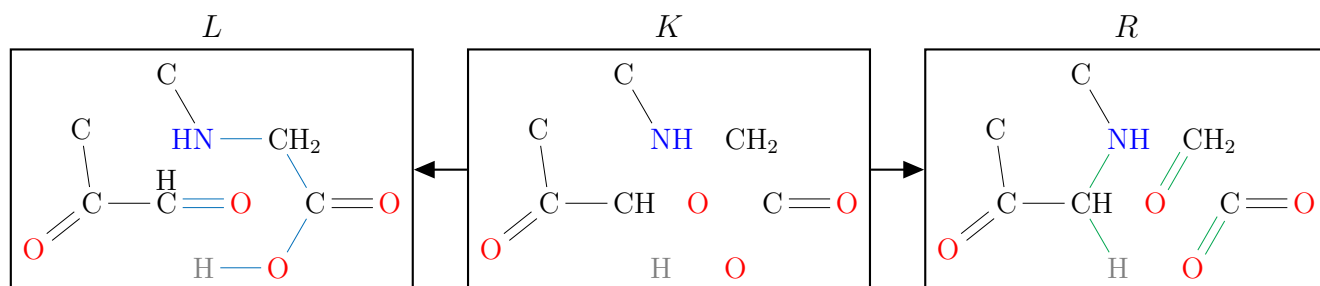
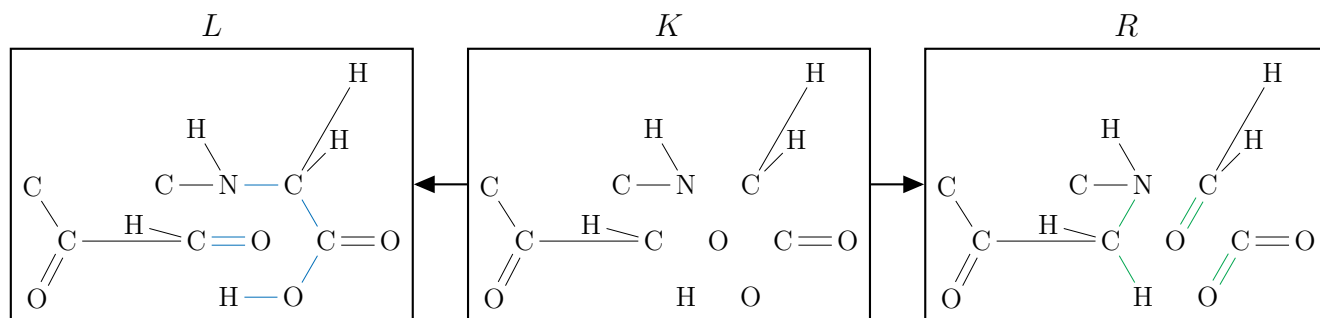
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

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

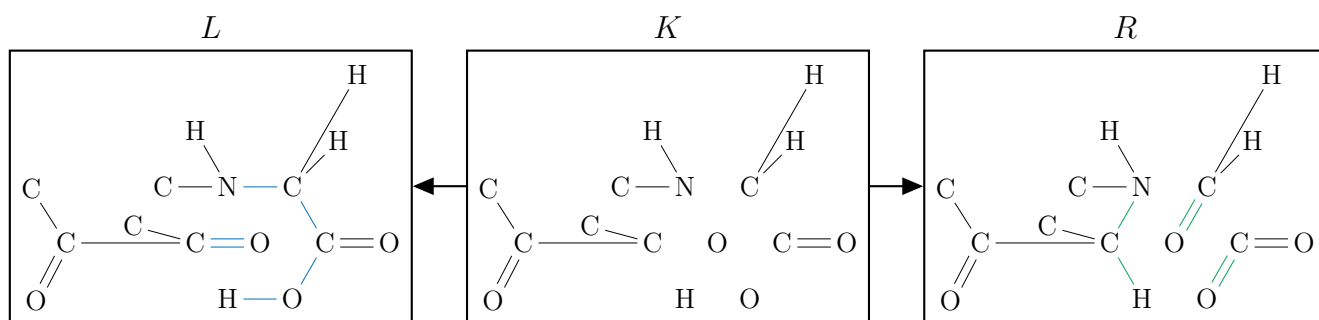


File: out/228_r_44_combined

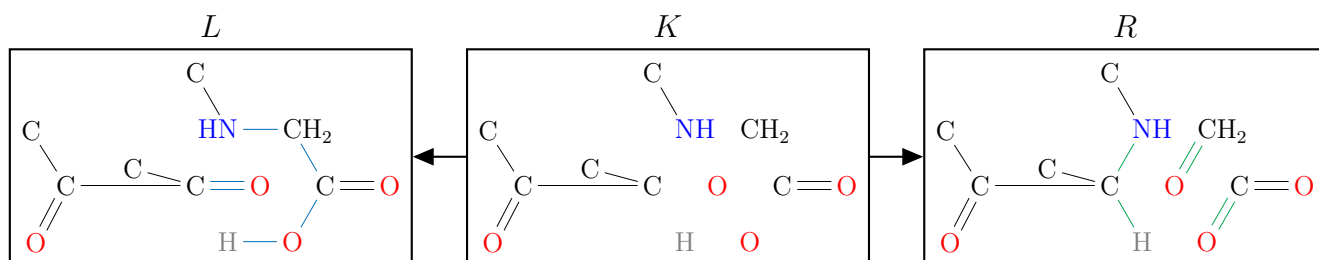
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

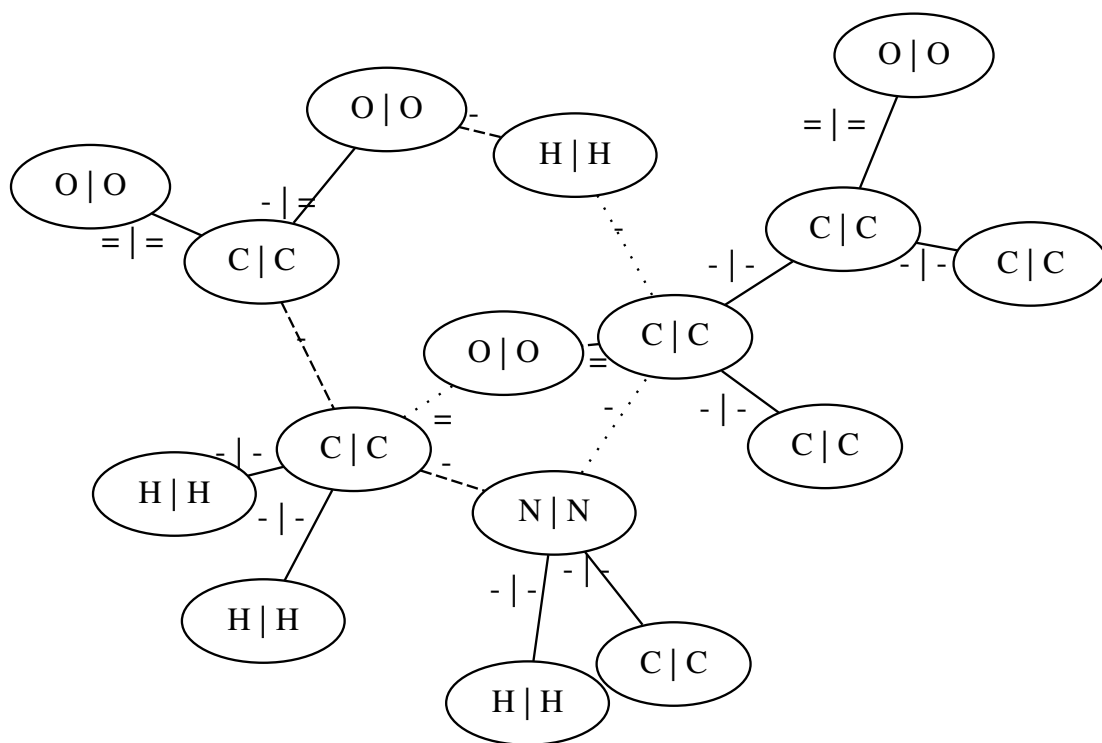
0.0.47 Strecker Degradation Dicarbonyl, H, C, C, C



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



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



File: out/233_r_45_combined

$$|\{e \in \text{outEdges}(9) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(10) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid$$

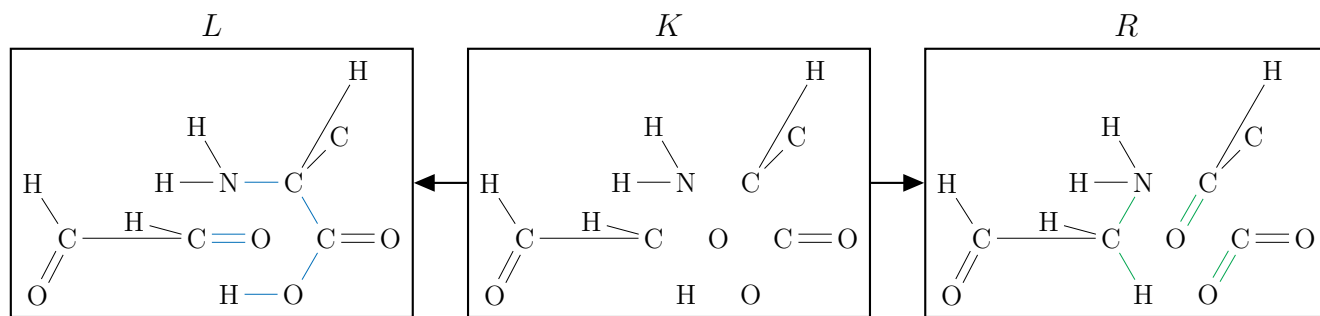
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

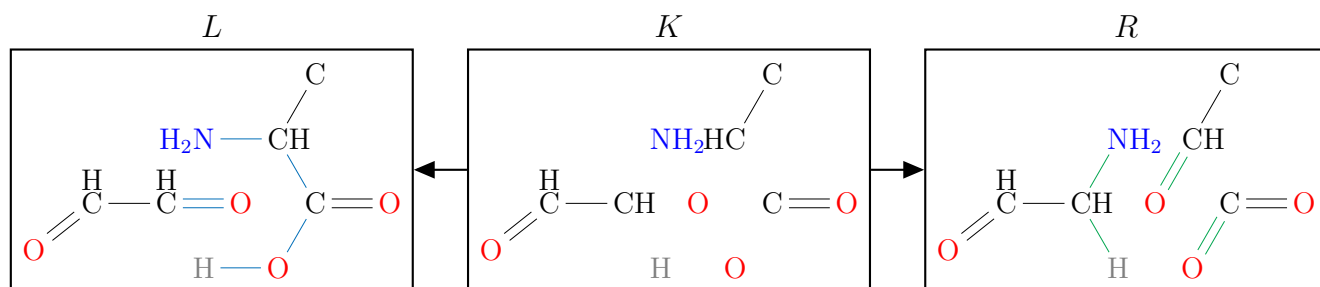
$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

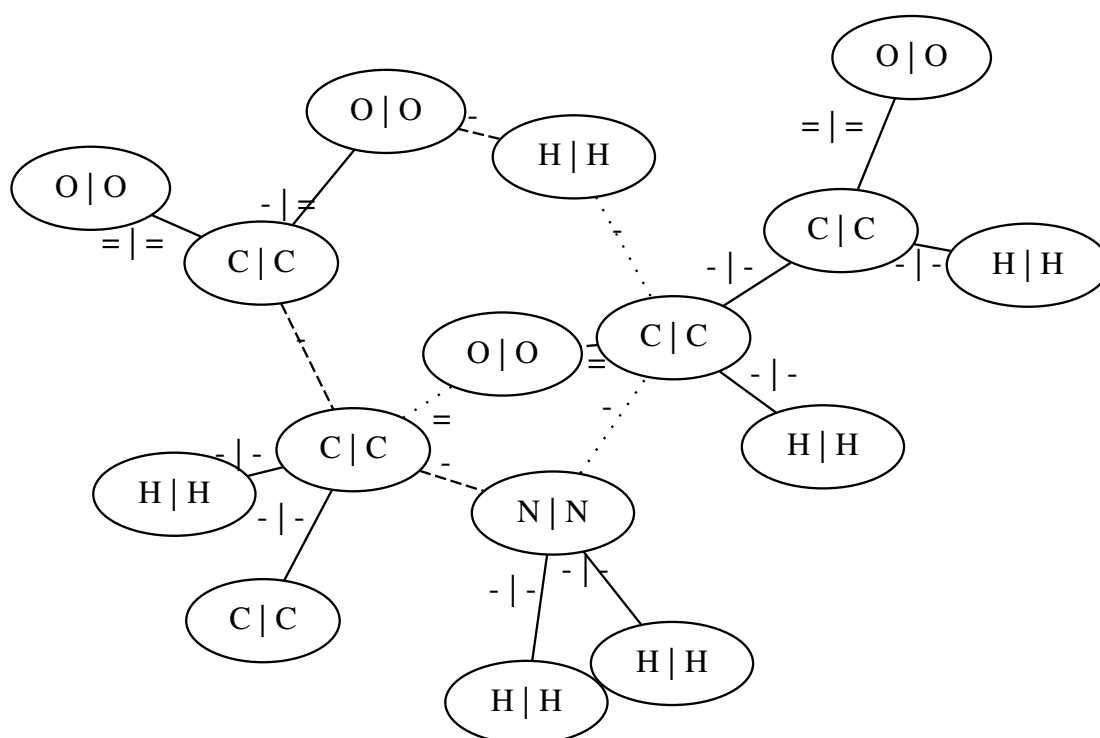
0.0.48 Strecker Degradation Dicarbonyl, C, H, H, H



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



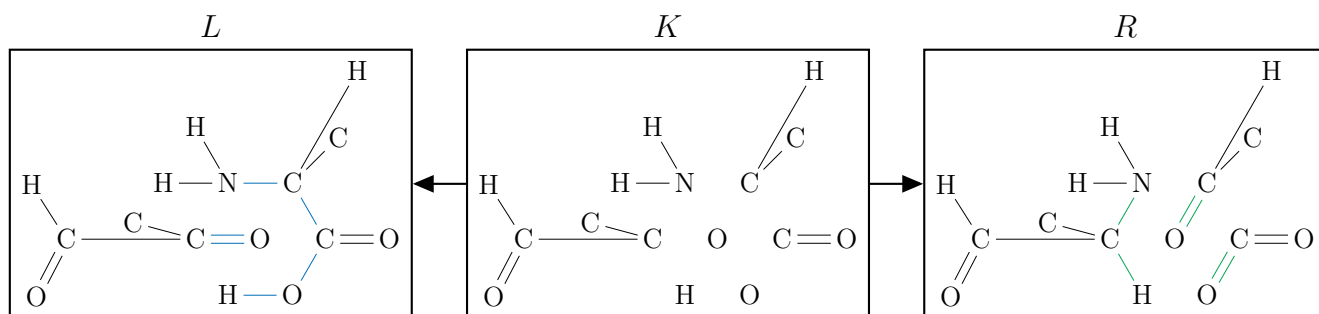
Files: out/237_r_46_11300100_{L, K, R}



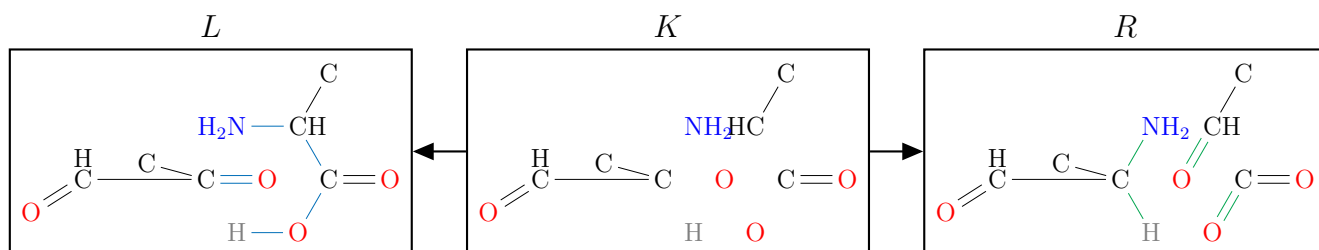
File: out/238_r_46_combined

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

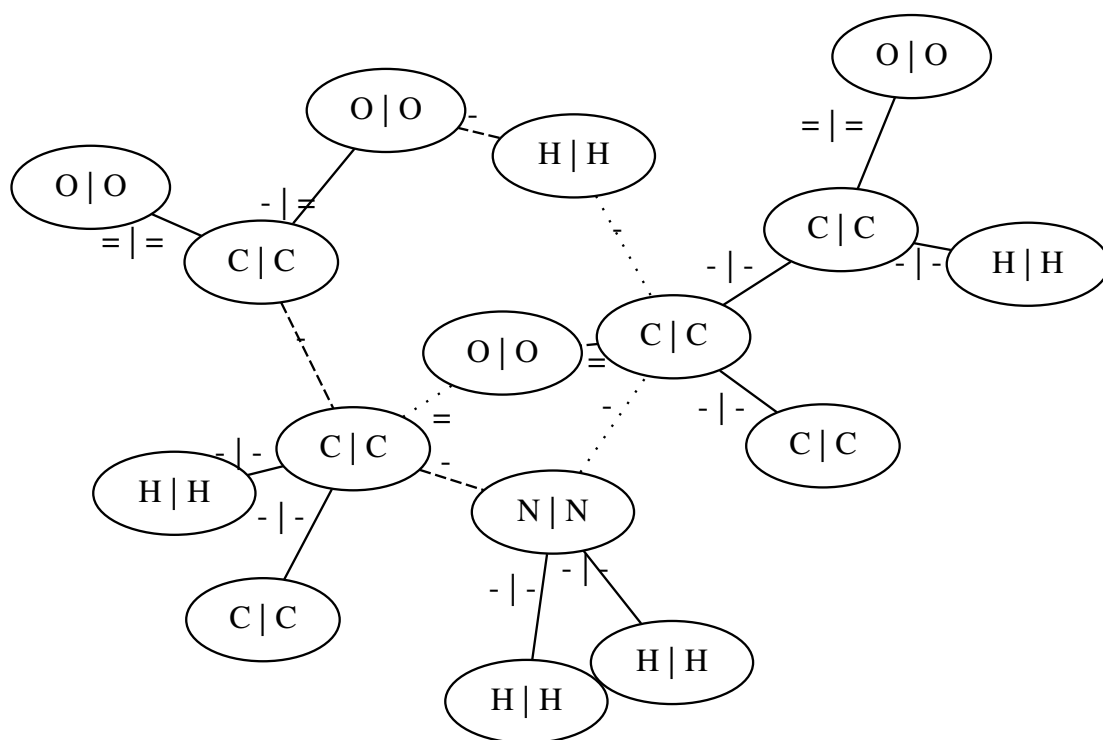
0.0.49 Strecker Degradation Dicarbonyl, C, H, H, C



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



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



File: out/243_r_47_combined

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid$$

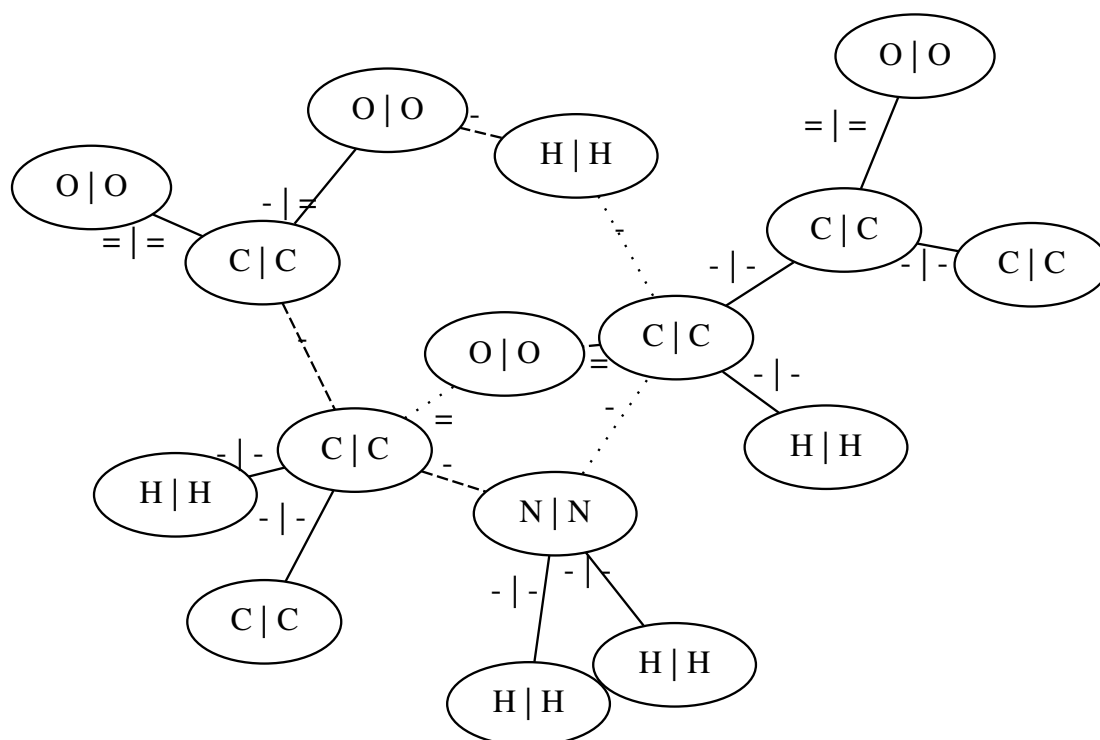
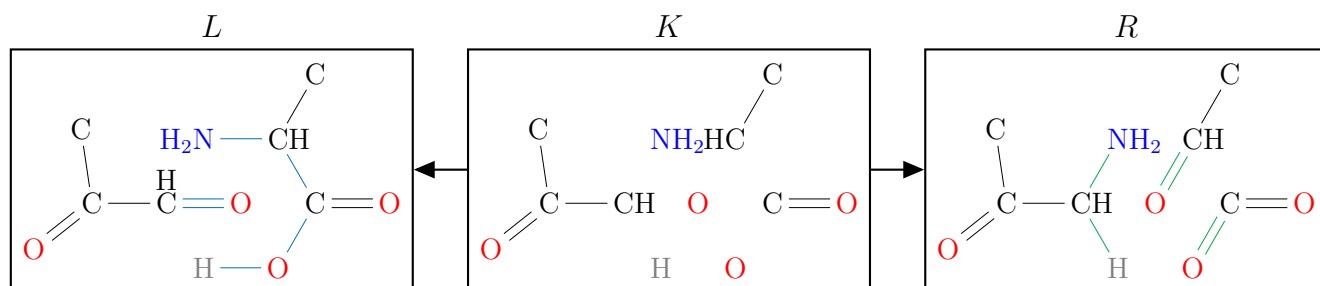
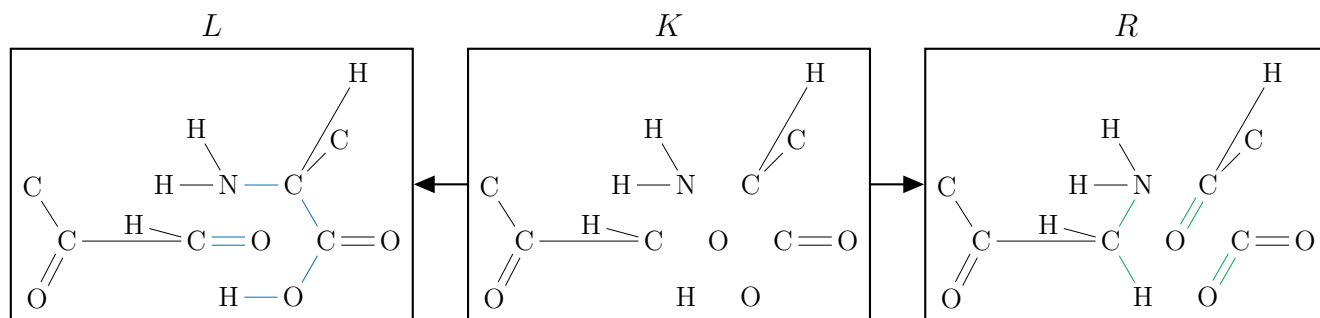
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

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

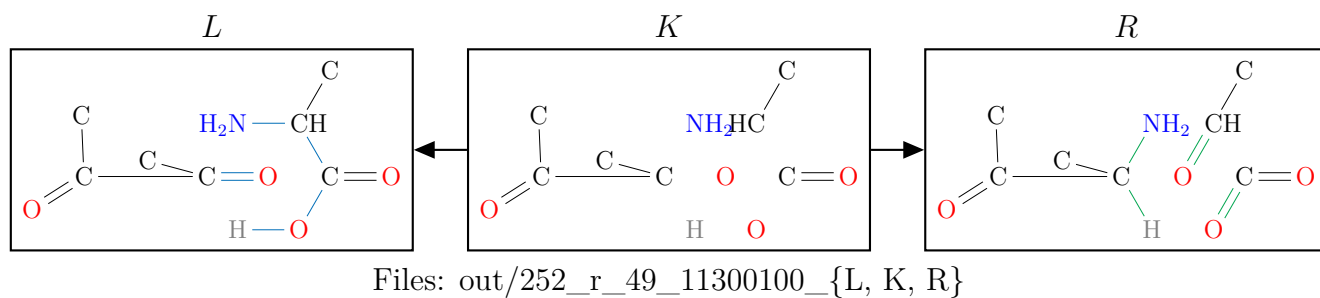
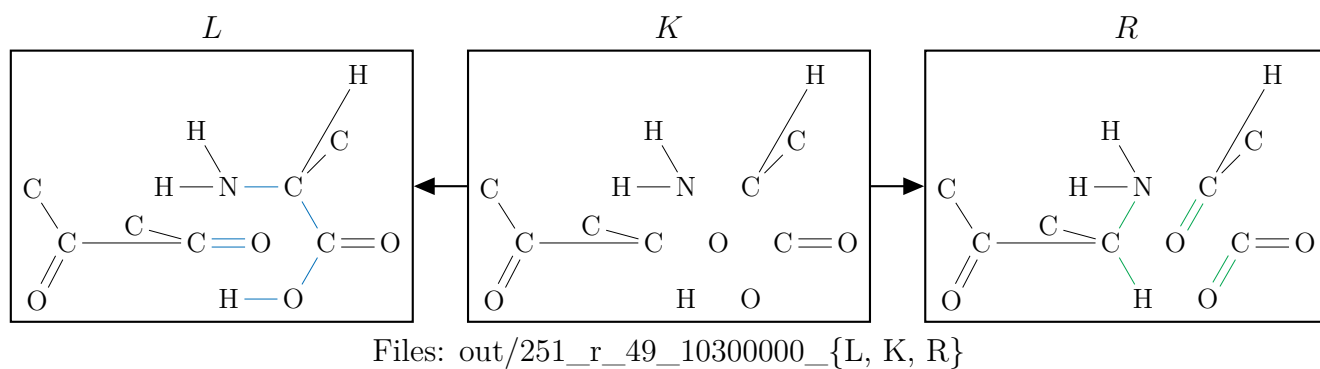


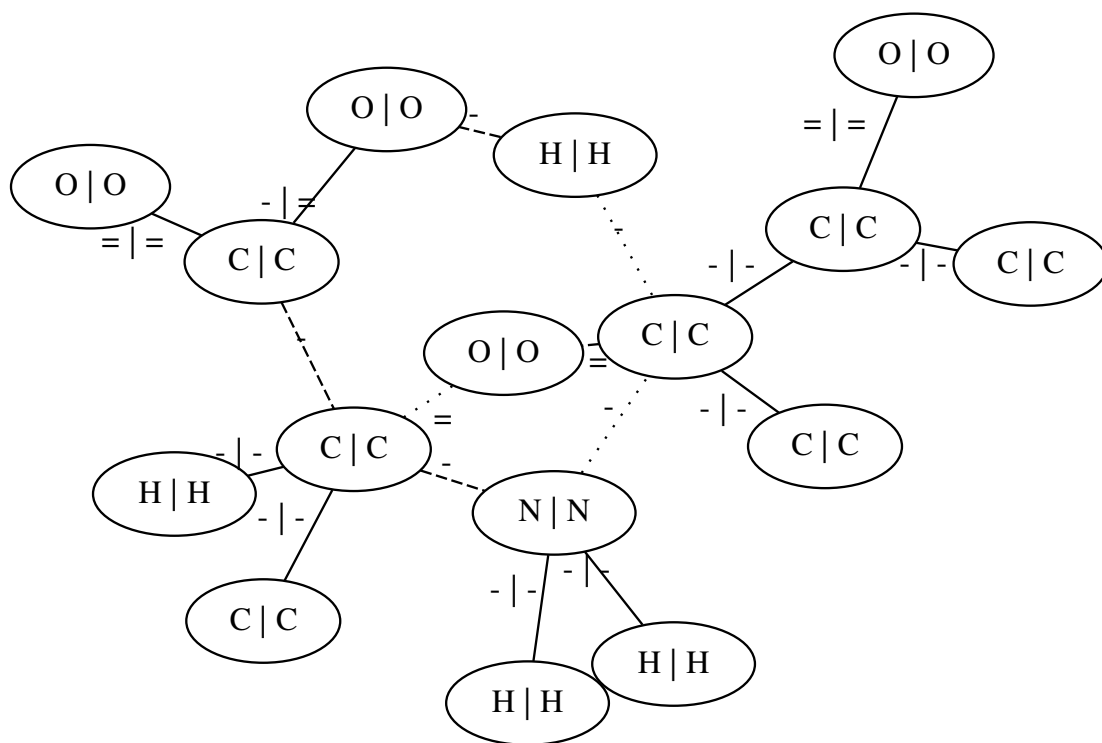
File: out/248_r_48_combined

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

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

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





File: out/253_r_49_combined

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(10) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid$$

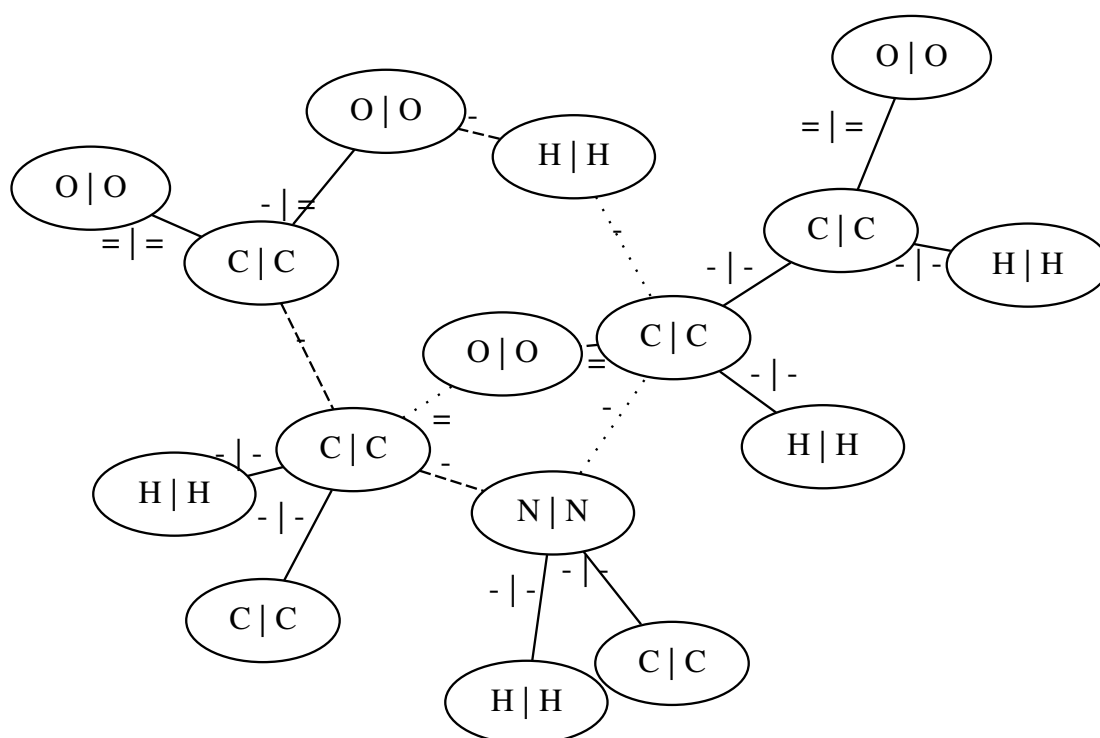
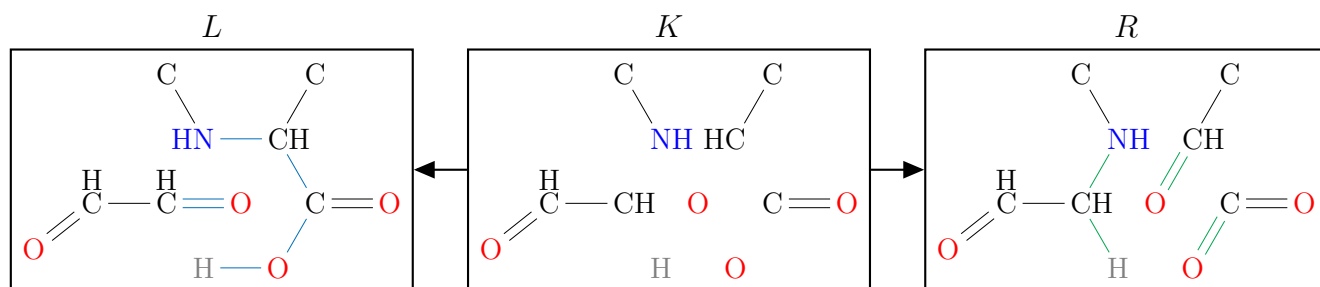
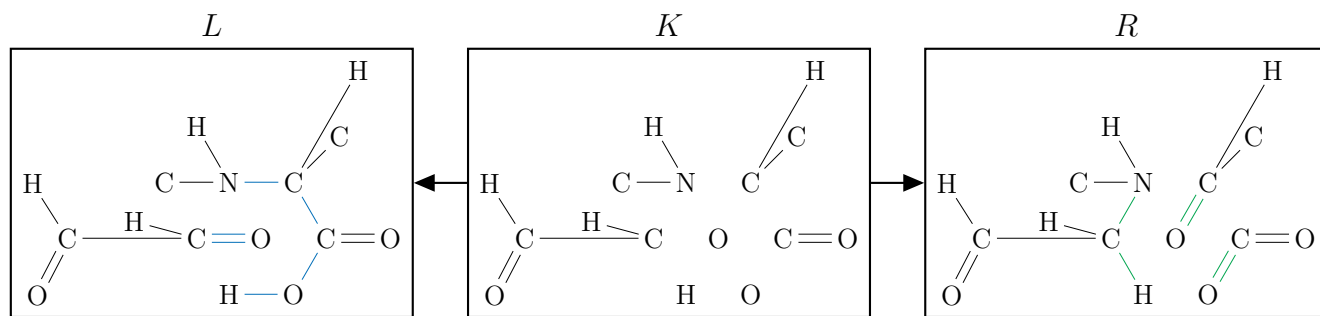
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

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

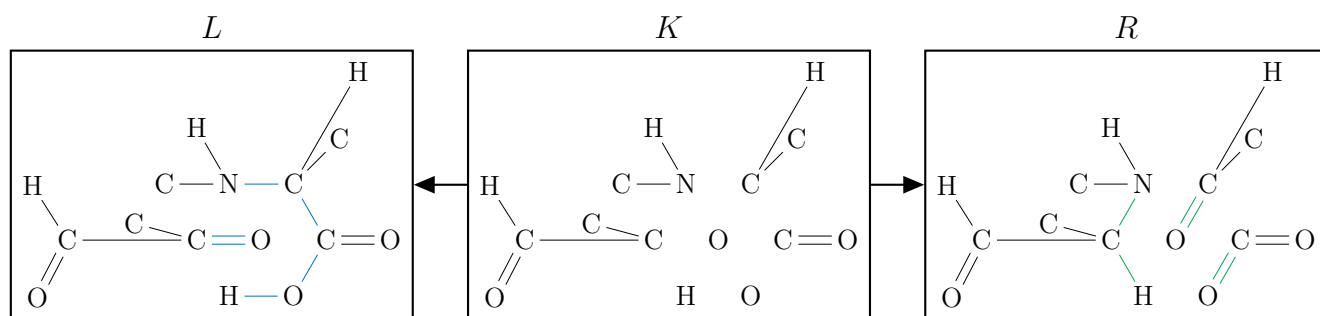


File: out/258_r_50_combined

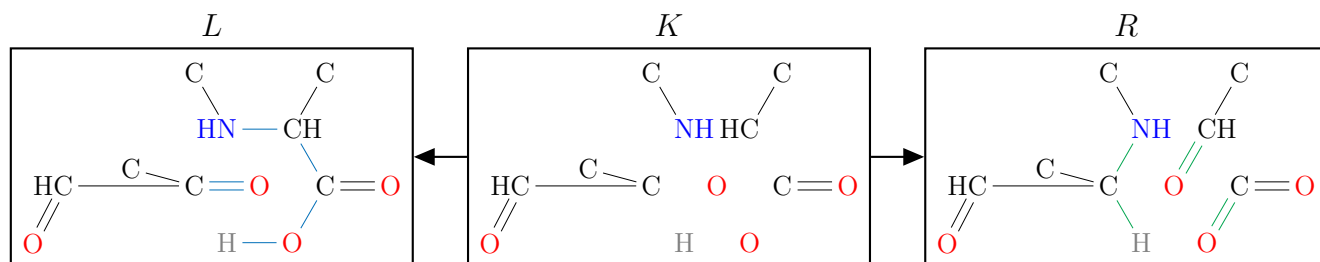
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

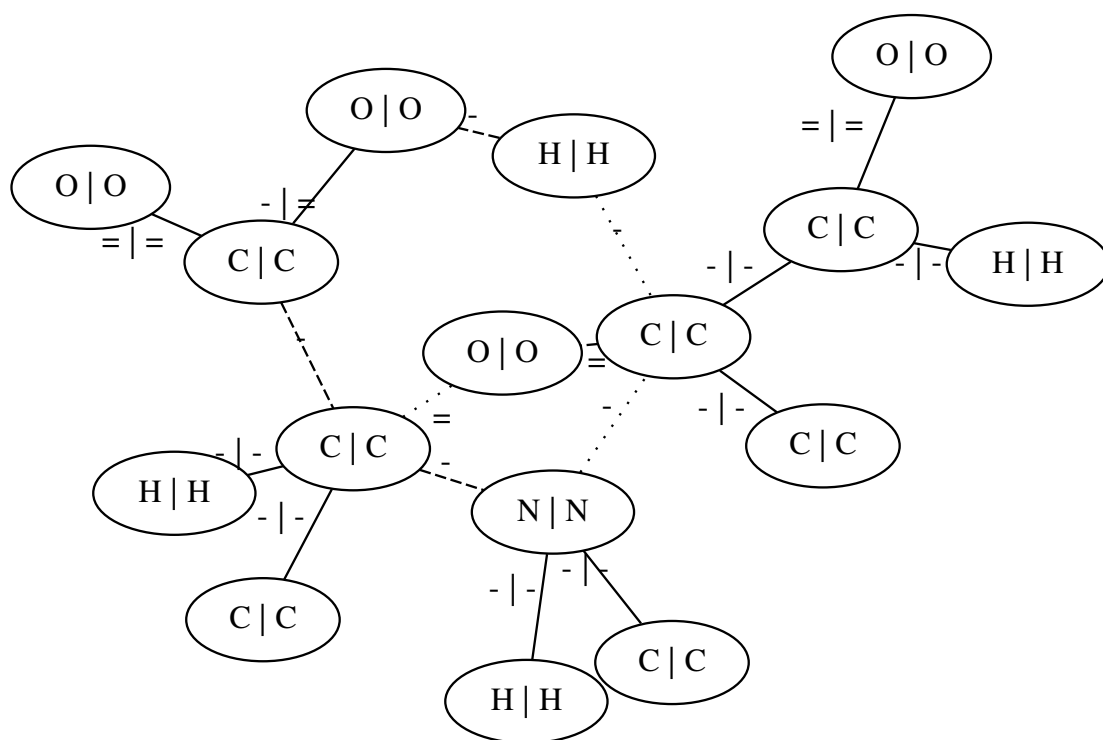
0.0.53 Strecker Degradation Dicarbonyl, C, C, H, C



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



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



File: out/263_r_51_combined

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(9) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(15) \mid$$

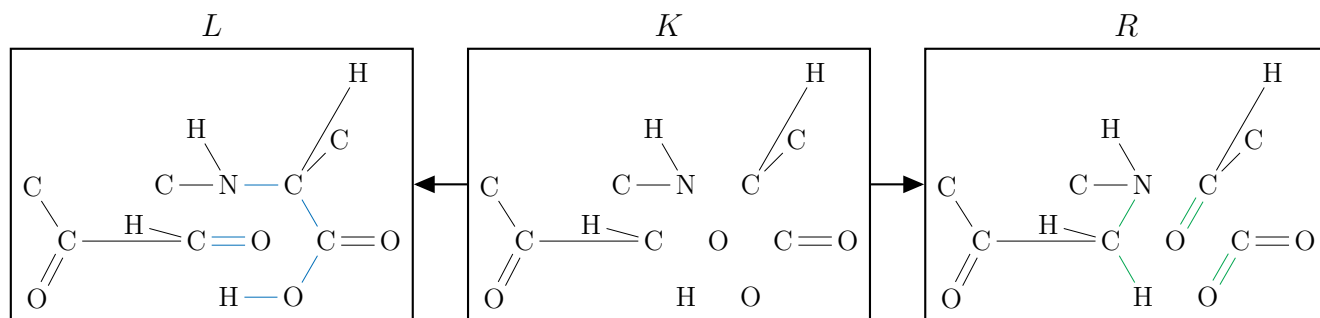
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

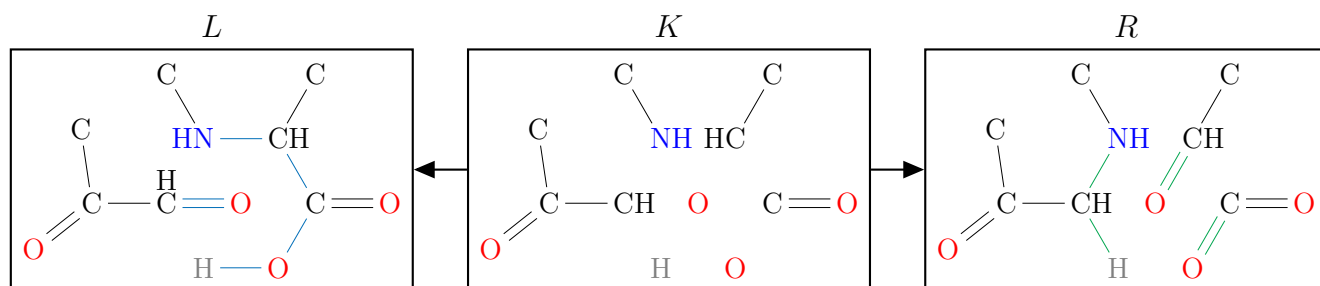
$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

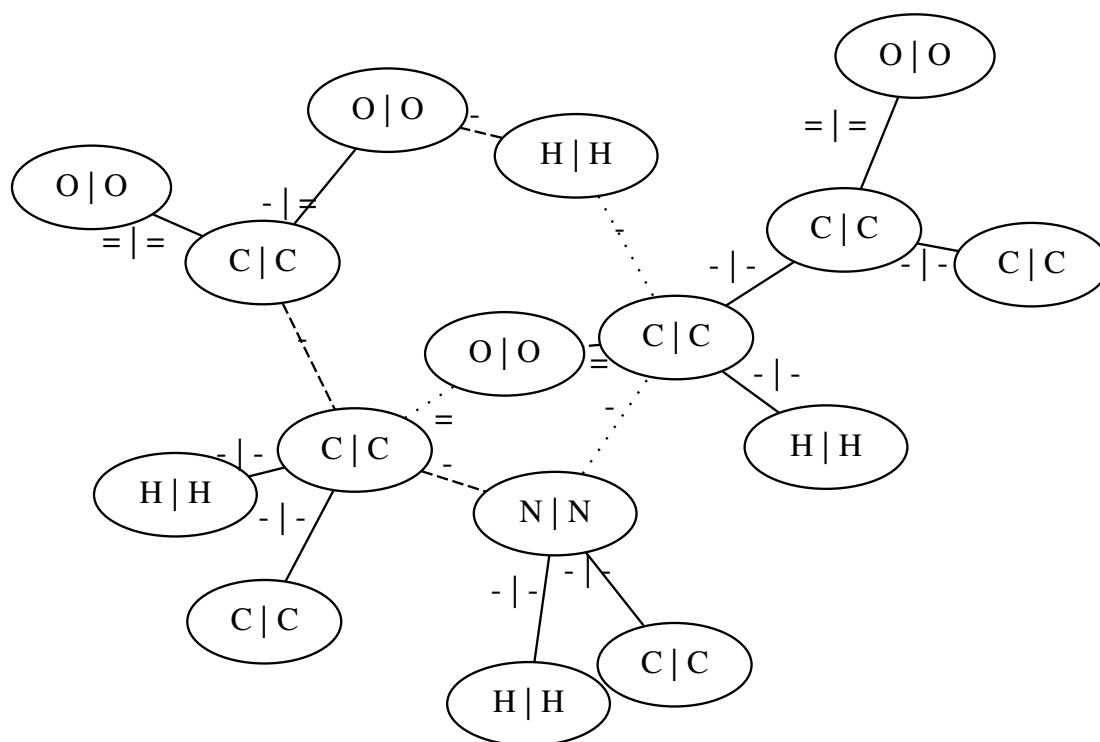
0.0.54 Strecker Degradation Dicarbonyl, C, C, C, H



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



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



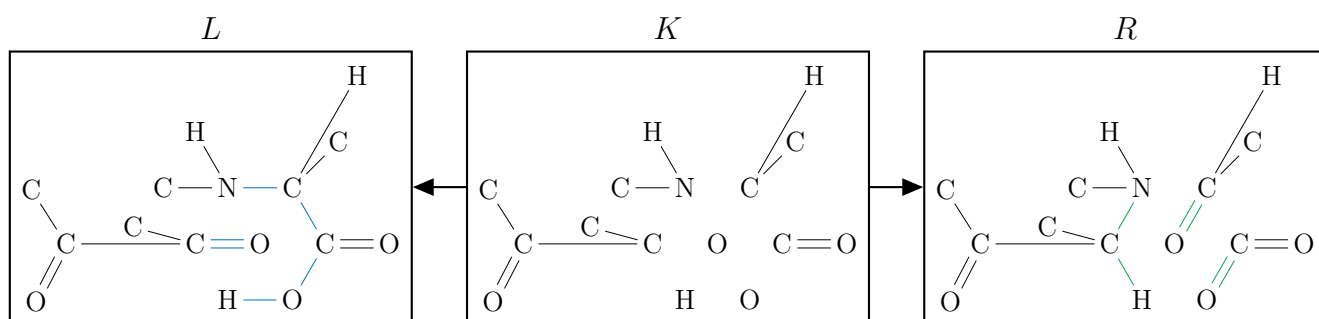
File: out/268_r_52_combined

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

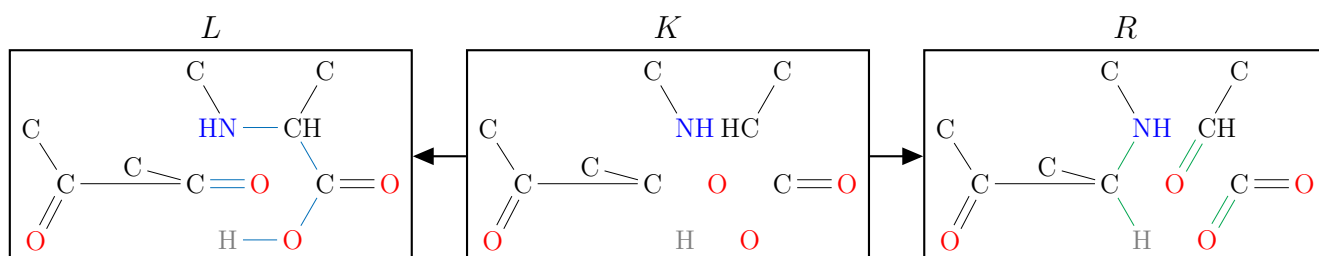
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

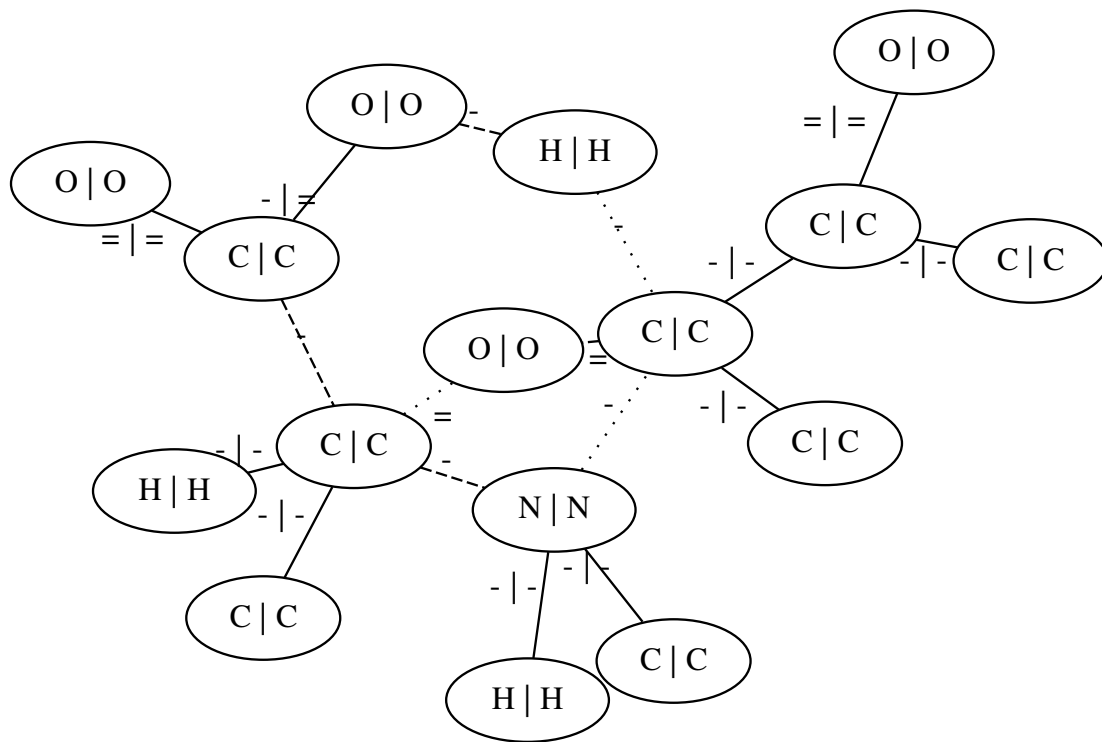
0.0.55 Strecker Degradation Dicarbonyl, C, C, C, C



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



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



File: out/273_r_53_combined

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(9) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(10) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

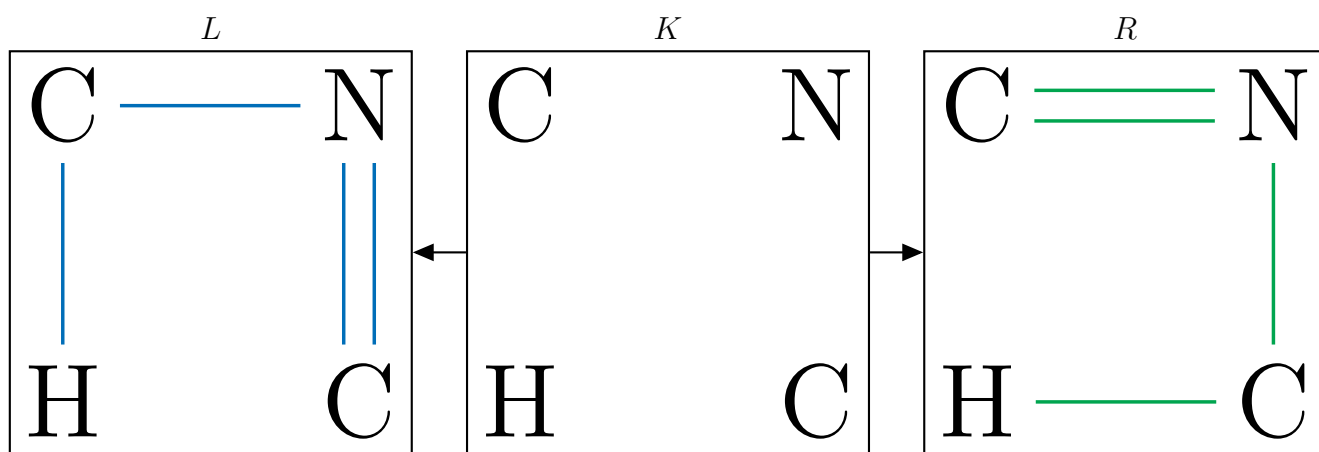
$$\wedge$$

$$\text{label}(e) \in \{'=\'}\}$$

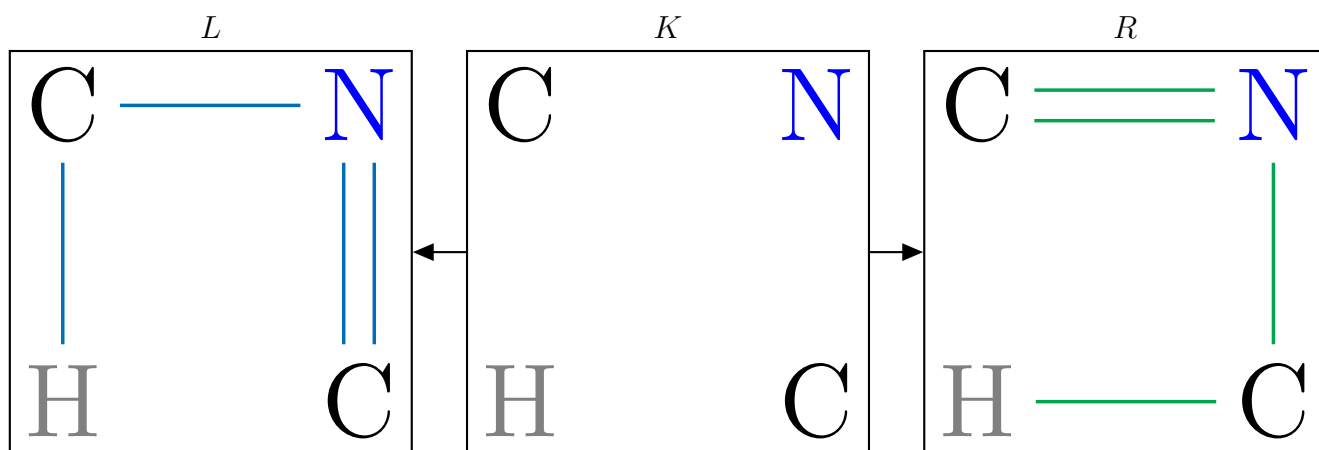
$$\}| = 0$$

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

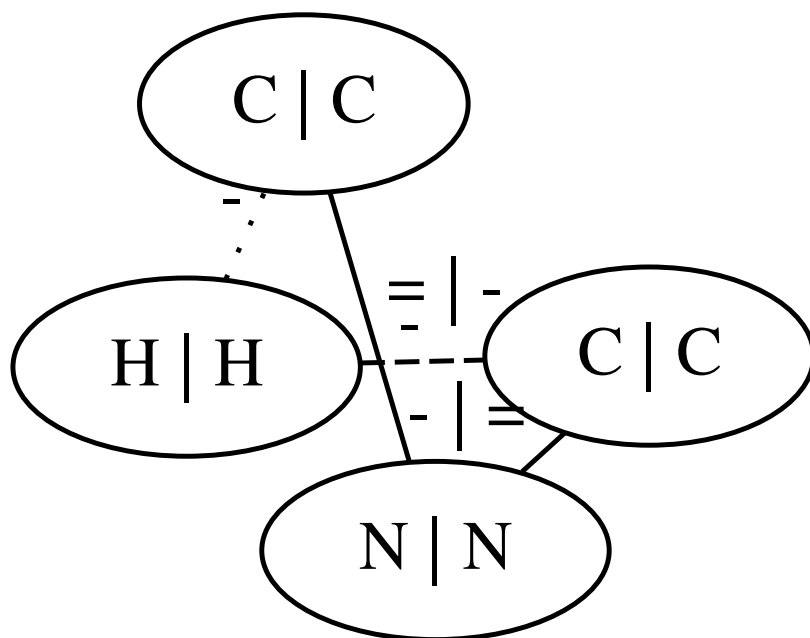
0.0.56 Schiff Tautomerization



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

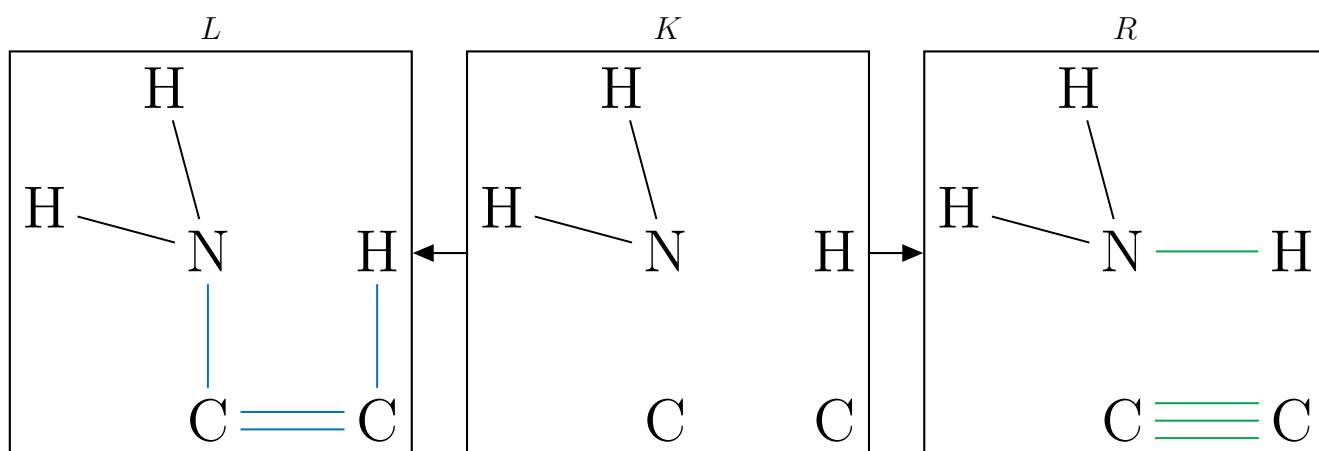


Files: out/277_r_54_11300100_{L, K, R}

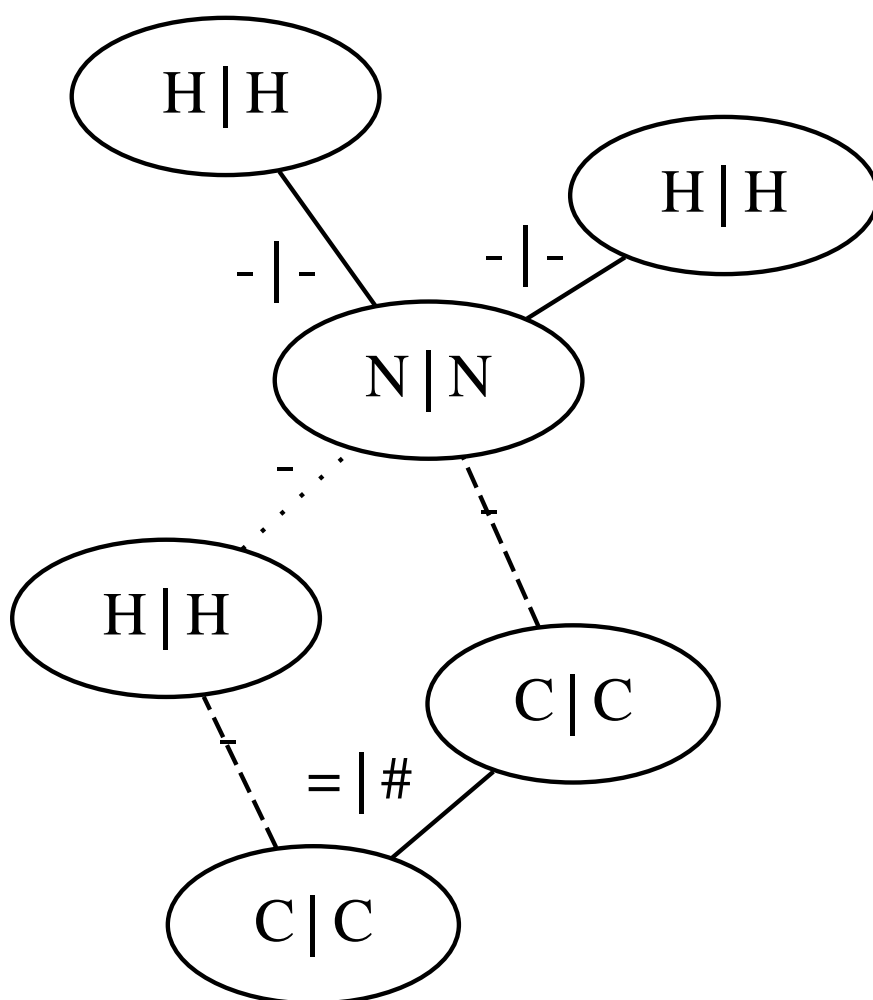
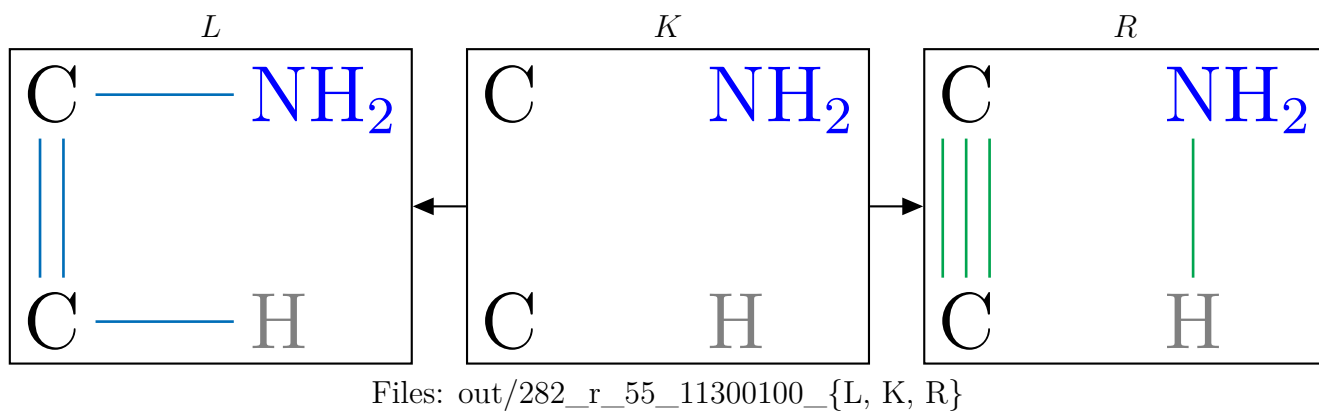


File: out/278_r_54_combined

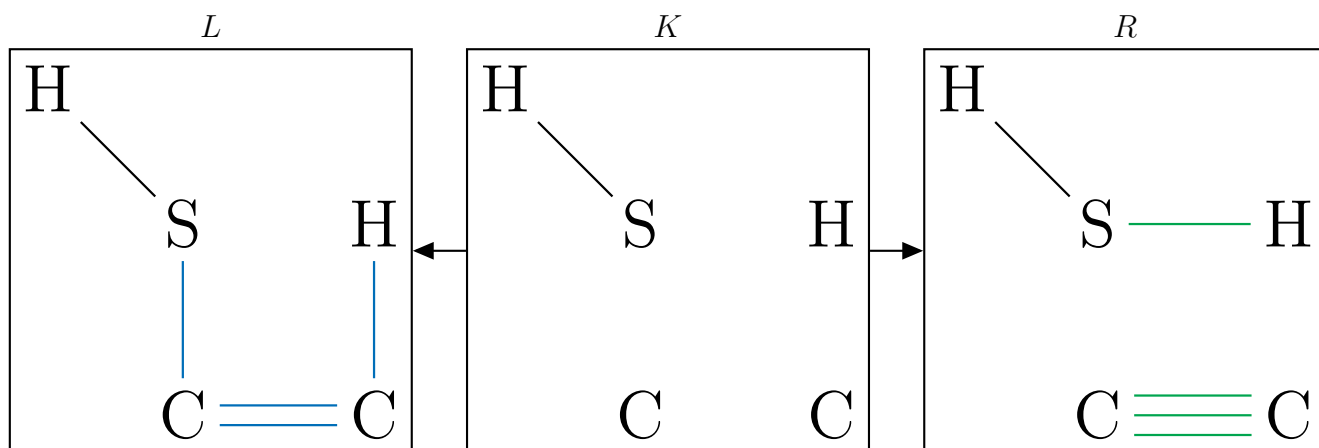
0.0.57 Alkyne Addition, N, HH, inverse



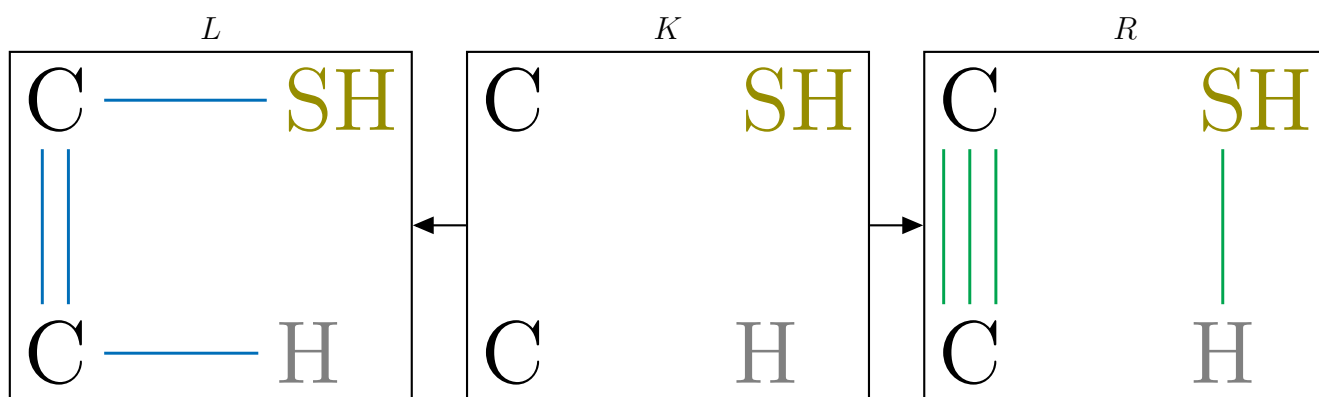
Files: out/281_r_55_10300000_{L, K, R}



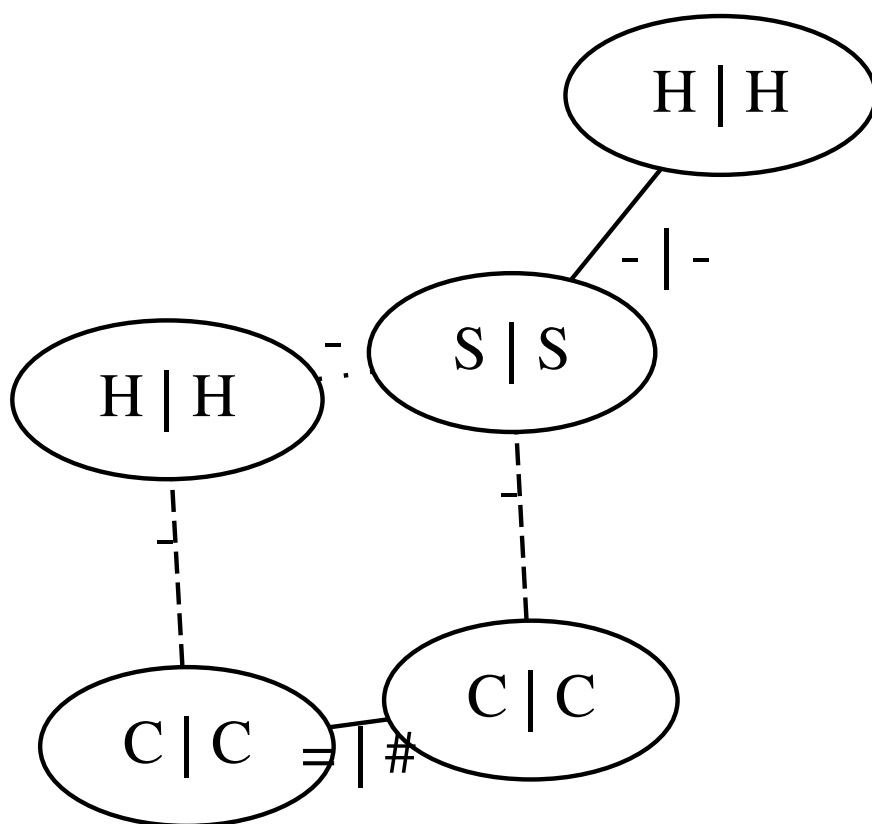
0.0.58 Alkyne Addition, S, H, inverse



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

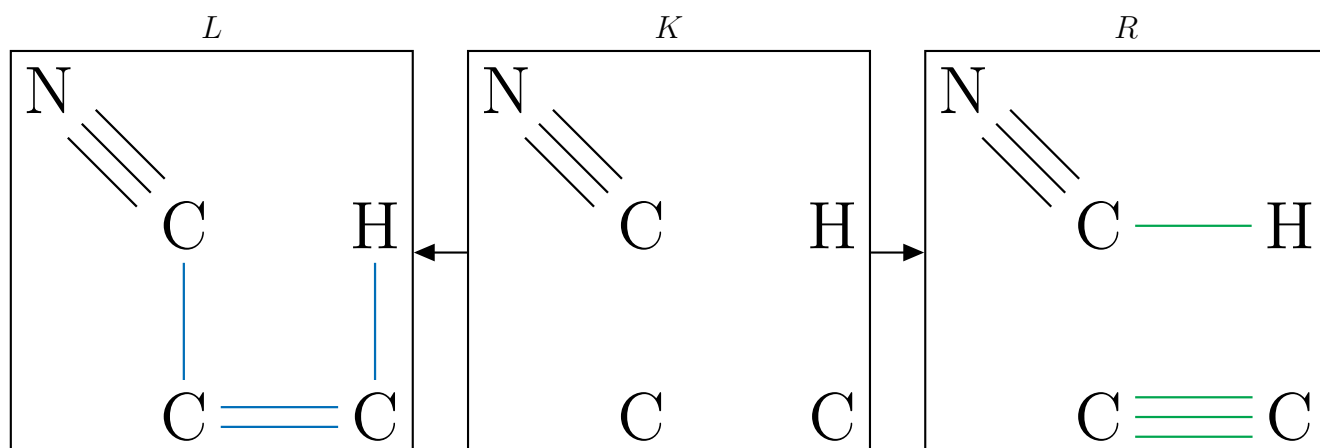


Files: out/287_r_56_11300100_{L, K, R}

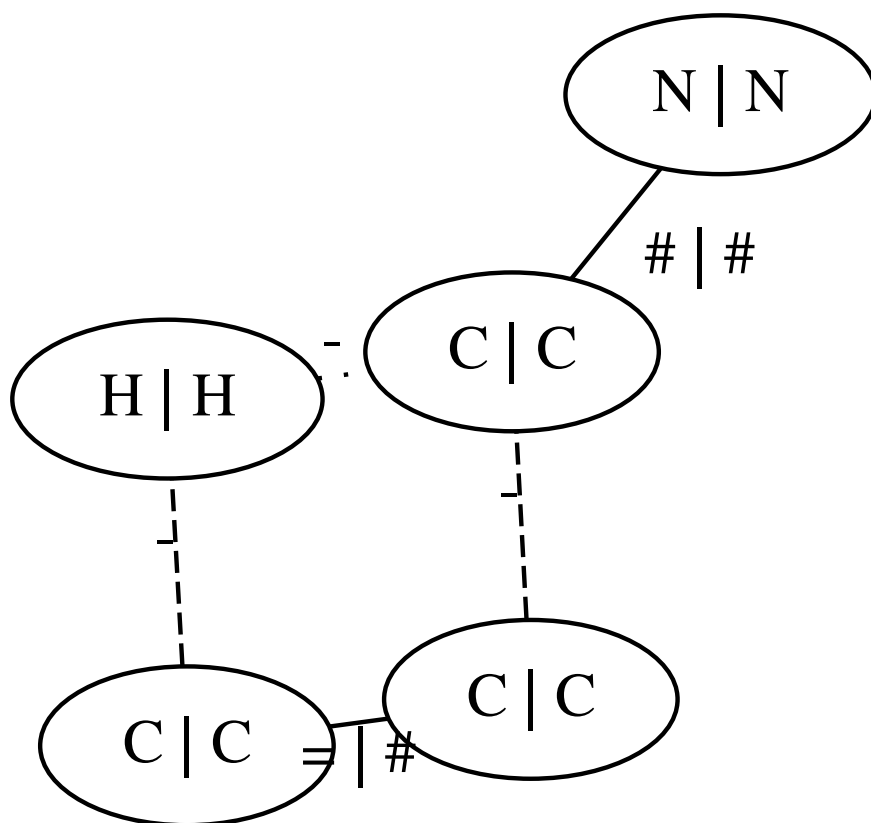
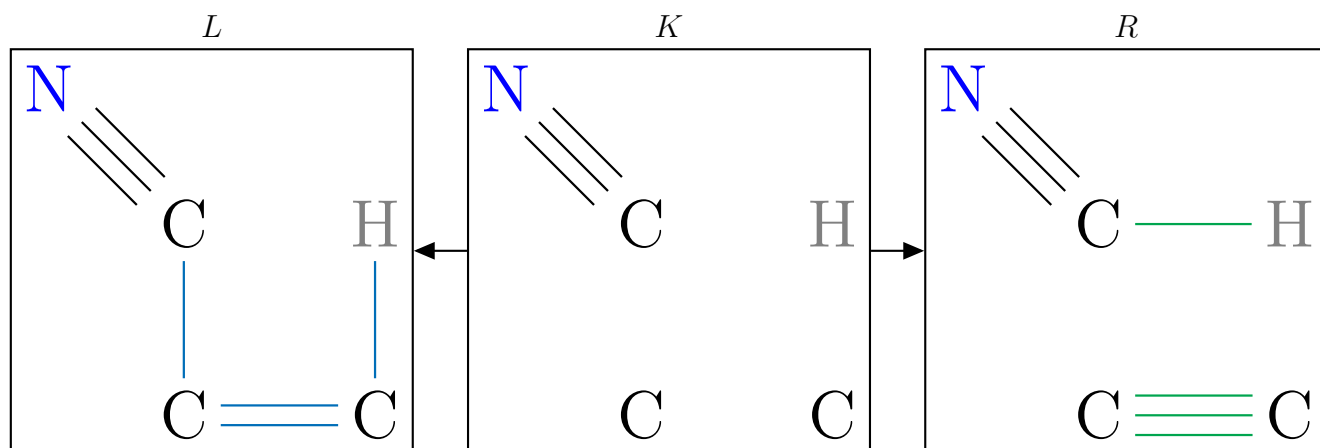


File: out/288_r_56_combined

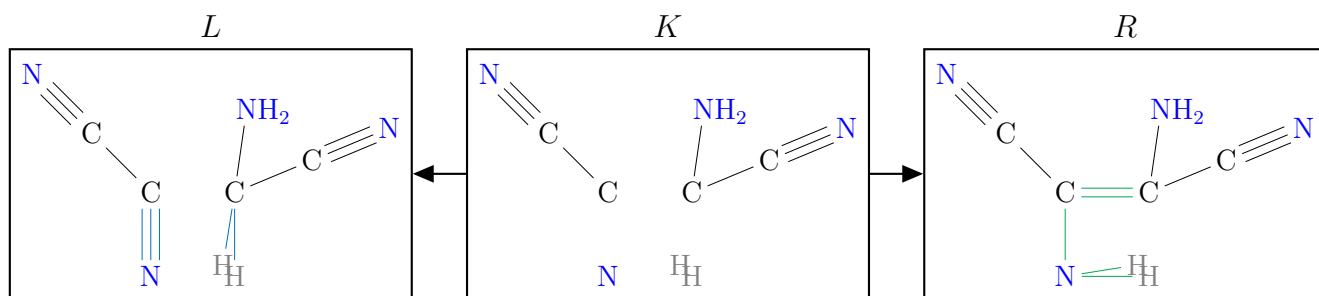
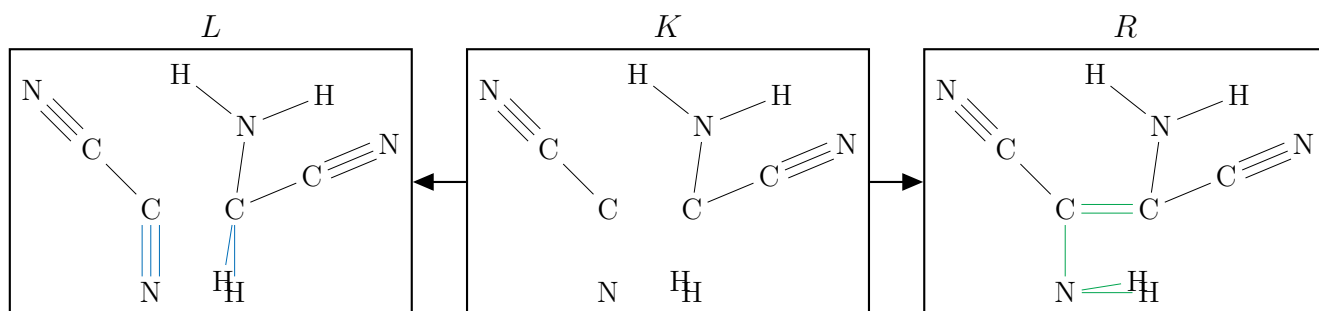
0.0.59 Alkyne Addition, C, inverse

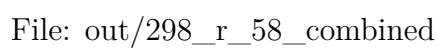


Files: out/291_r_57_10300000_{L, K, R}

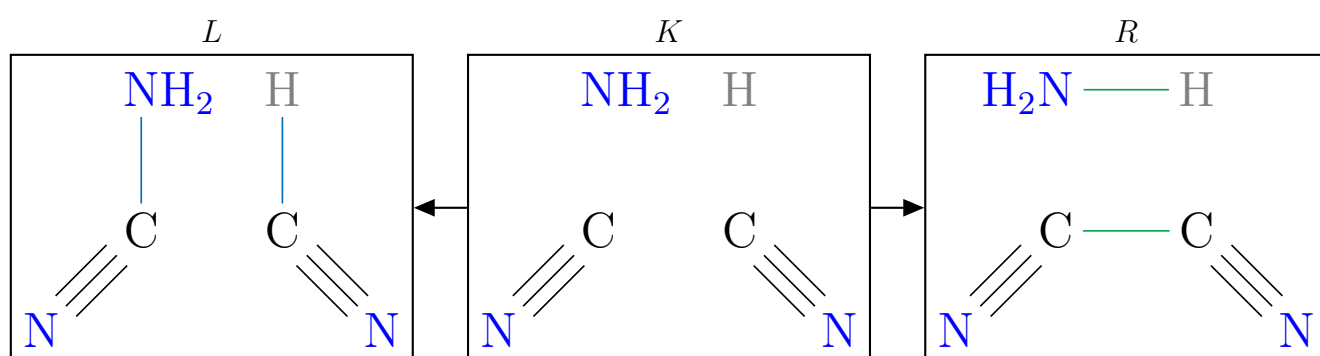
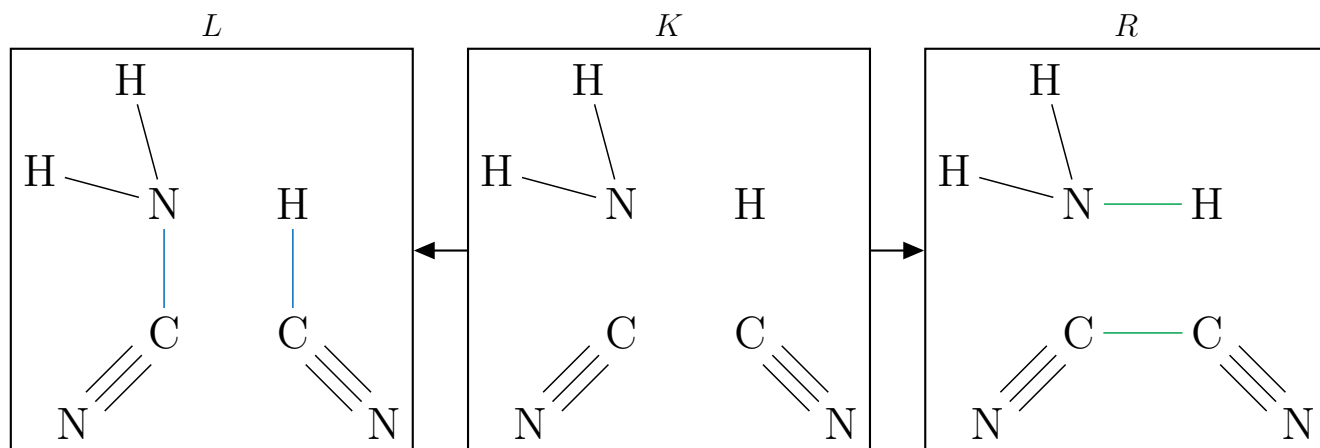


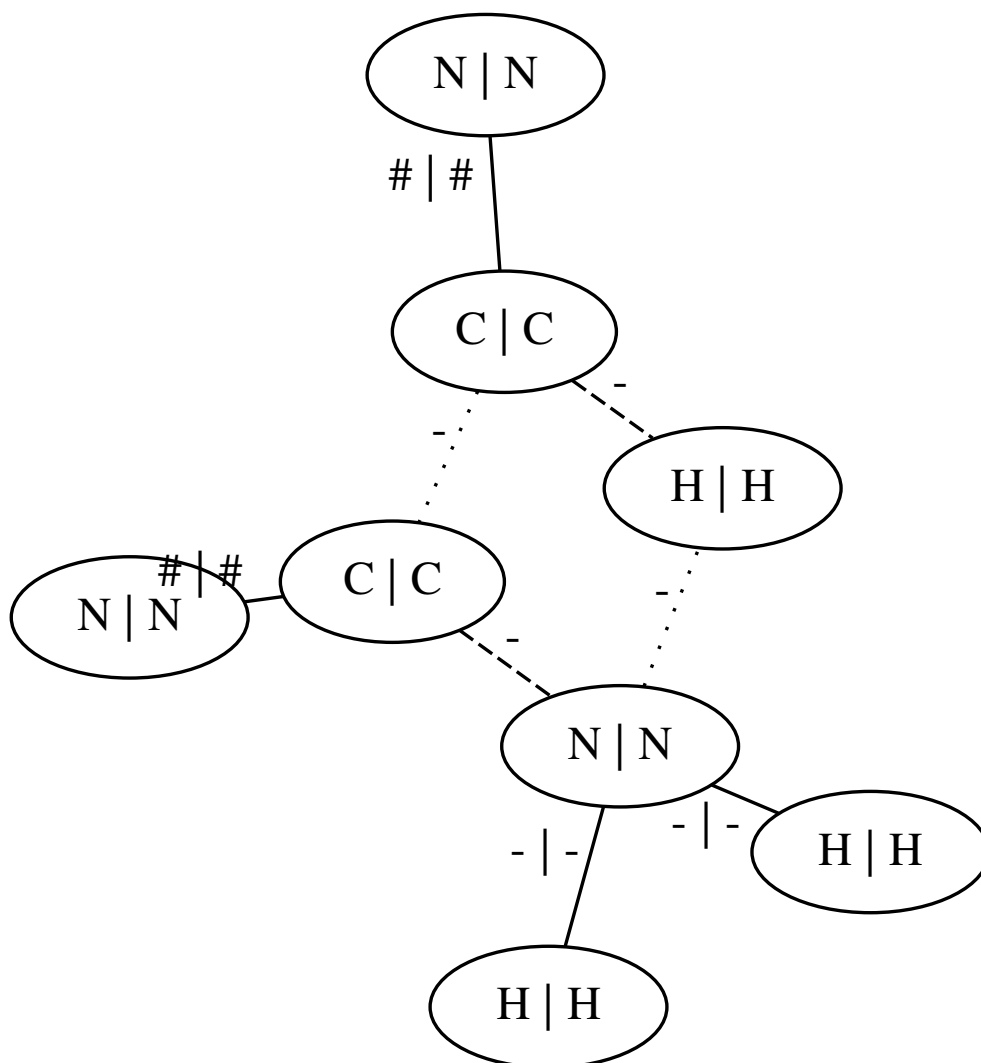
0.0.60 DAMN Scission, inverse





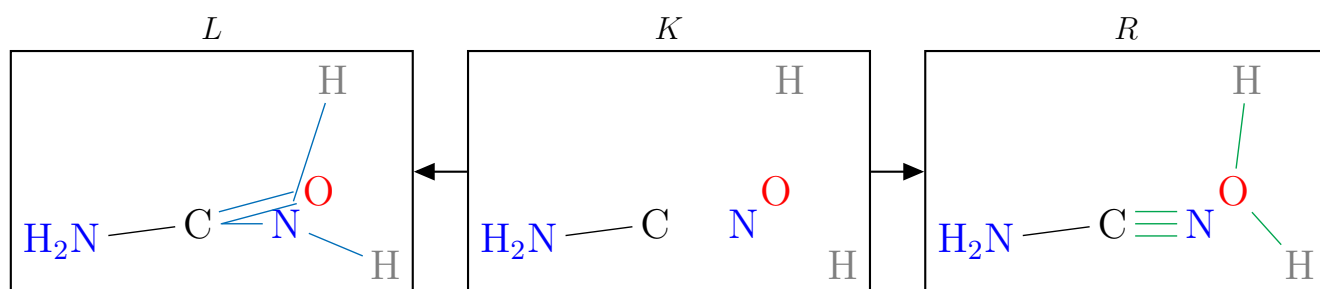
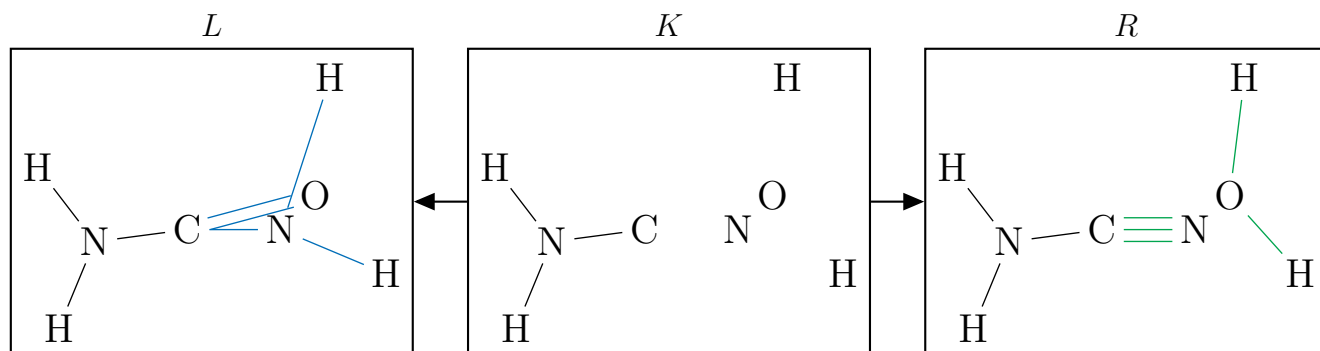
0.0.61 Cyanogen Ammonolysis, inverse

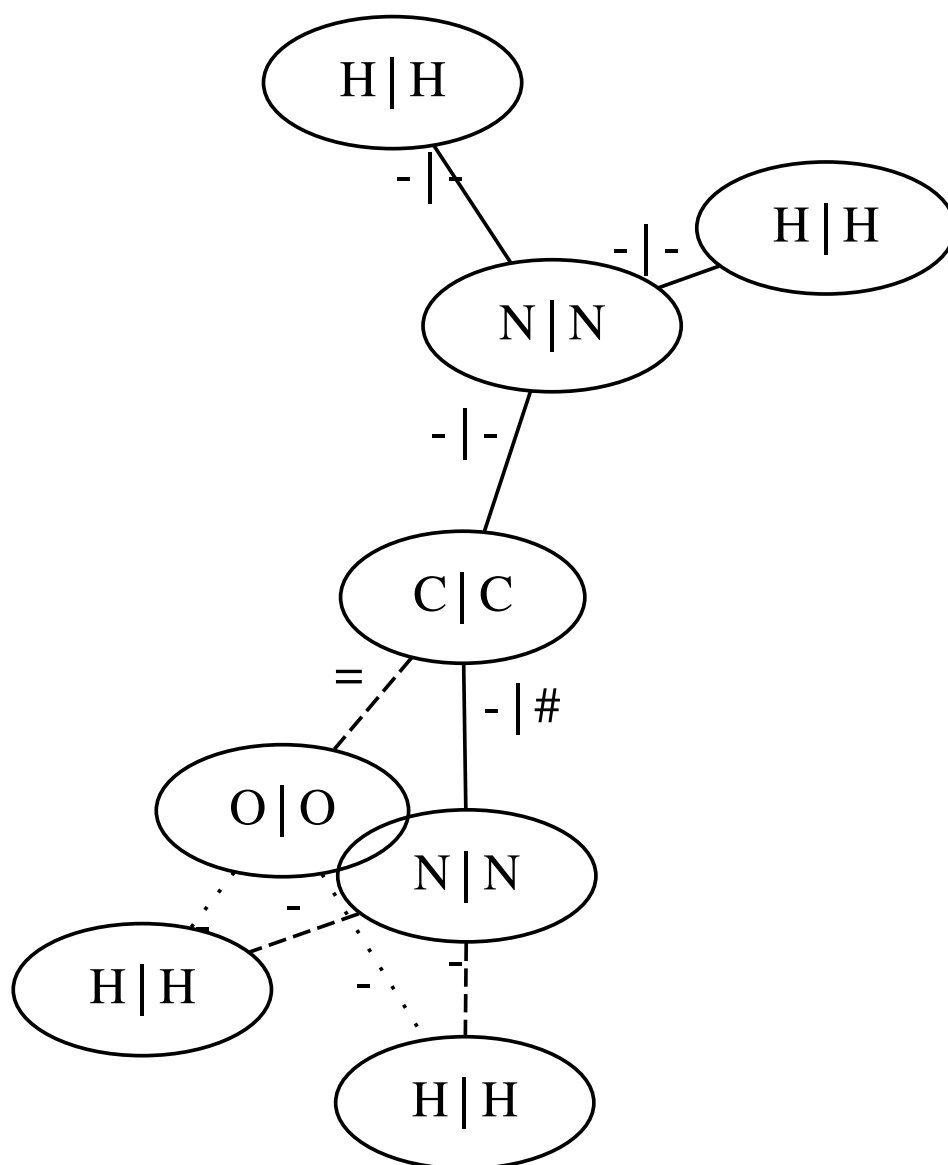




File: out/303_r_59_combined

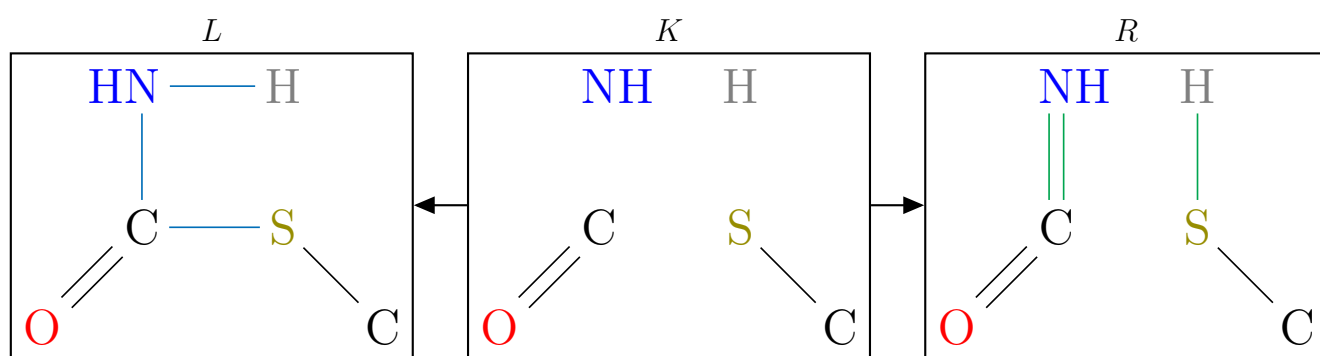
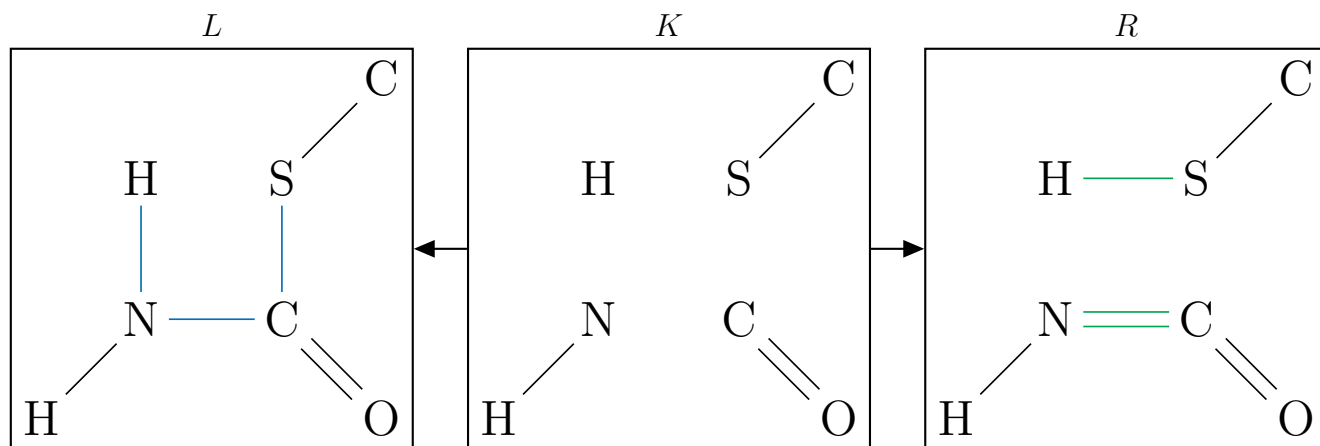
0.0.62 Cyanamide Hydration, inverse

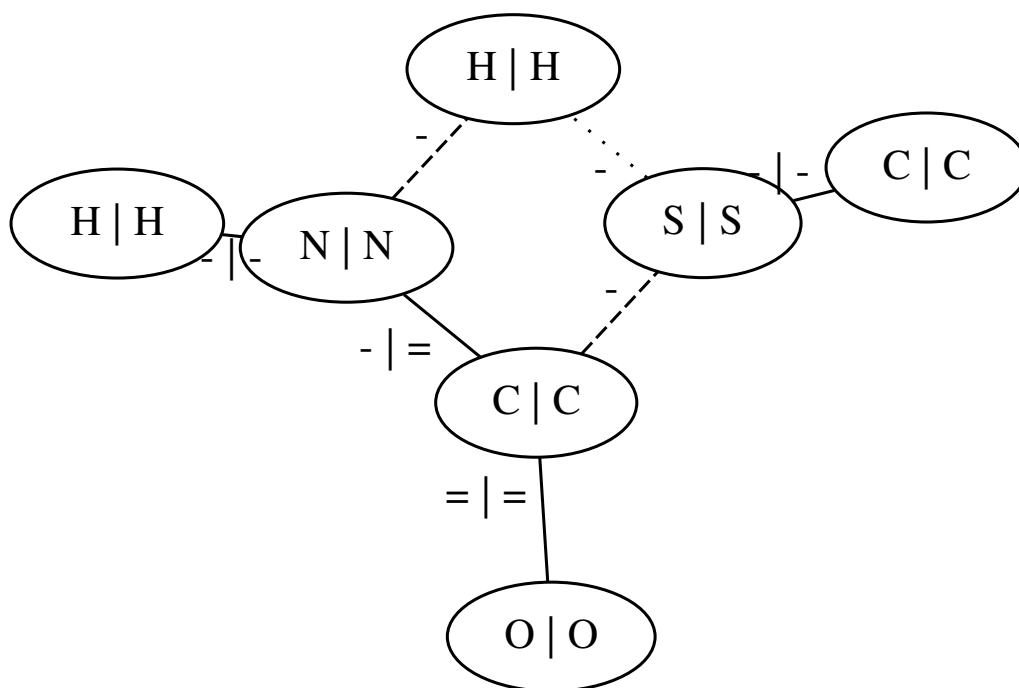




File: out/308_r_60_combined

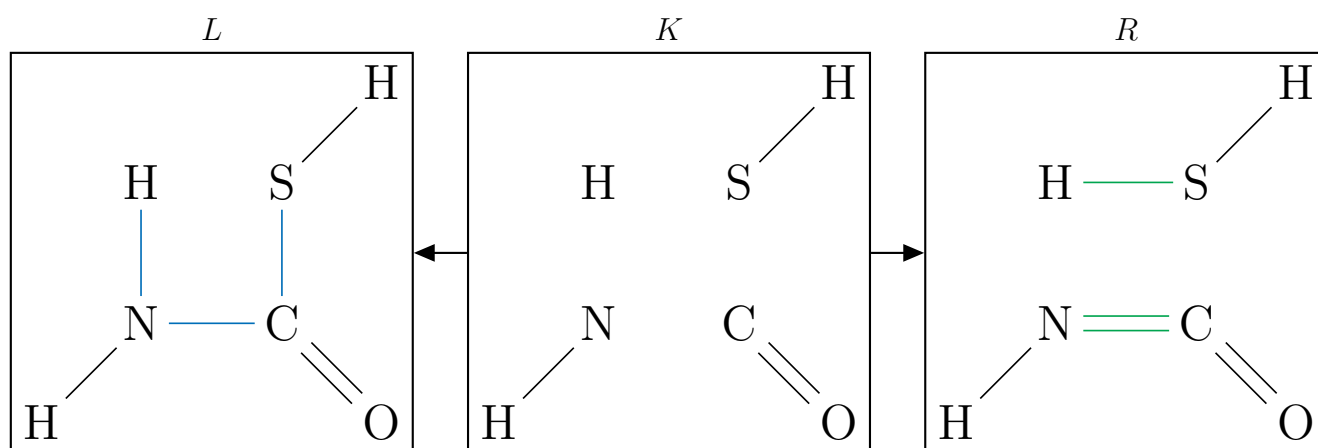
0.0.63 Carbamylation, SC, inverse



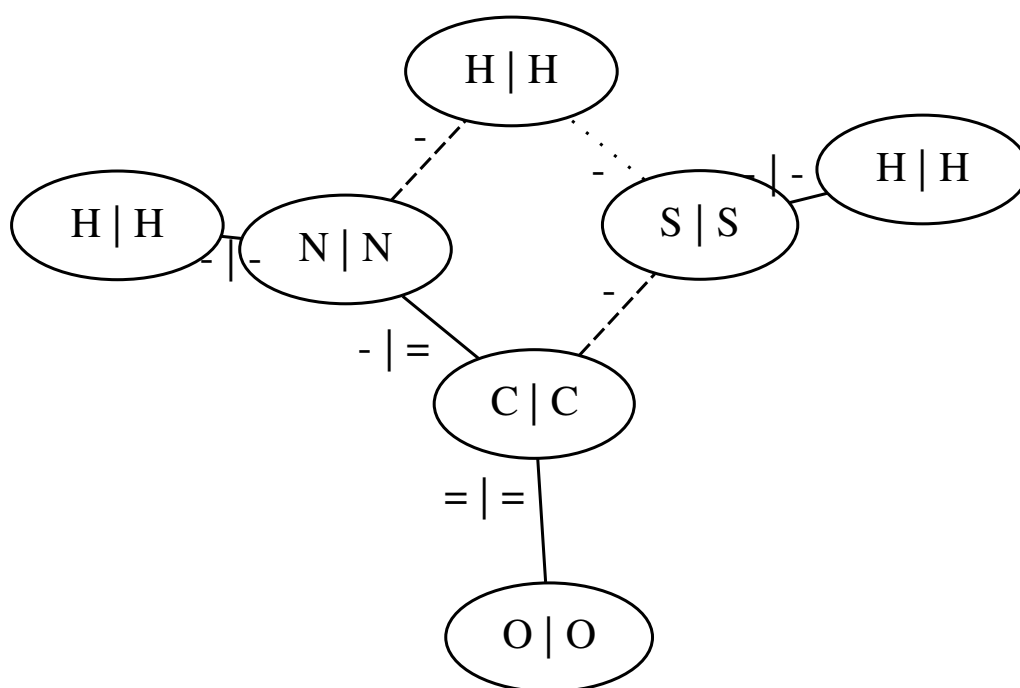
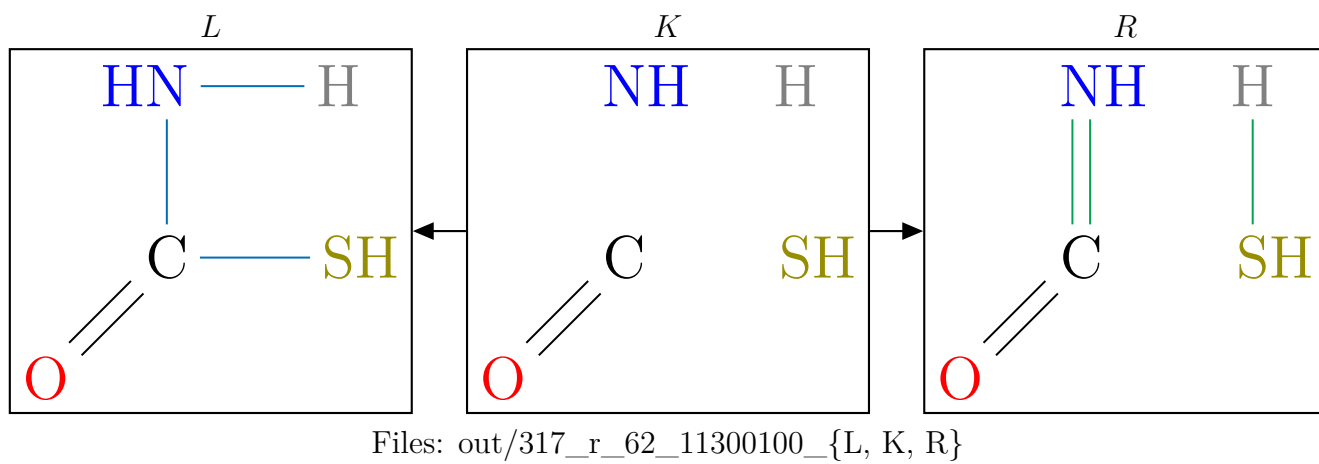


File: out/313_r_61_combined

0.0.64 Carbamylation, SH, inverse

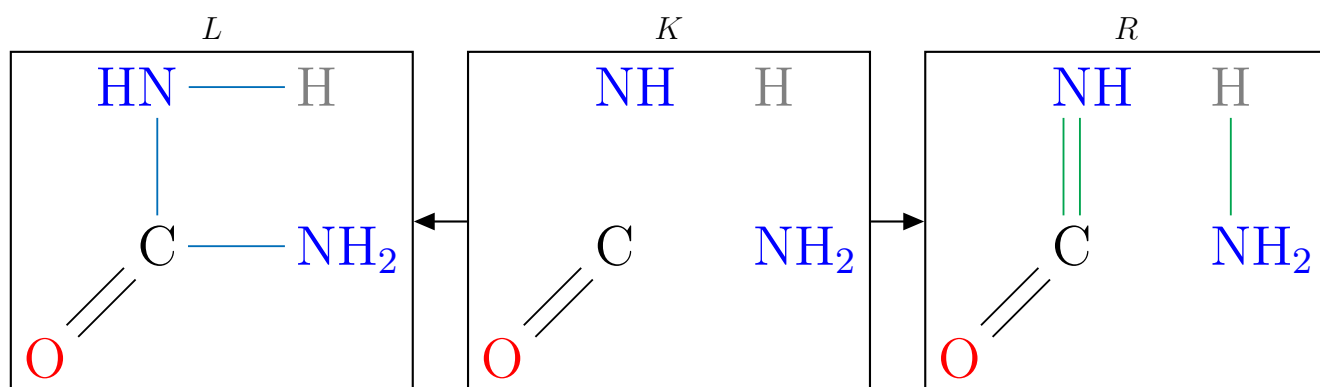
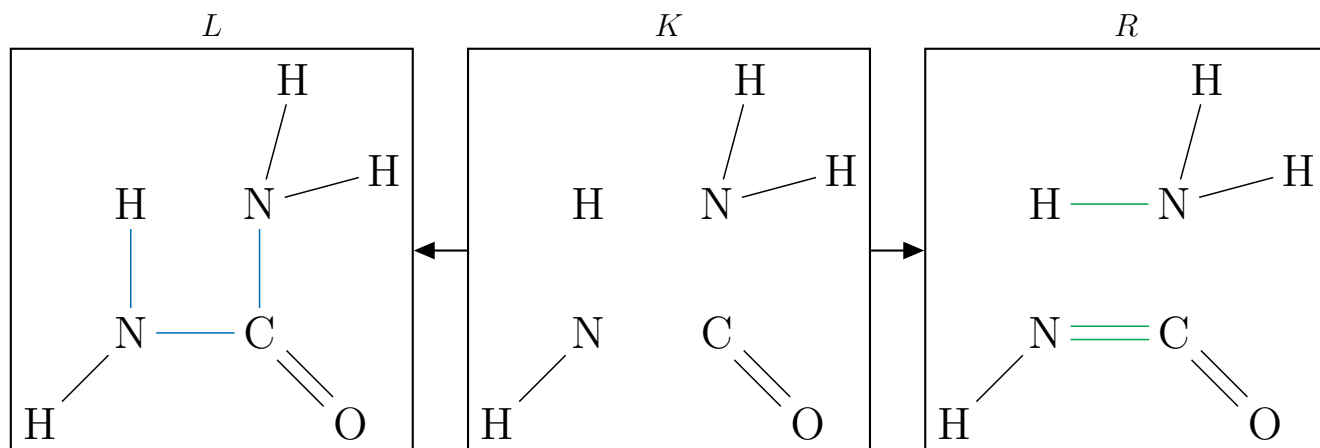


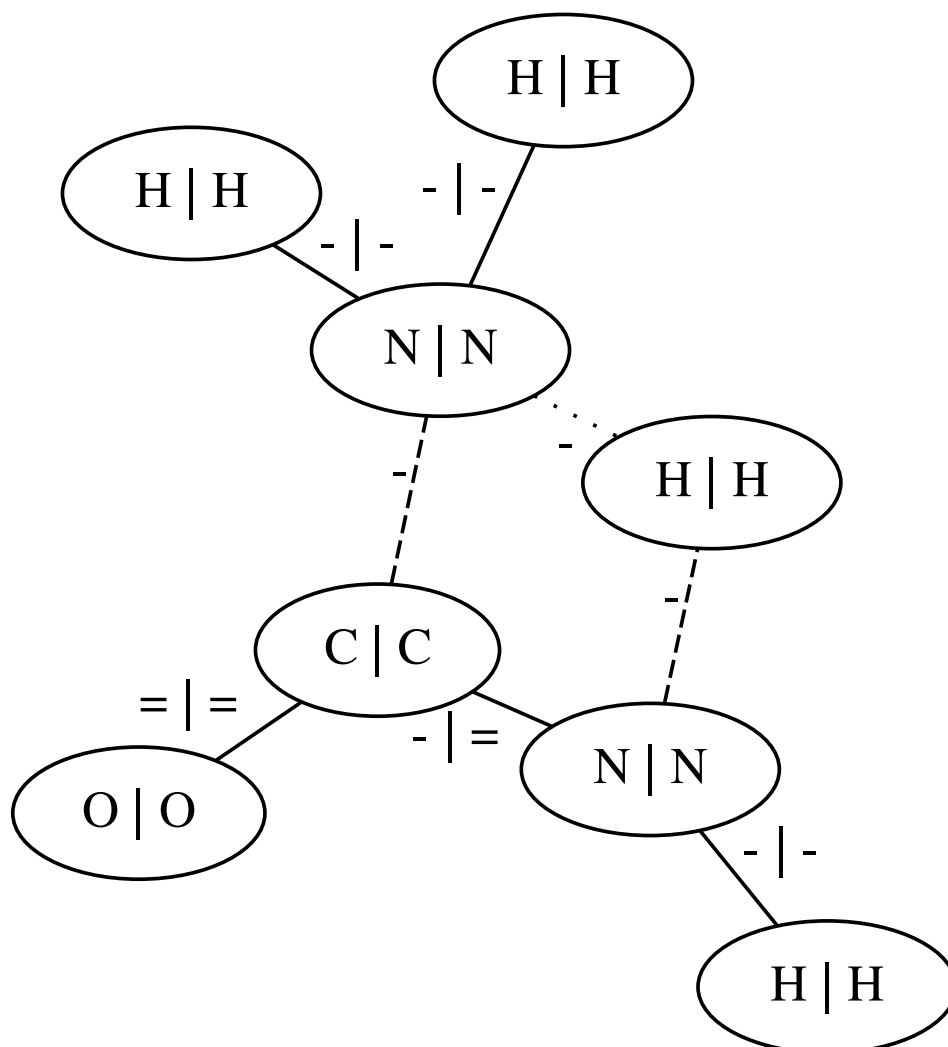
Files: out/316_r_62_10300000_{L, K, R}



File: out/318_r_62_combined

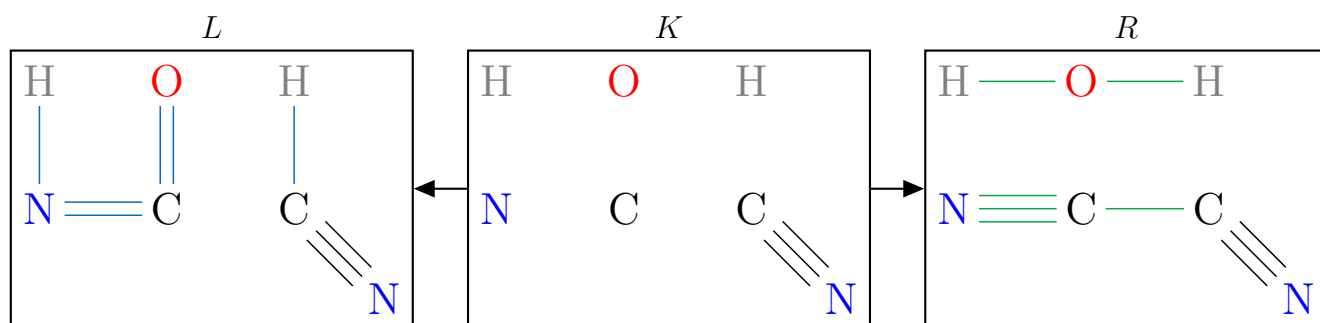
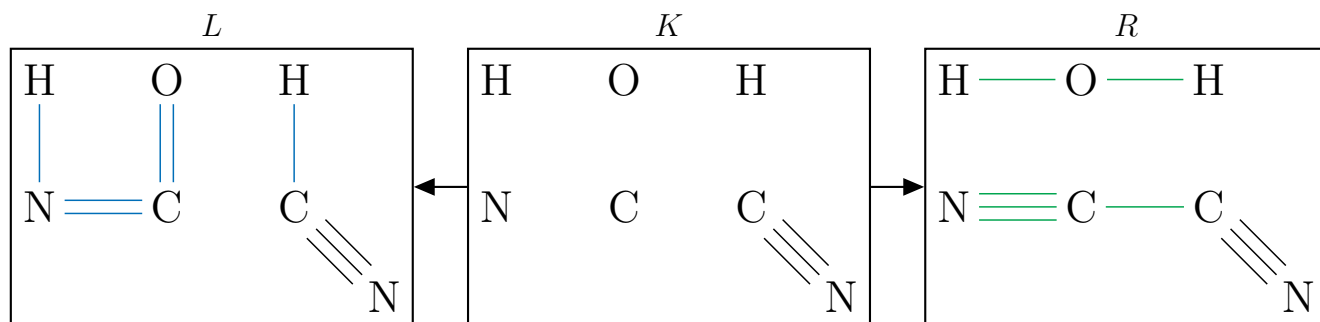
0.0.65 Carbamylation, N, HH, inverse

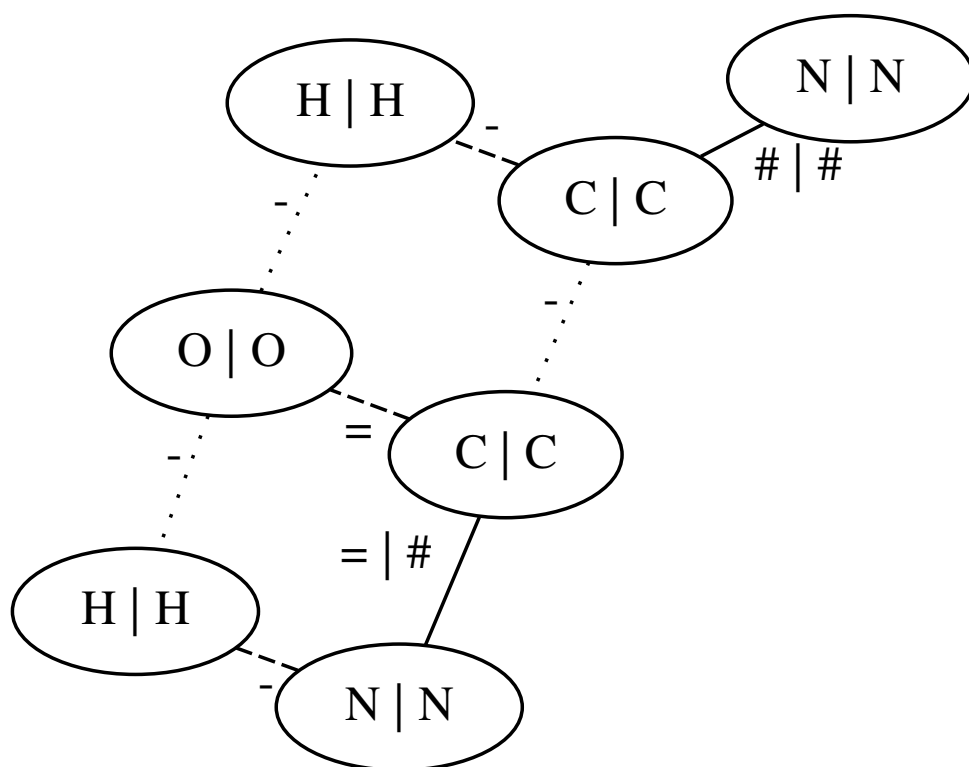




File: out/323_r_63_combined

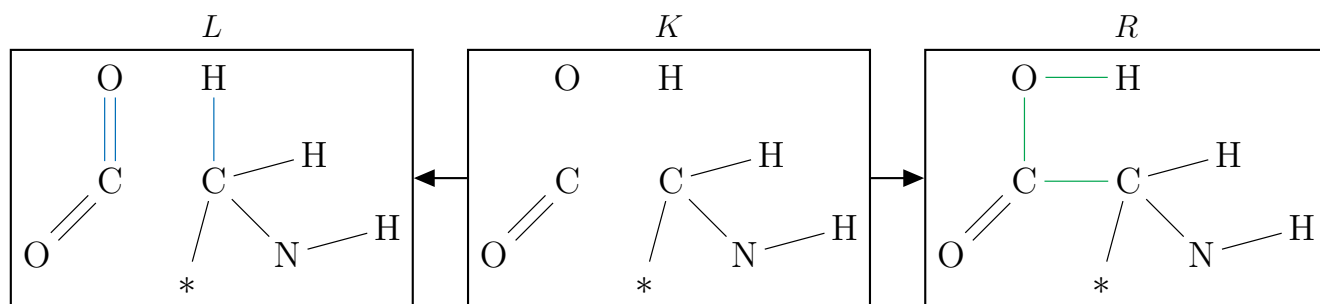
0.0.66 Cyanate from cyanogen, inverse



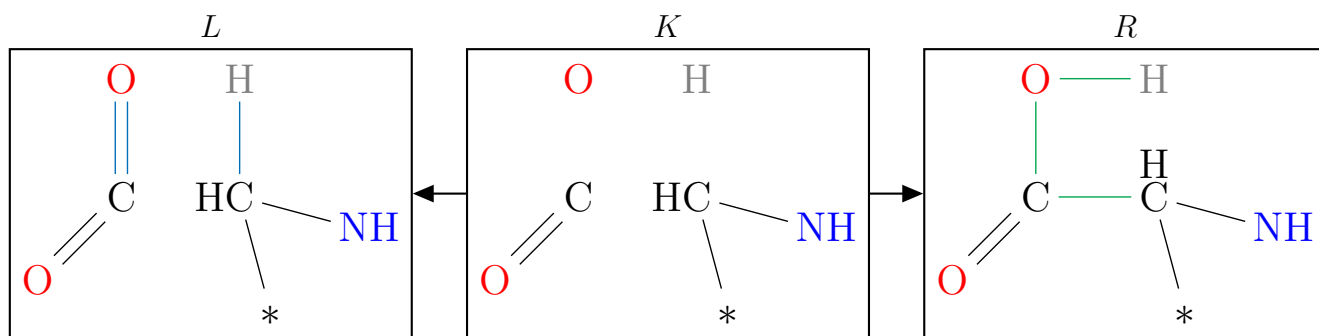


File: out/328_r_64_combined

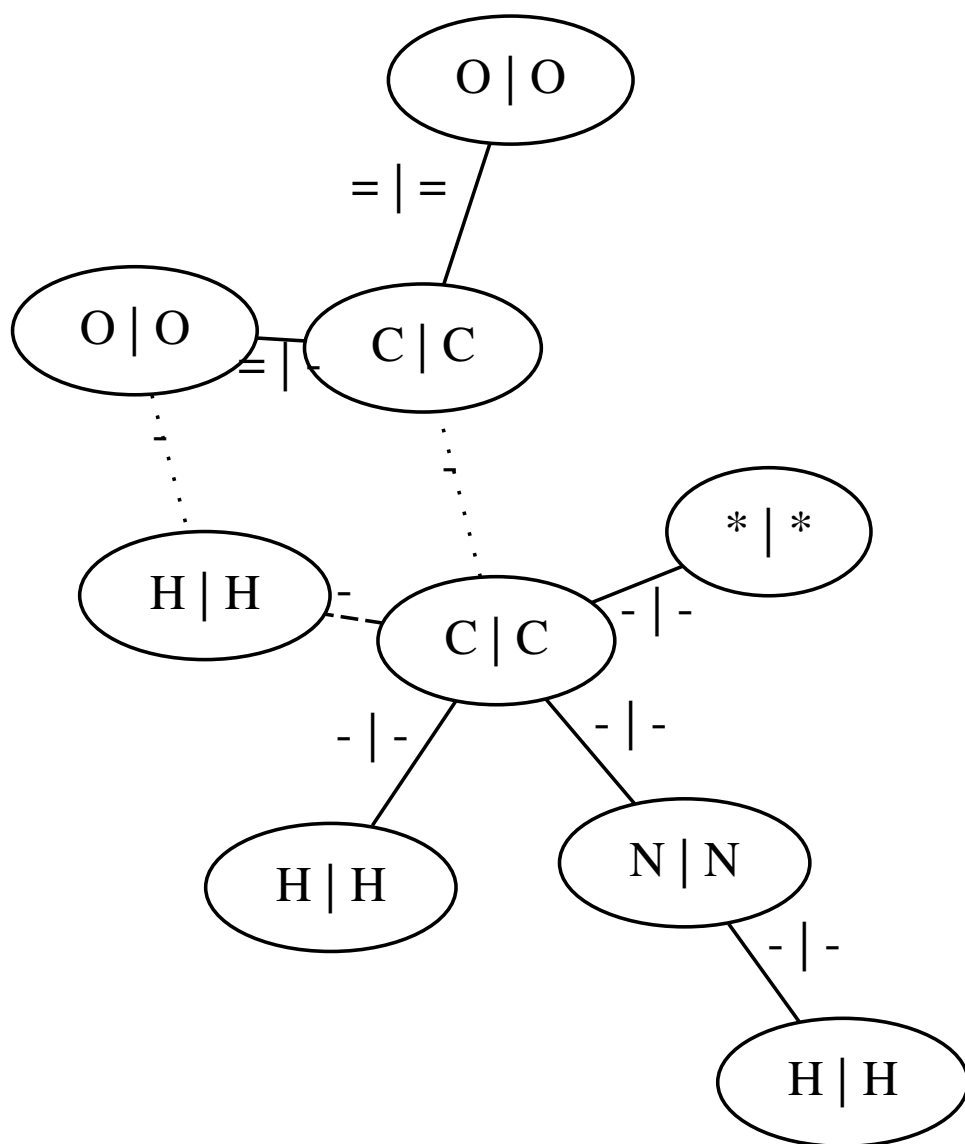
0.0.67 Ketone-Catalyzed Decarboxylation, inverse



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

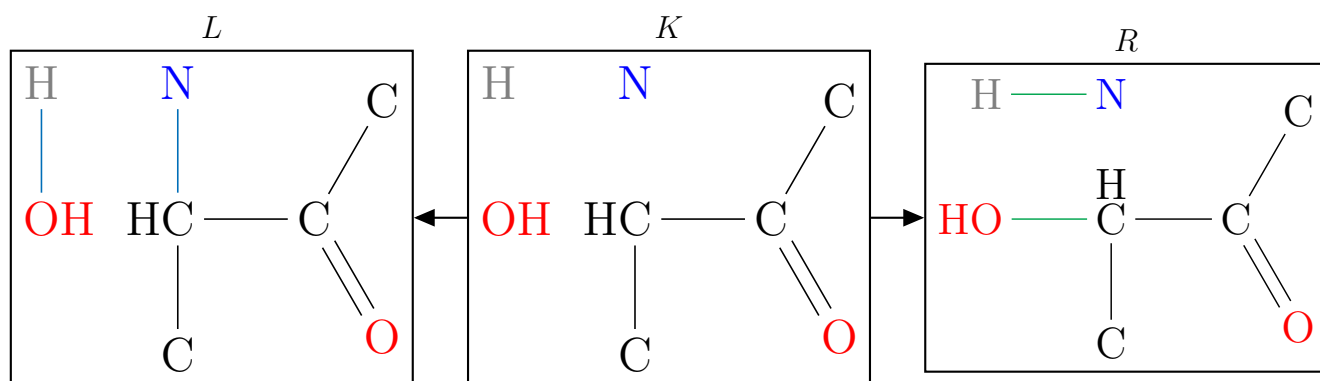
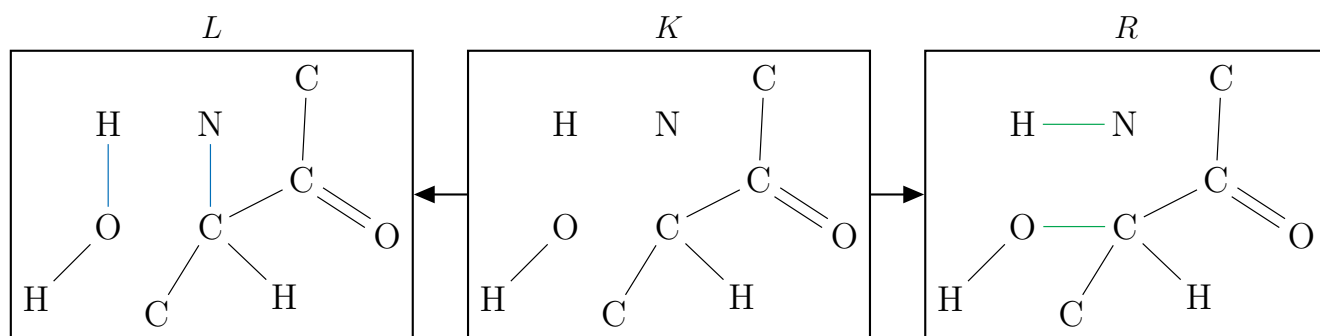


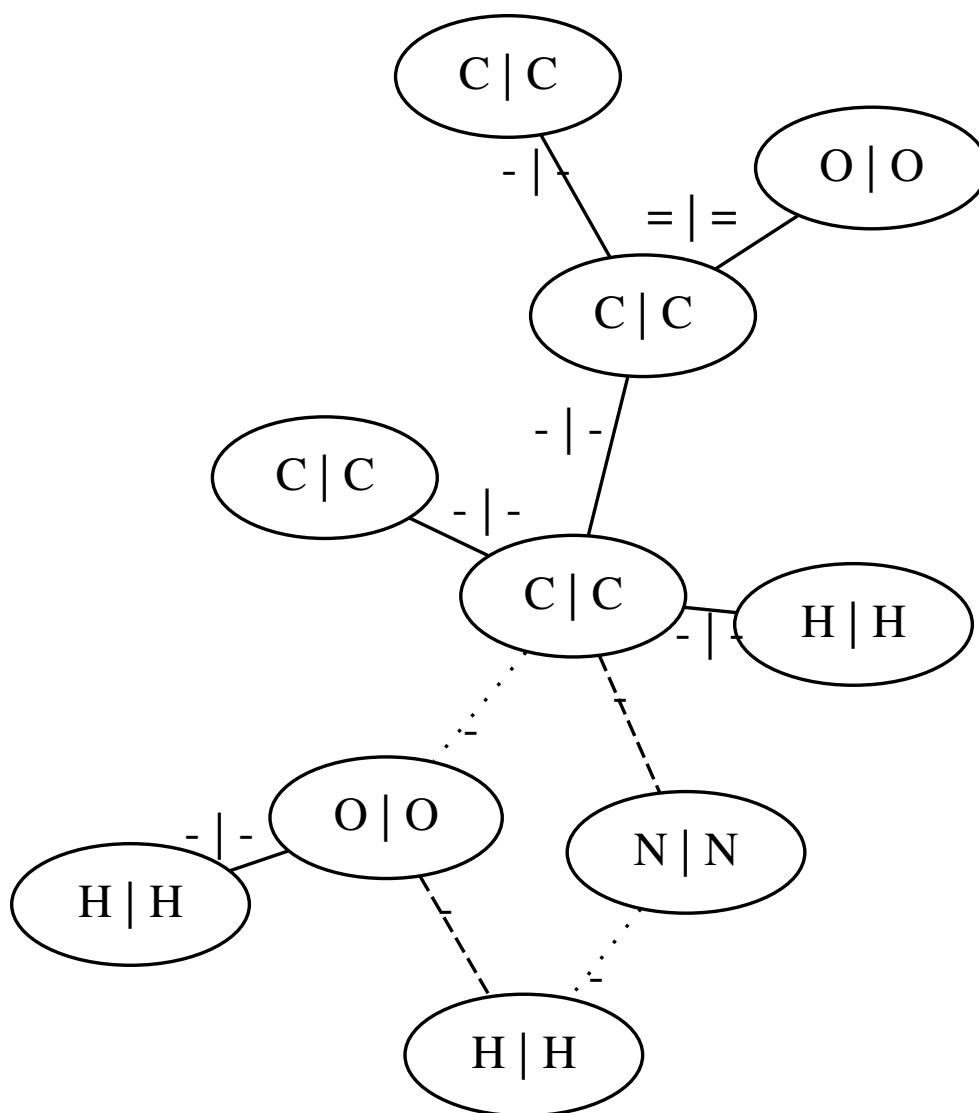
Files: out/332_r_65_11300100_{L, K, R}



File: out/333_r_65_combined

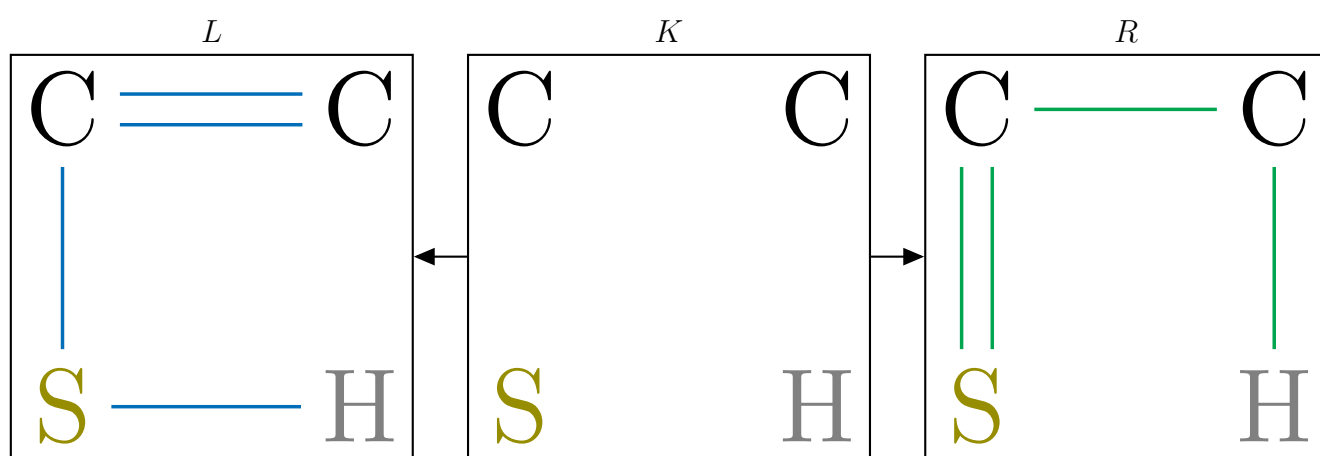
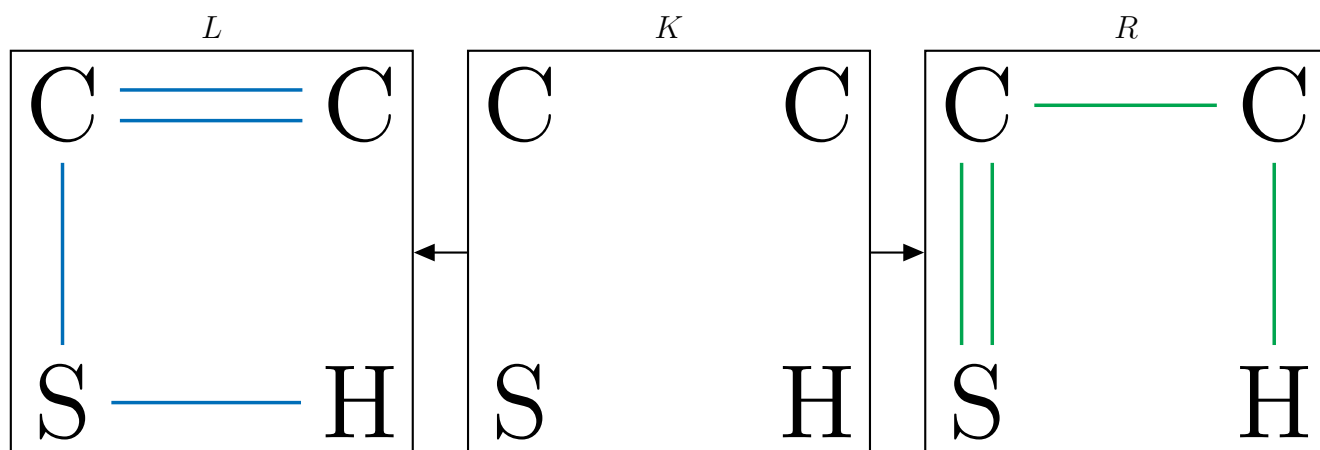
0.0.68 Amadori Rearrangement, inverse

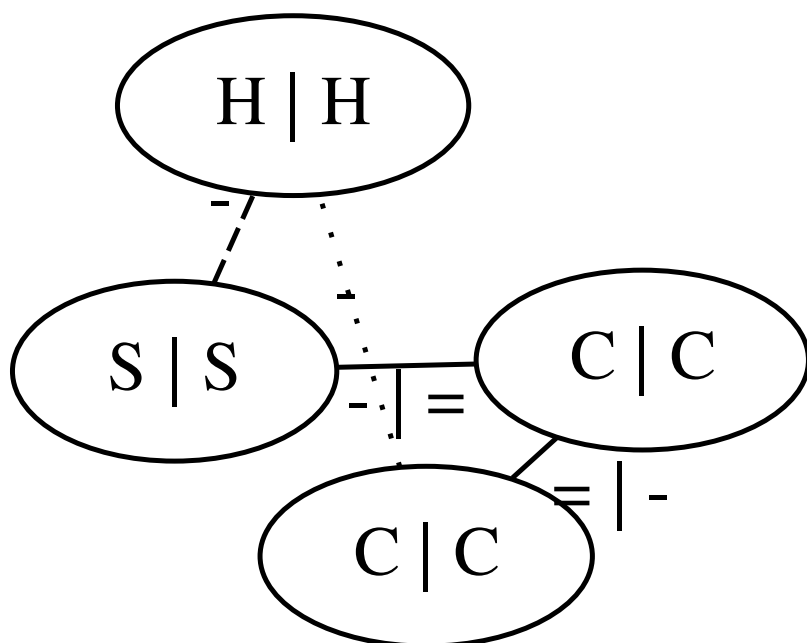




File: out/338_r_66_combined

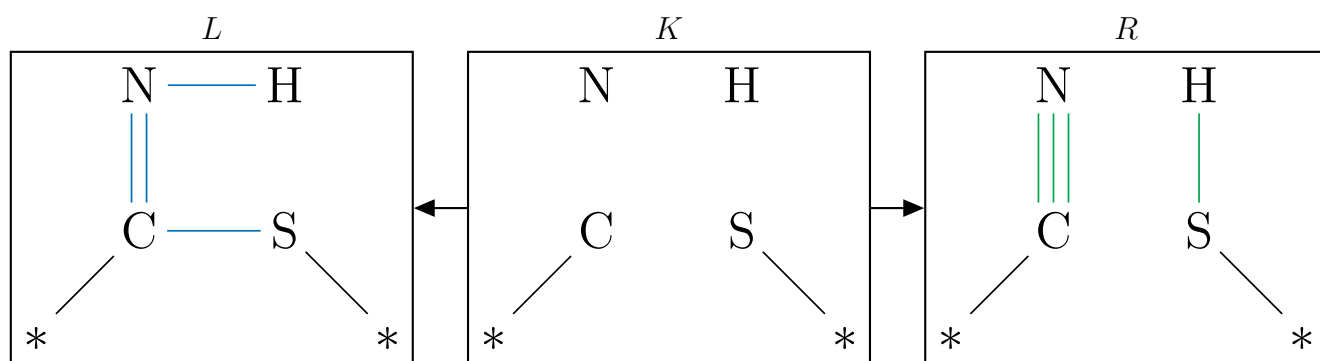
0.0.69 Thial -> Thiene, inverse



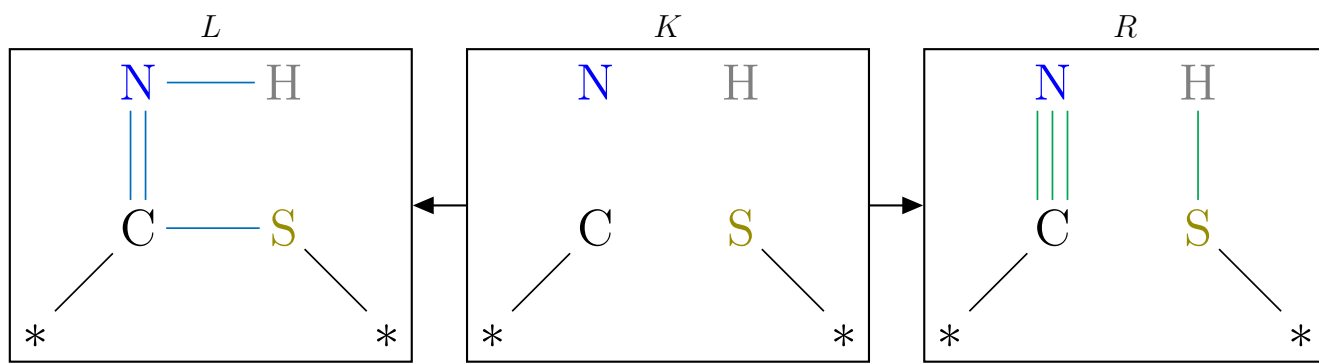


File: out/343_r_67_combined

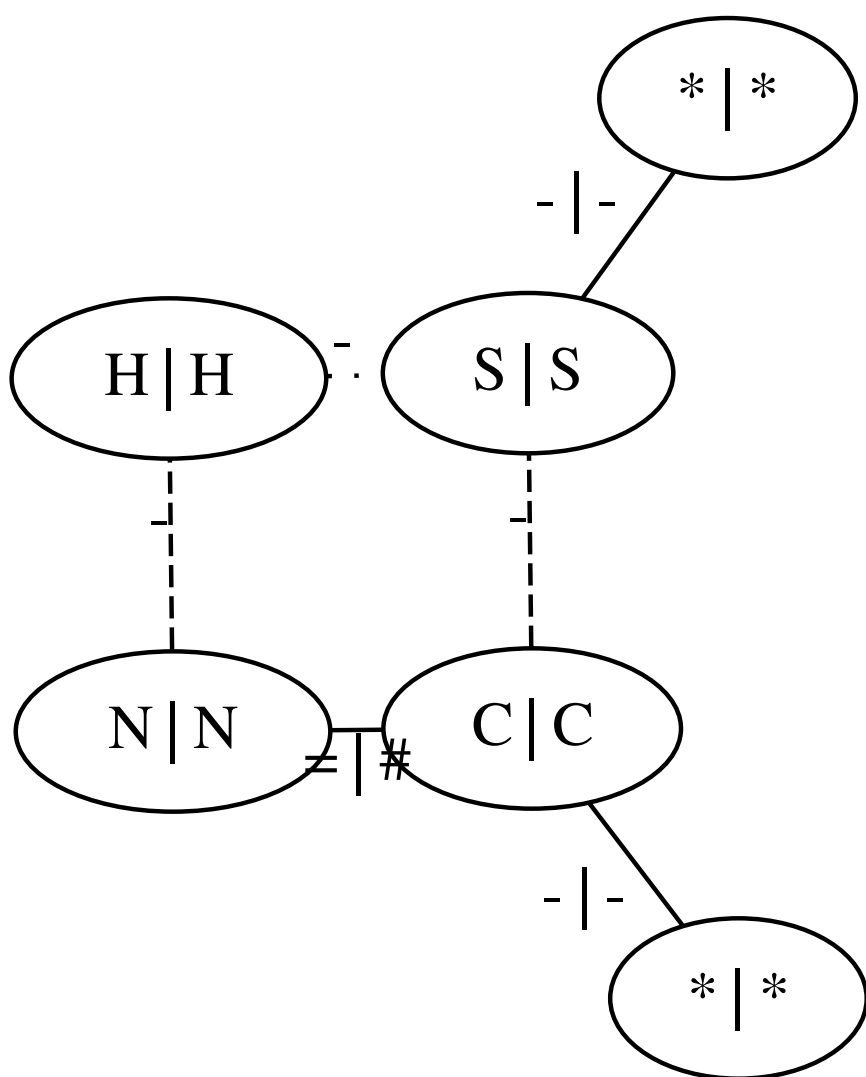
0.0.70 Sulfide to Nitrile Addition, inverse



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

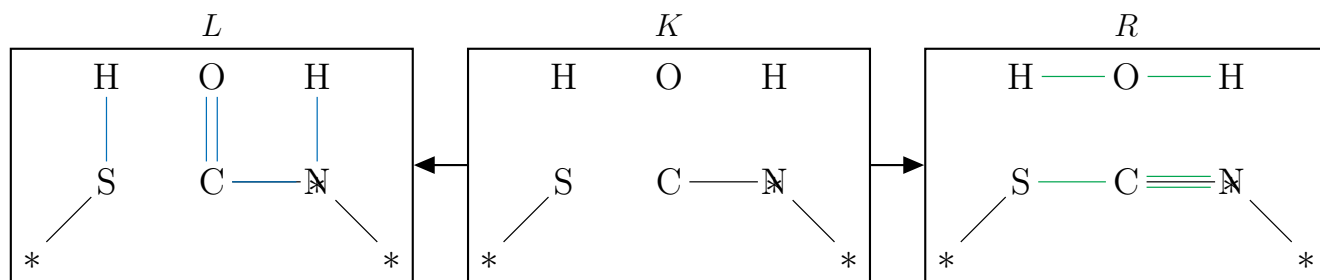


Files: out/347_r_68_11300100_{L, K, R}

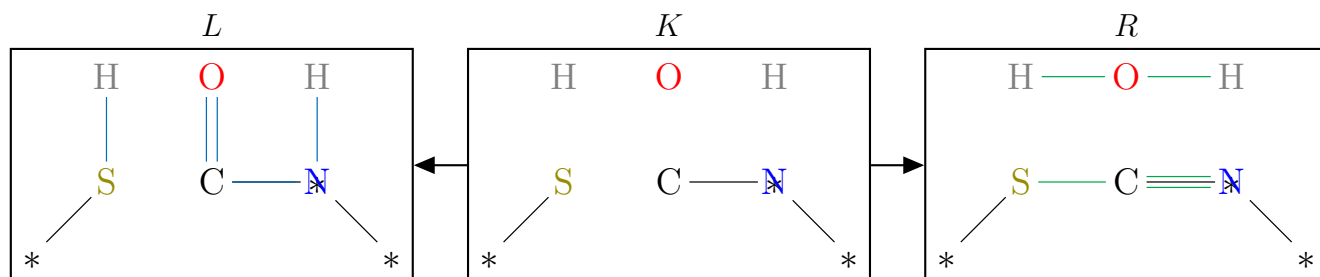


File: out/348_r_68_combined

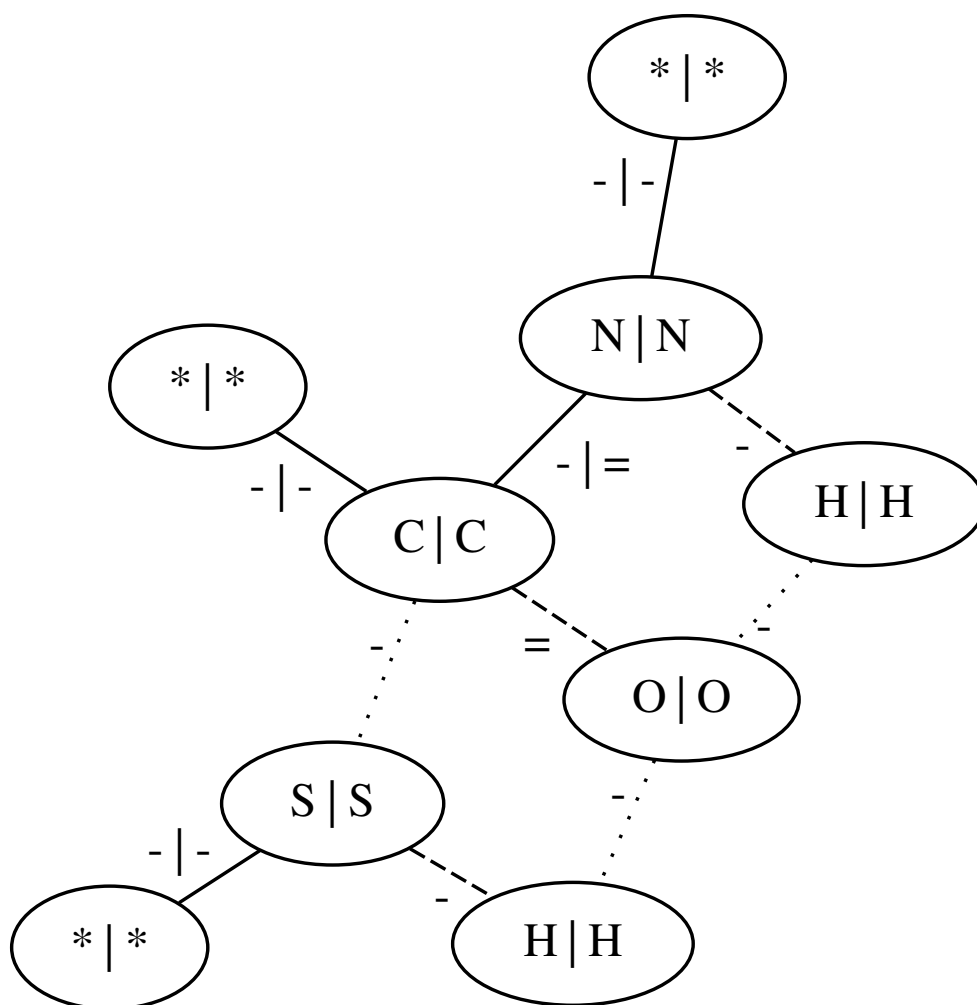
0.0.71 Thioamidine to Amide Hydrolysis, inverse



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

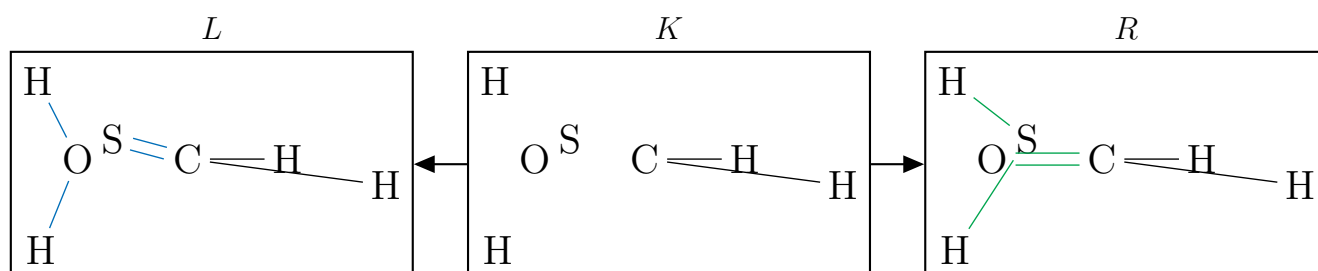


Files: out/352_r_69_11300100_{L, K, R}

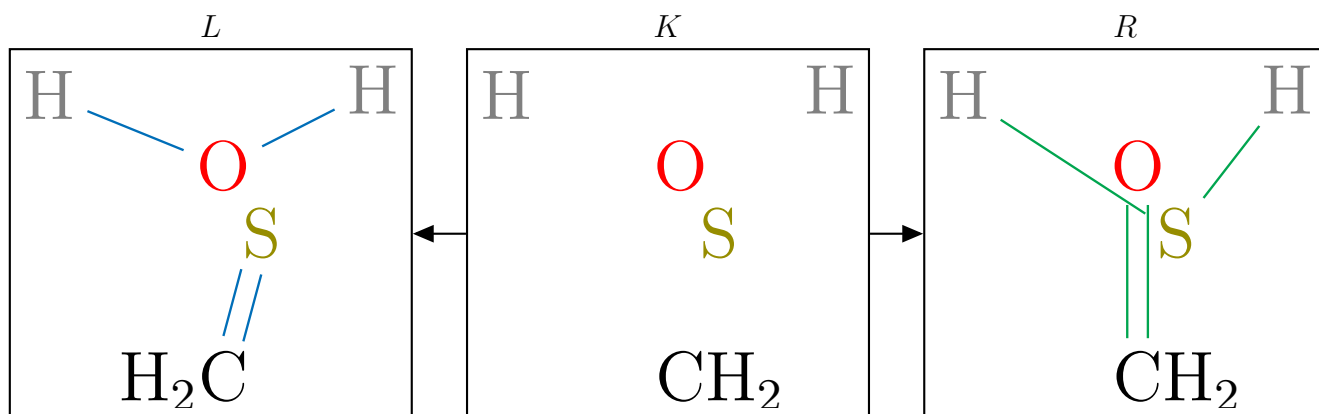


File: out/353_r_69_combined

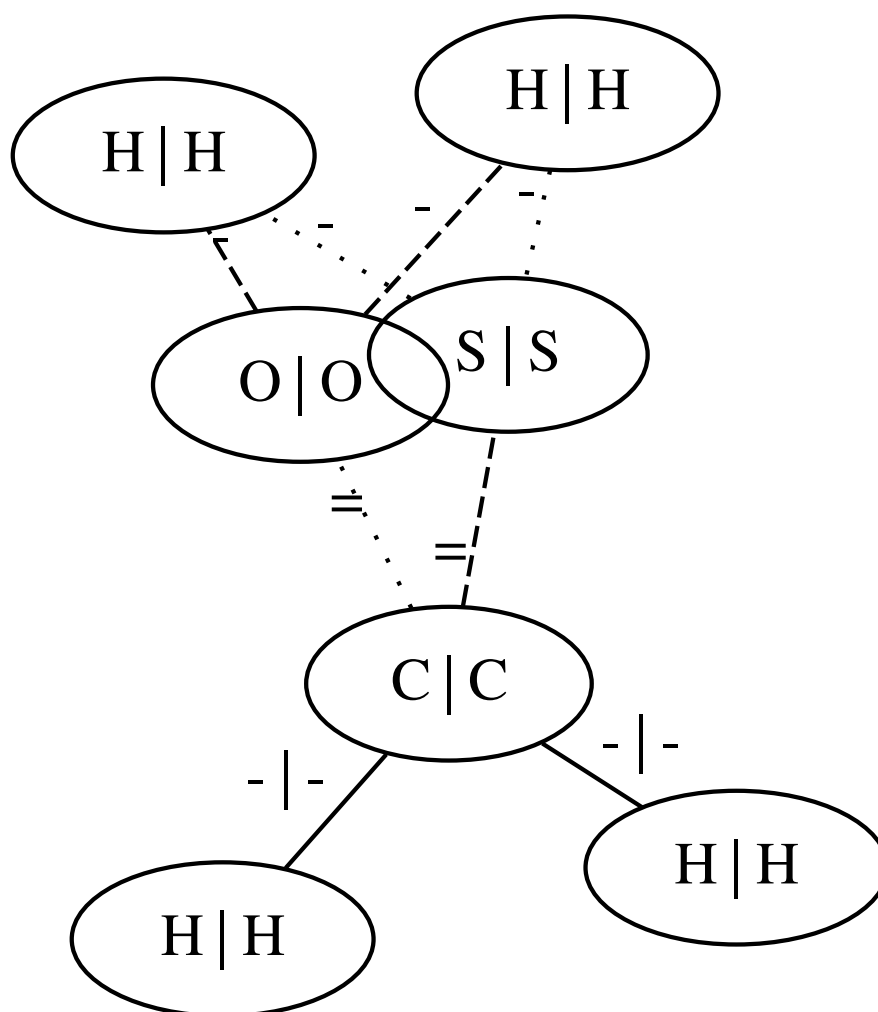
0.0.72 Ketone/Aldehyde to Thioketone/Thial, HH, inverse



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

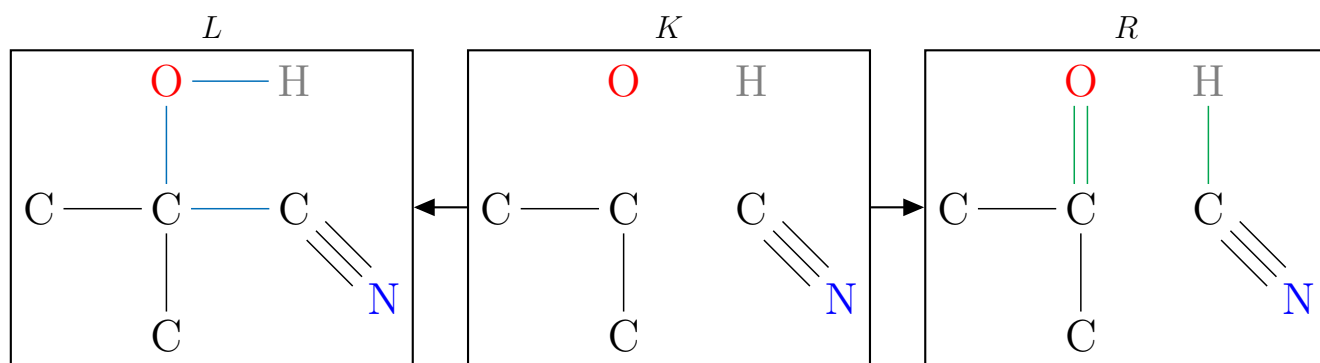
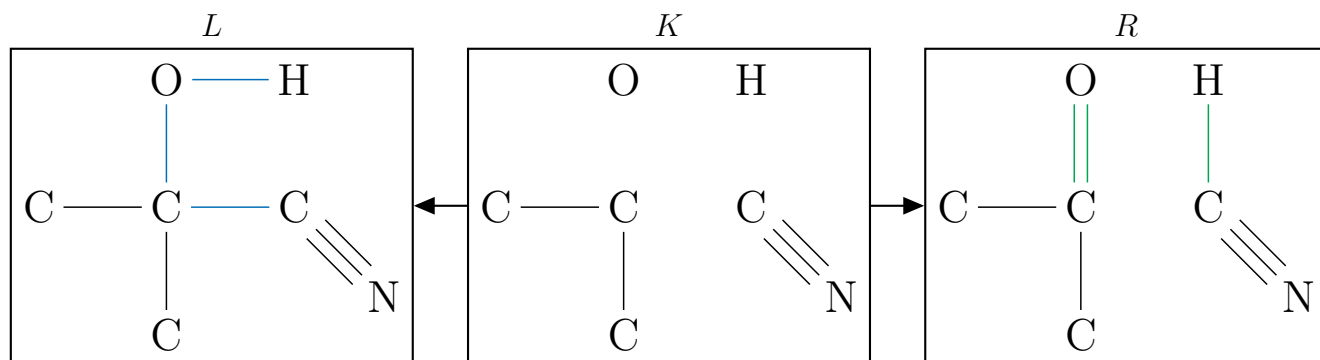


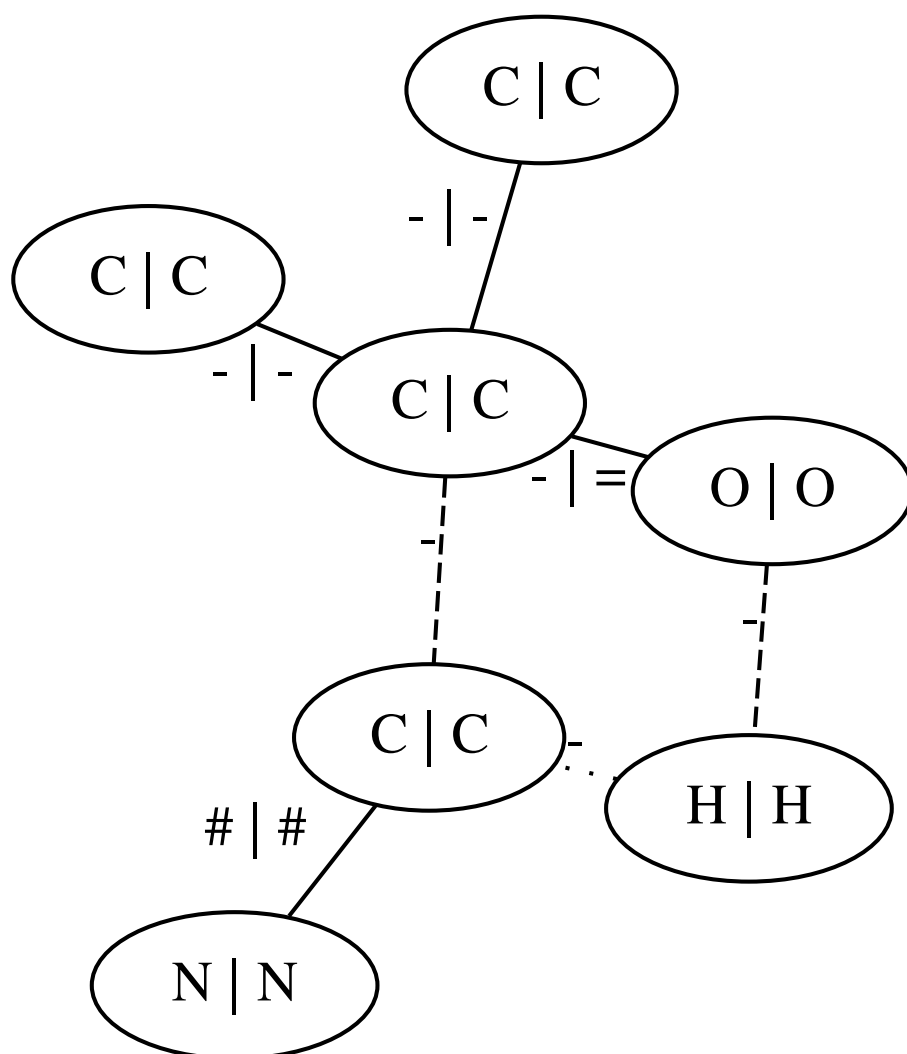
Files: out/357_r_70_11300100_{L, K, R}



File: out/358_r_70_combined

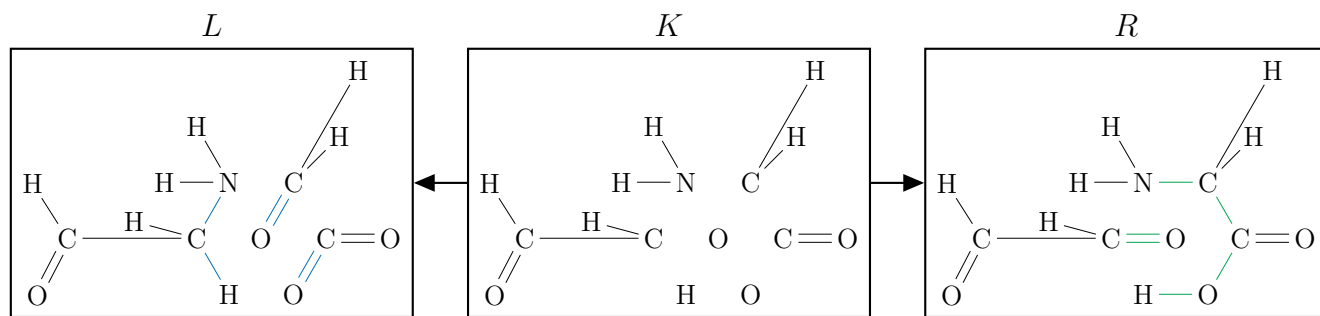
0.0.73 HCN to Ketone, inverse



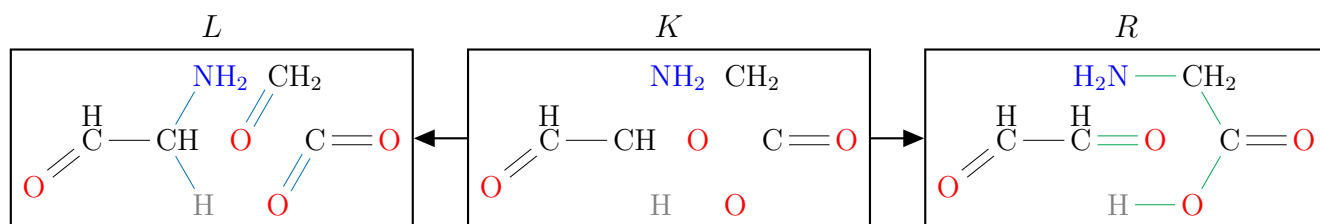


File: out/363_r_71_combined

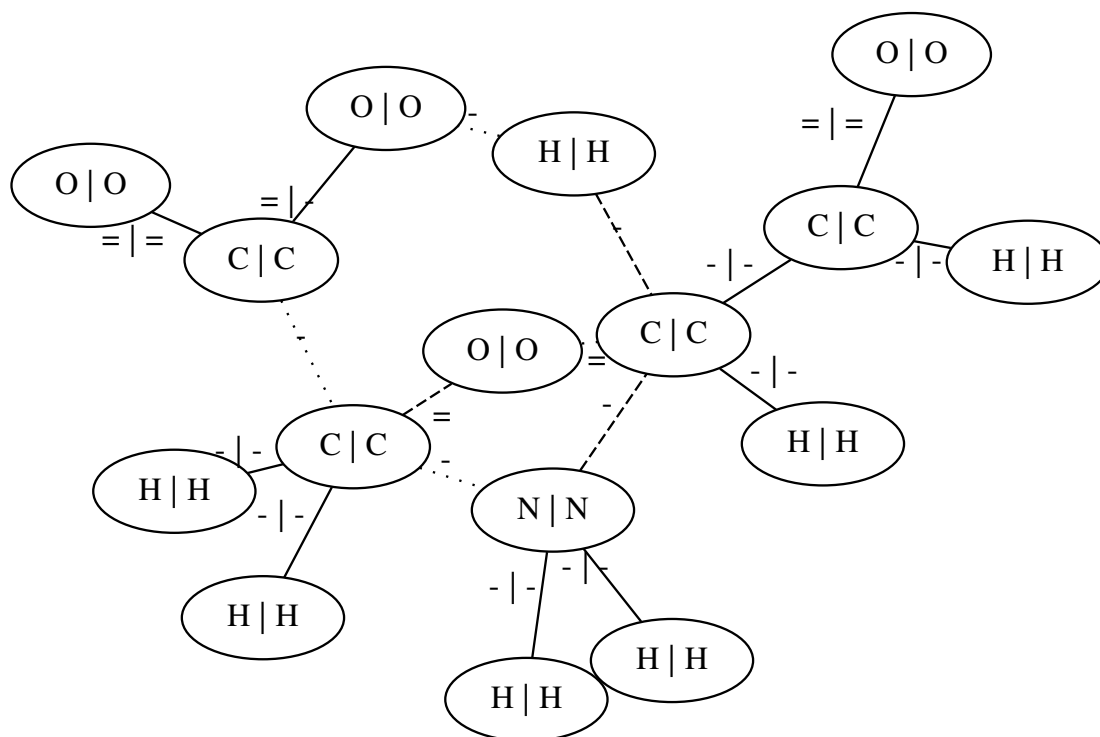
0.0.74 Strecker Degradation Dicarbonyl, H, H, H, H, inverse



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

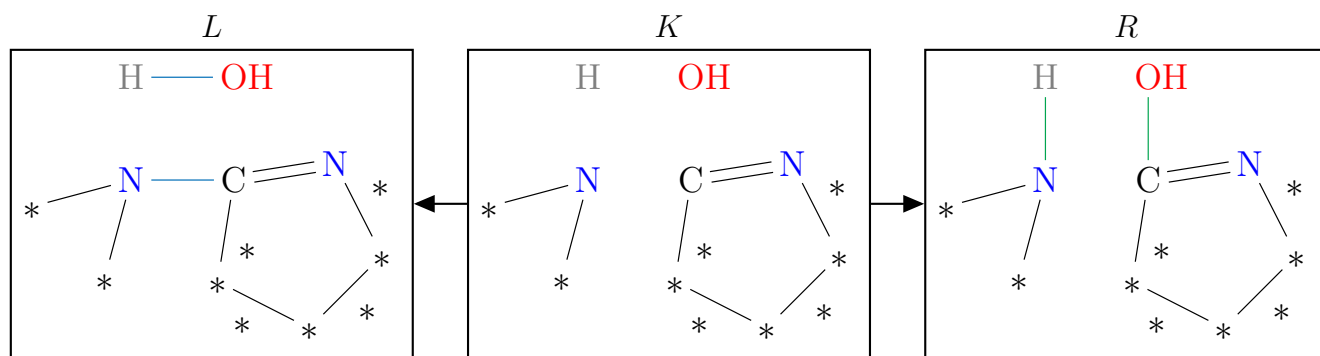
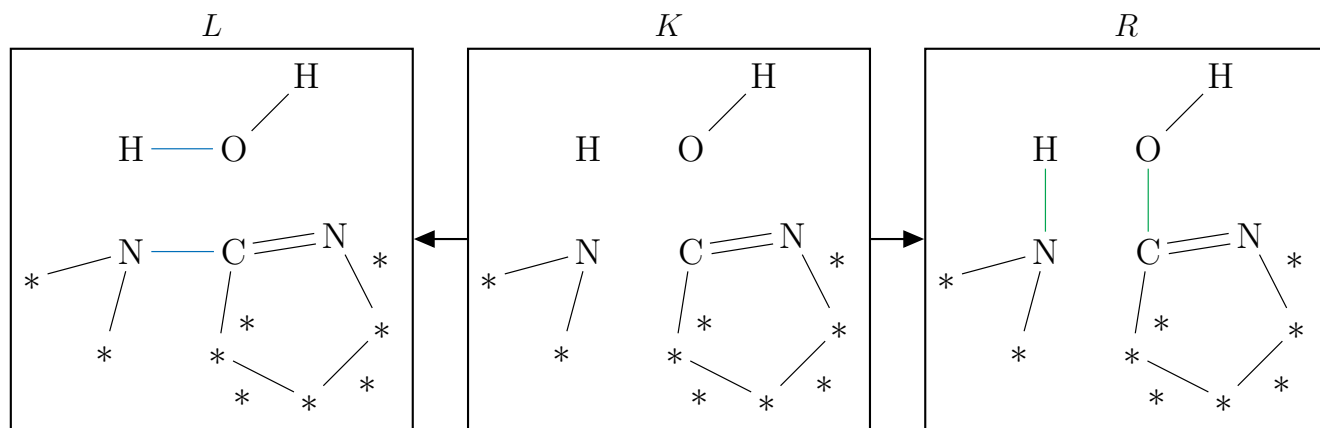


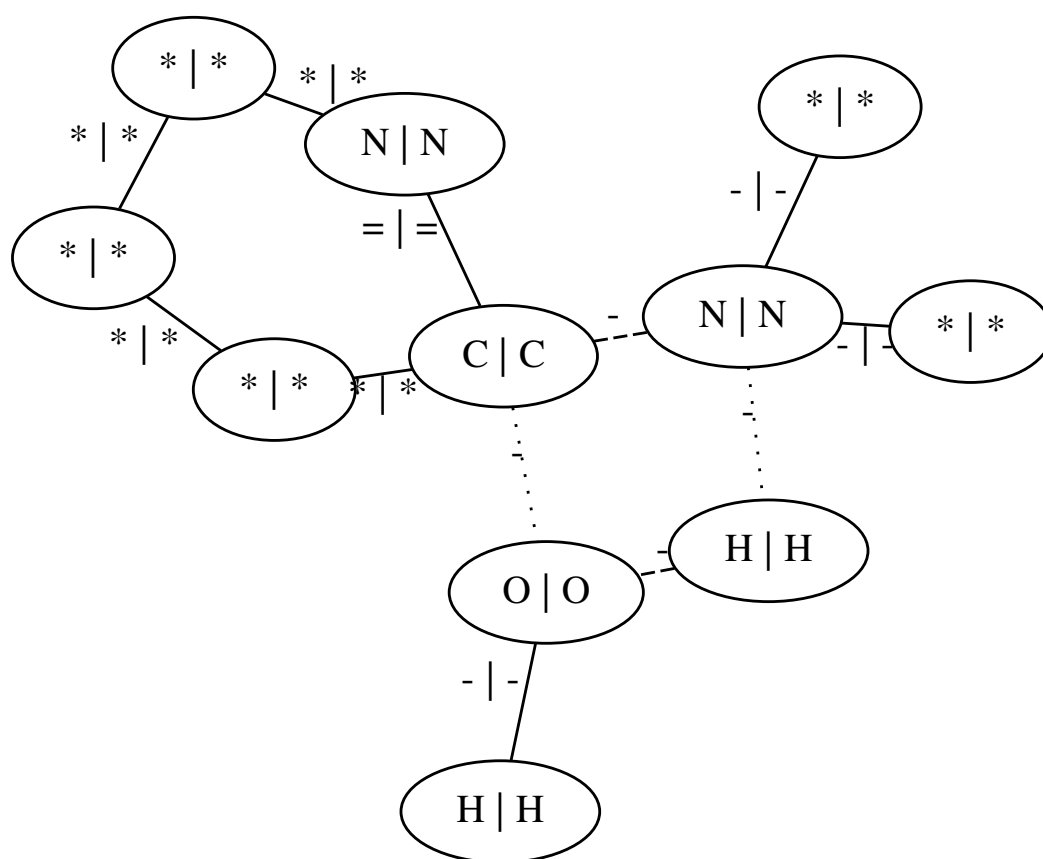
Files: out/367_r_72_11300100_{L, K, R}



File: out/368_r_72_combined

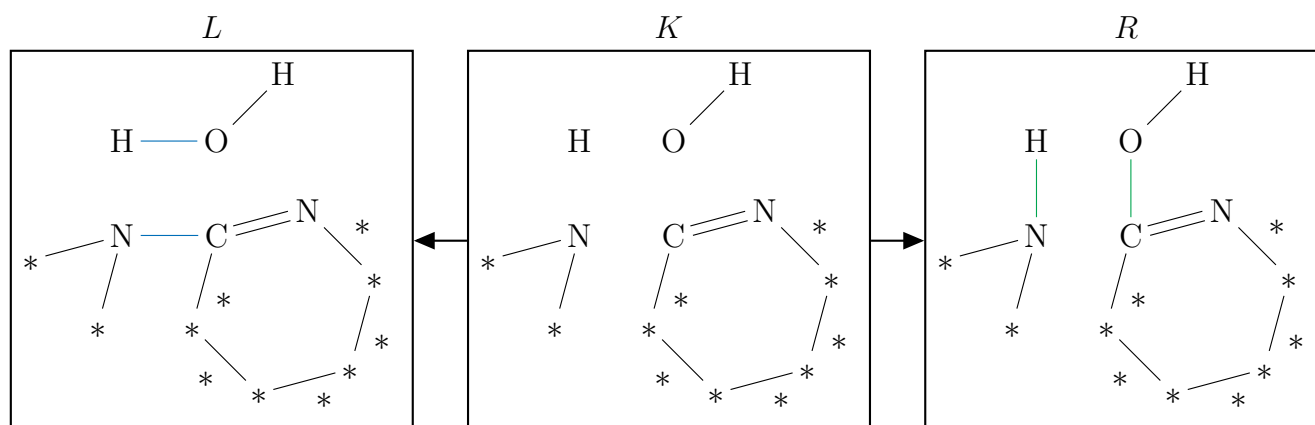
0.0.75 5 Membered Ring Exoamine Hydrolysis



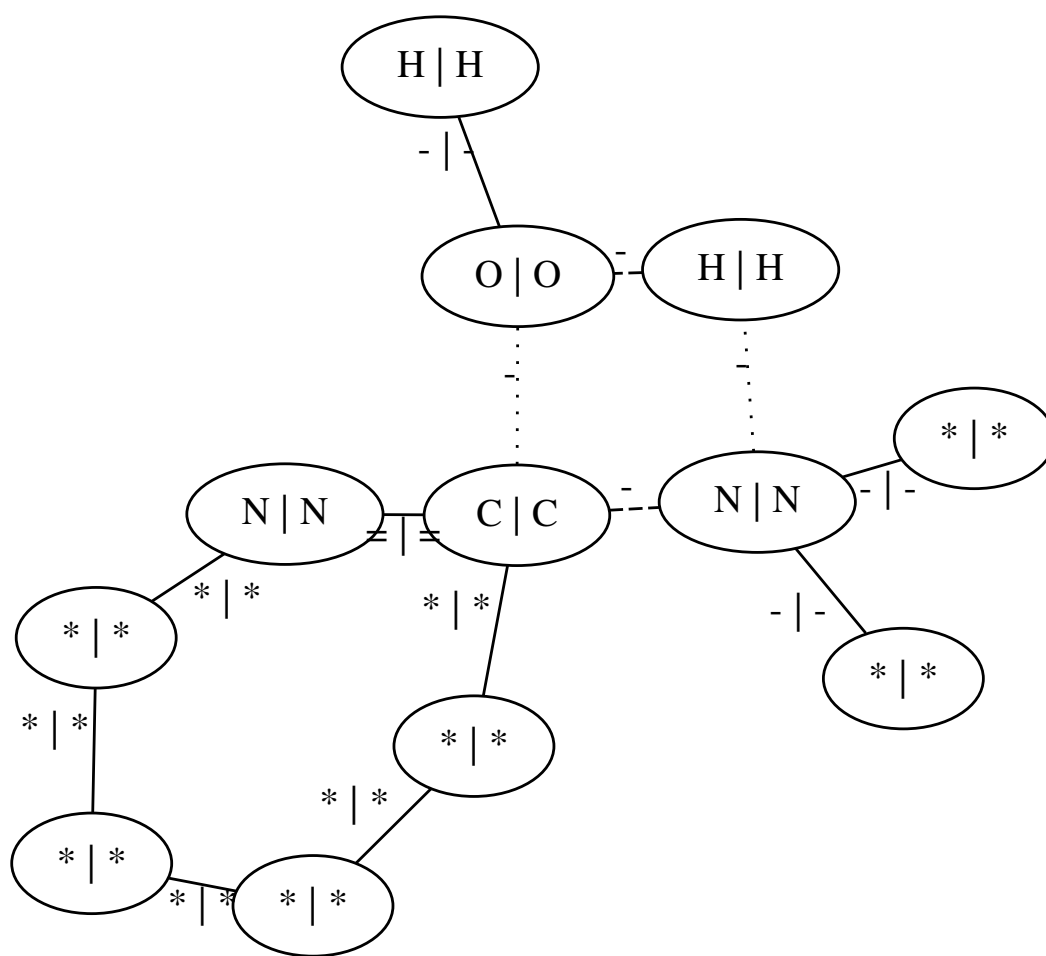
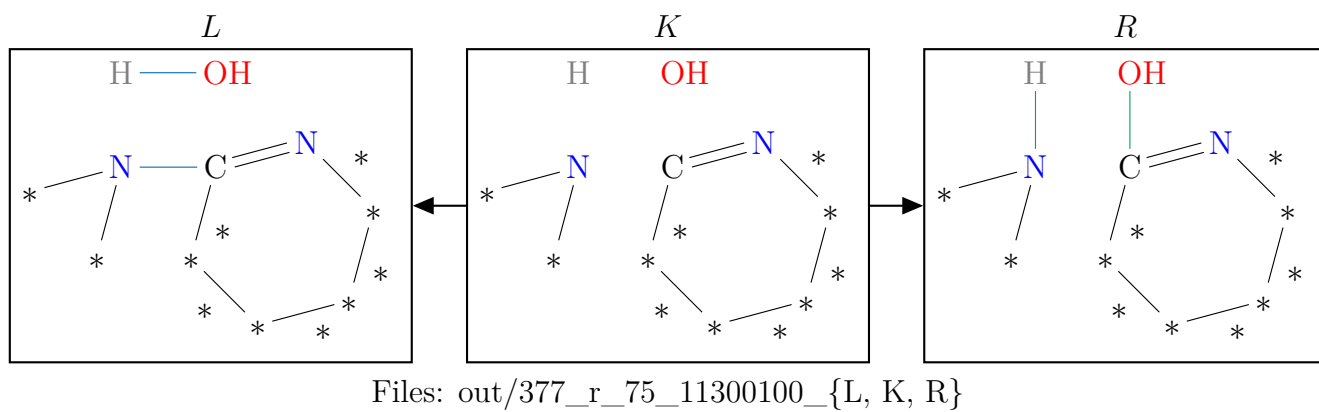


File: out/373_r_74_combined

0.0.76 6 Membered Ring Exoamine Hydrolysis

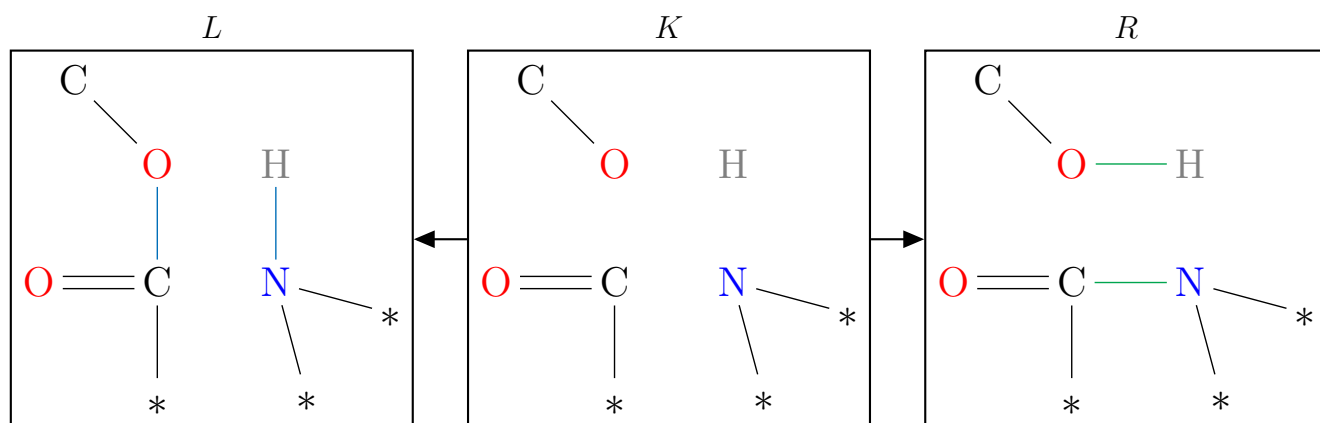
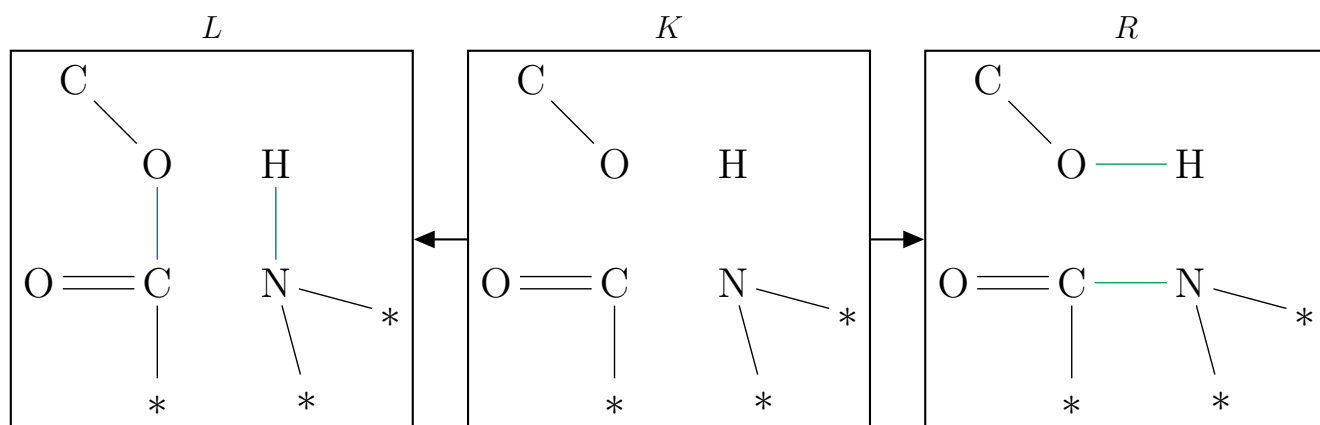


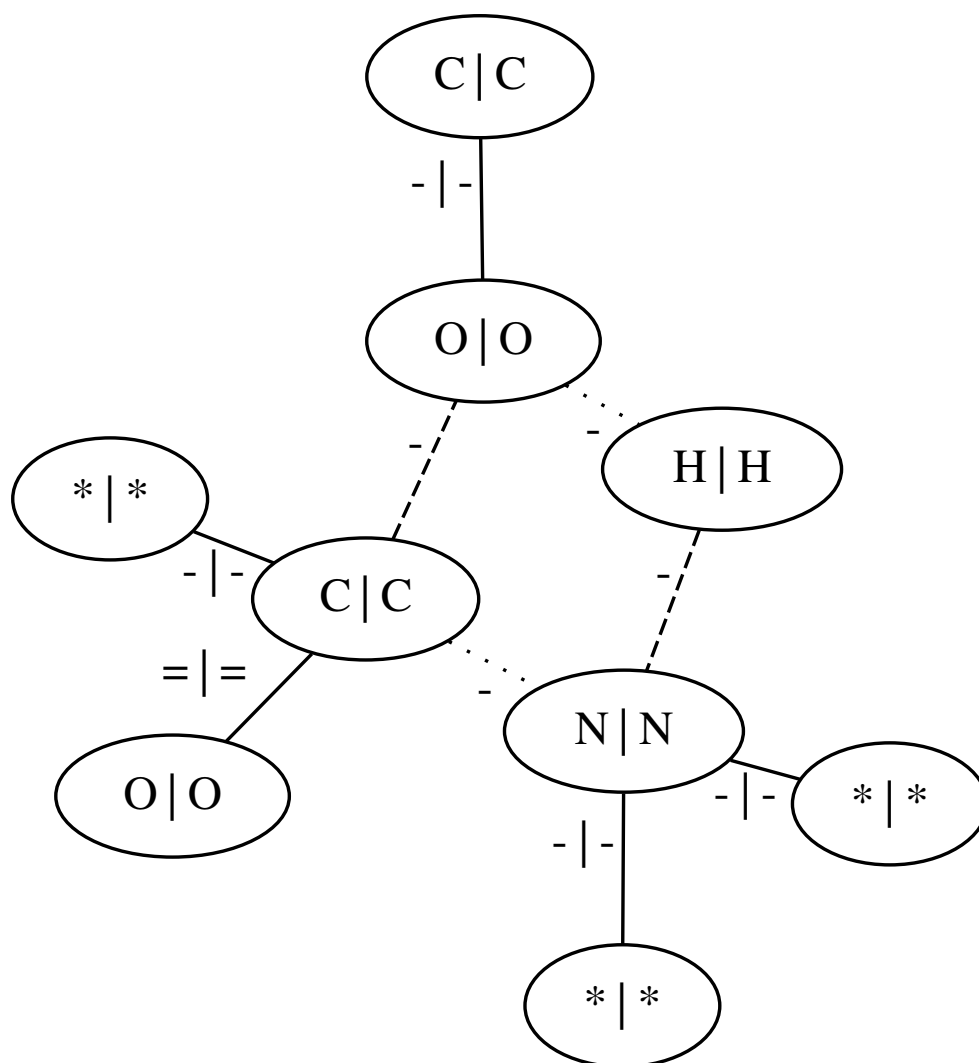
Files: out/376_r_75_10300000_{L, K, R}



File: out/378_r_75_combined

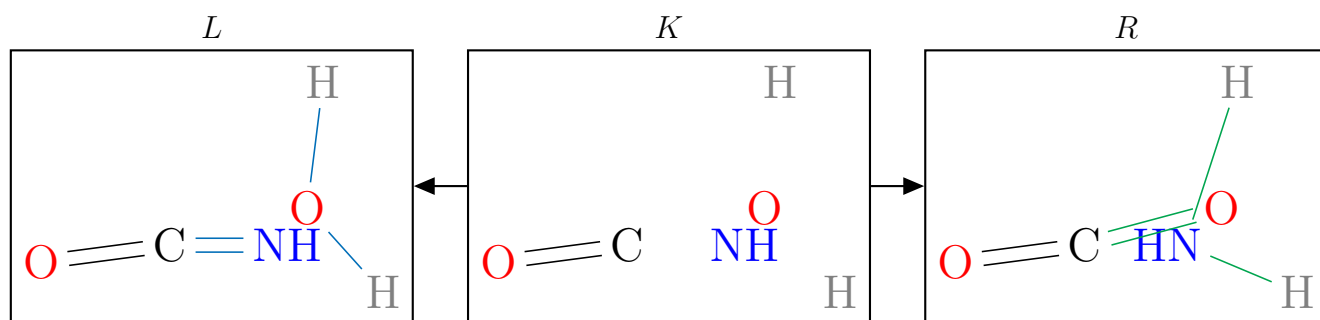
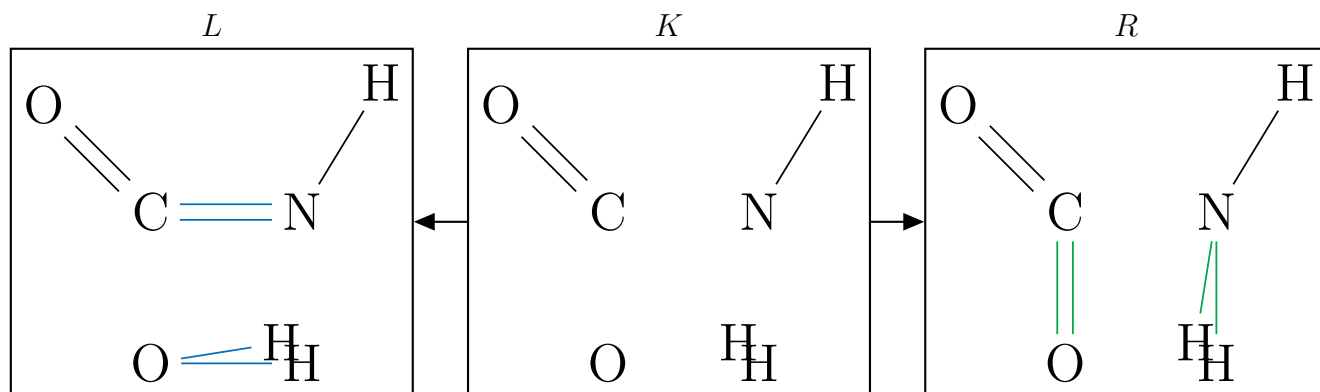
0.0.77 Ammonolysis of Esters

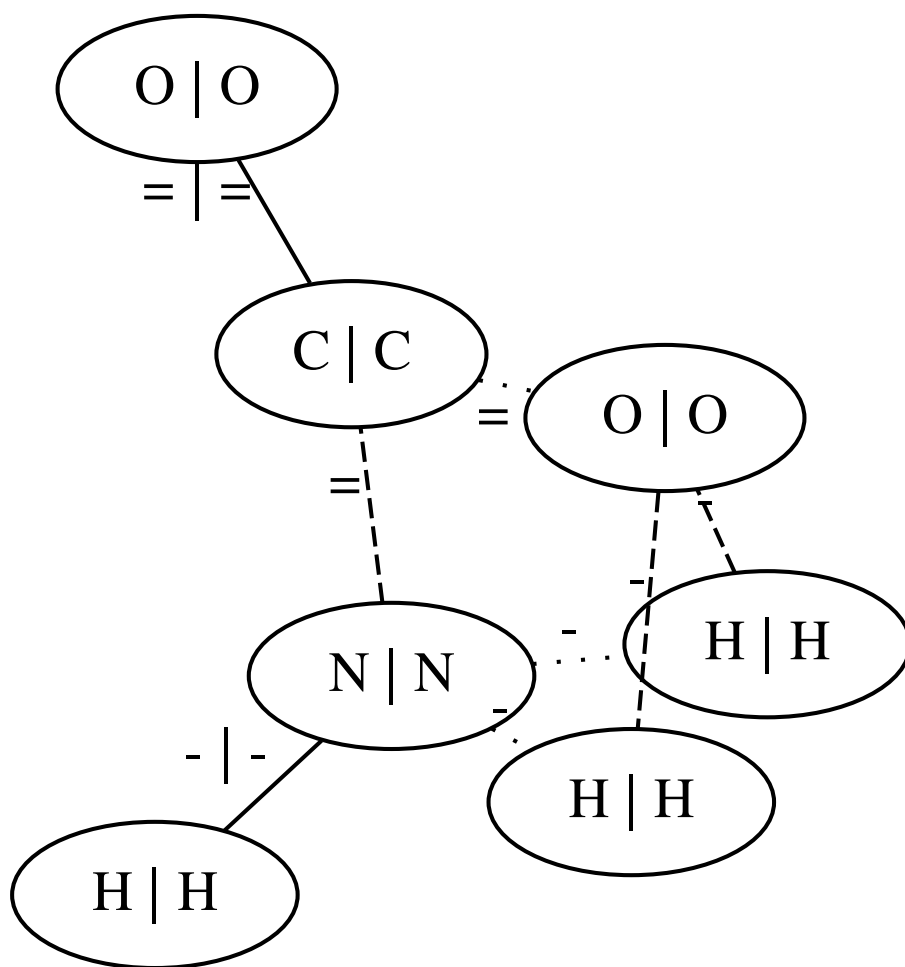




File: out/383_r_76_combined

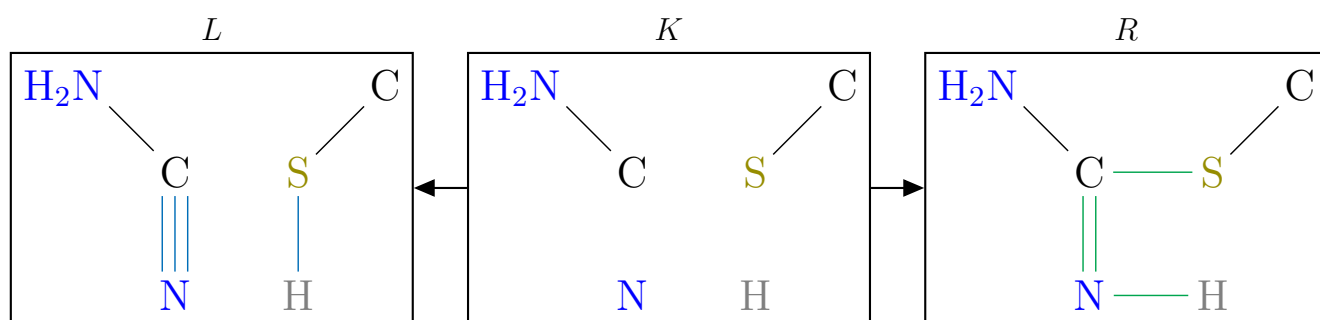
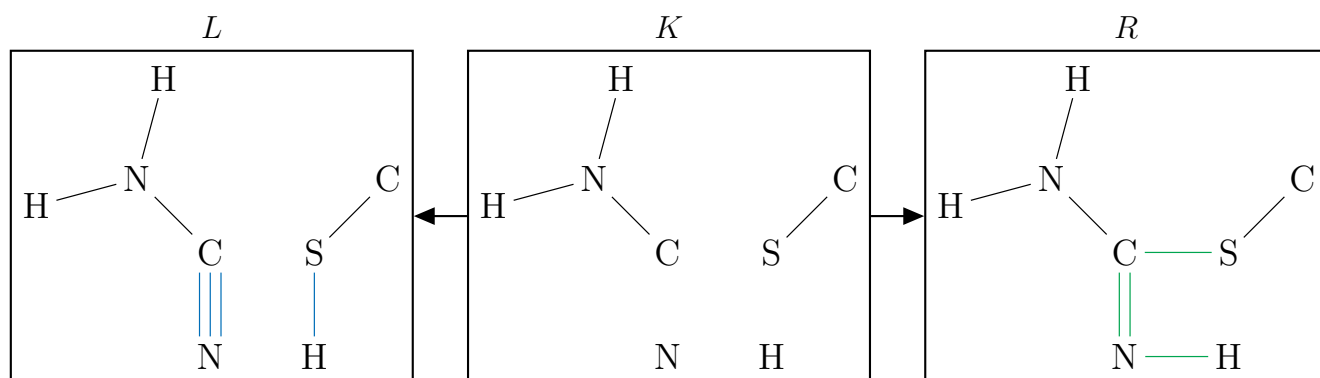
0.0.78 Isocyanate Hydrolysis

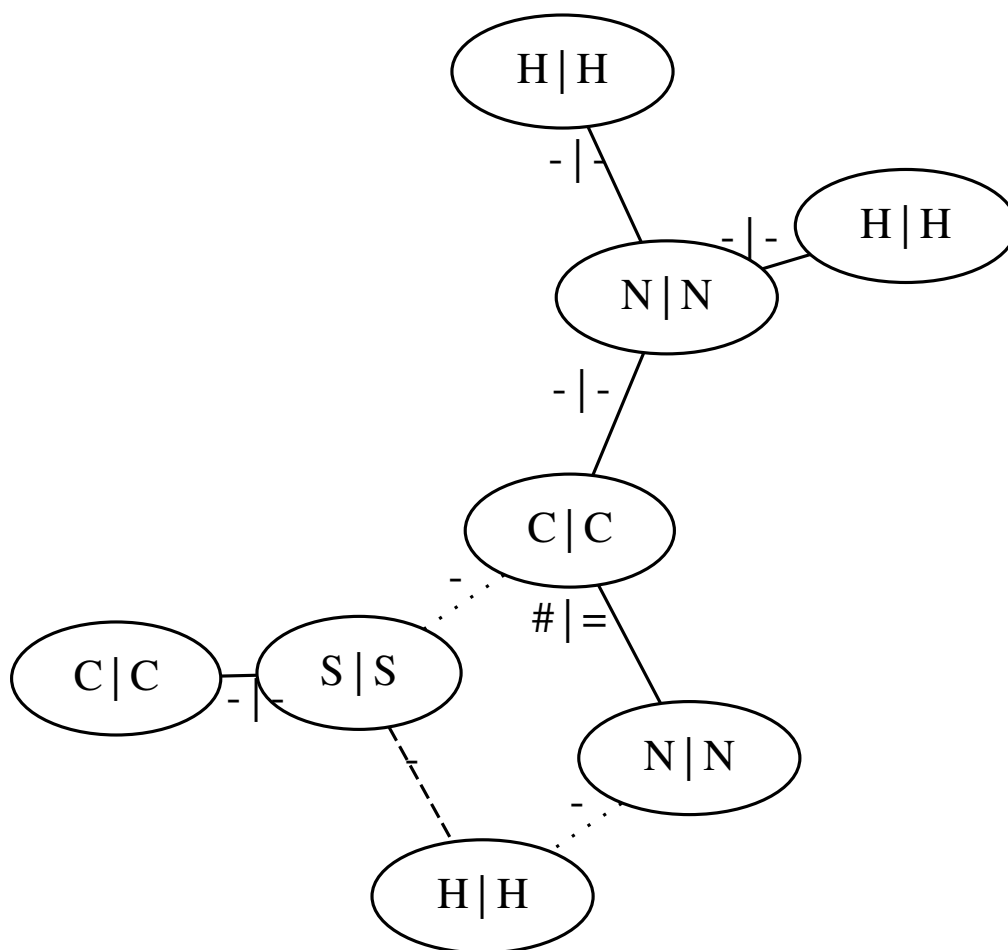




File: out/388_r_77_combined

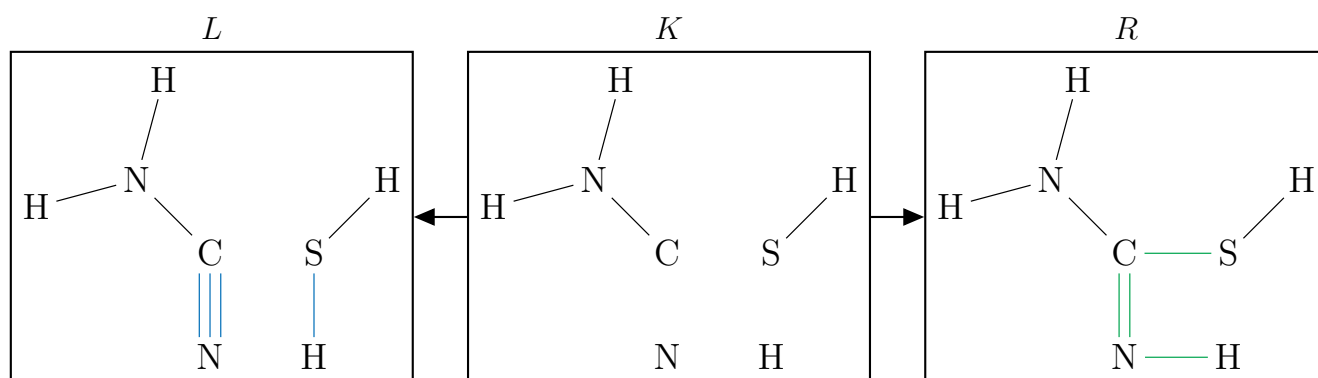
0.0.79 Cyanamidation, SC



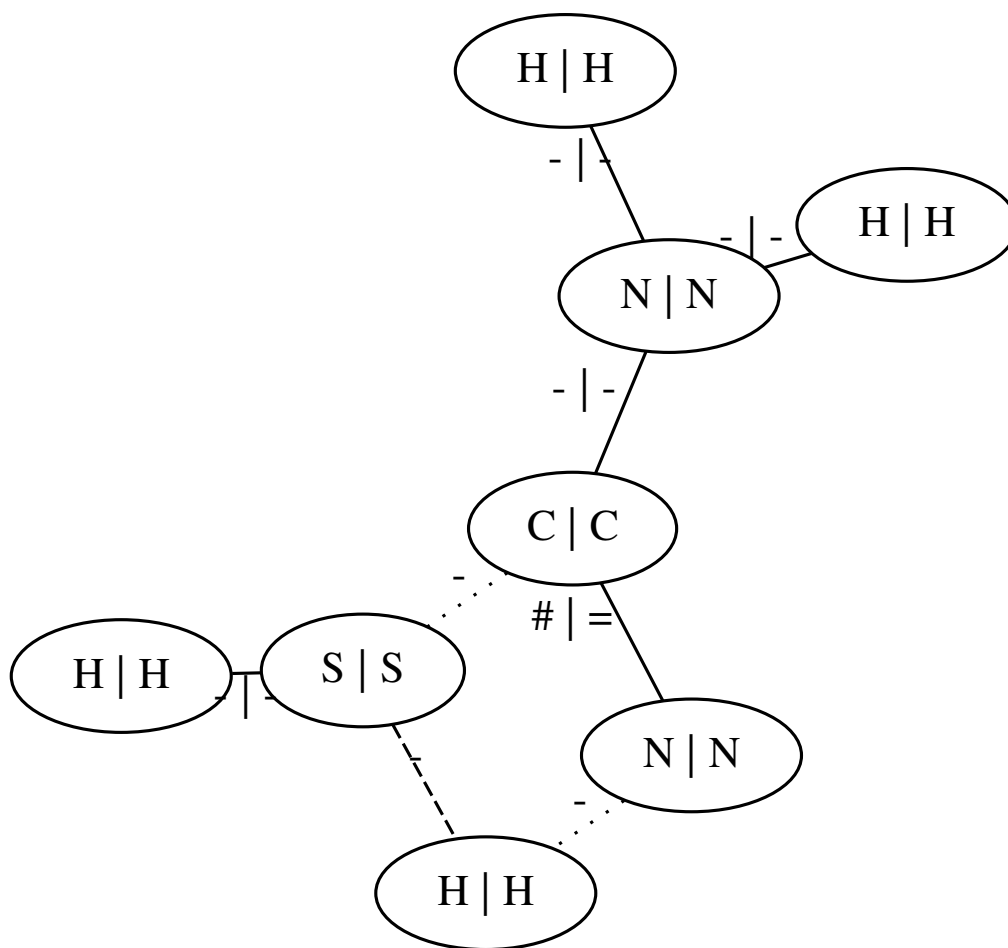
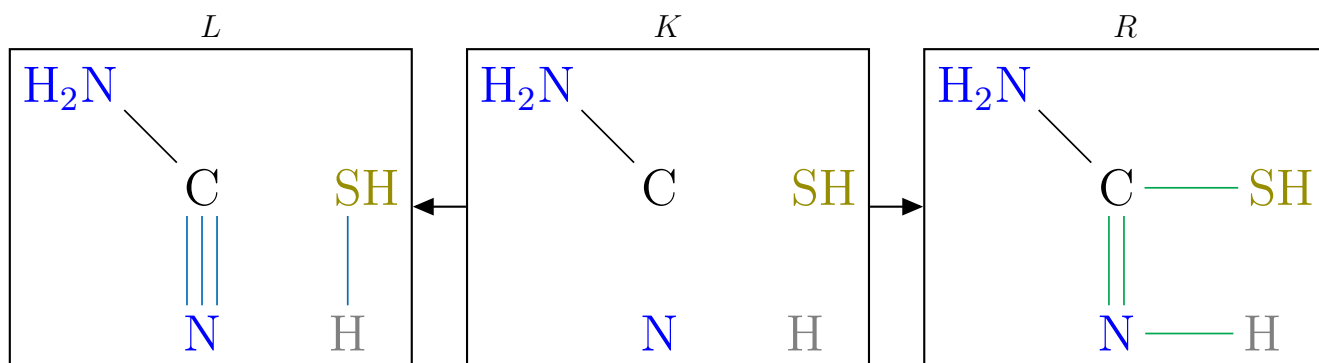


File: out/393_r_78_combined

0.0.80 Cyanamidation, SH

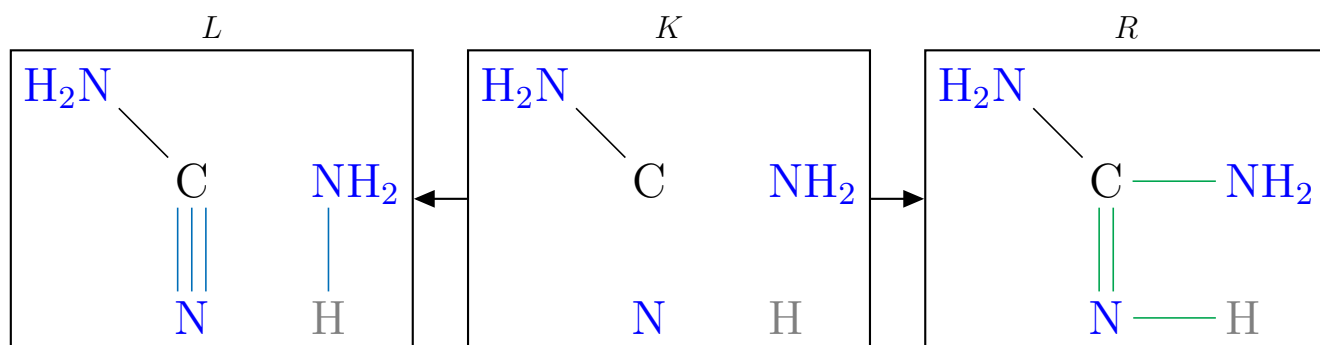
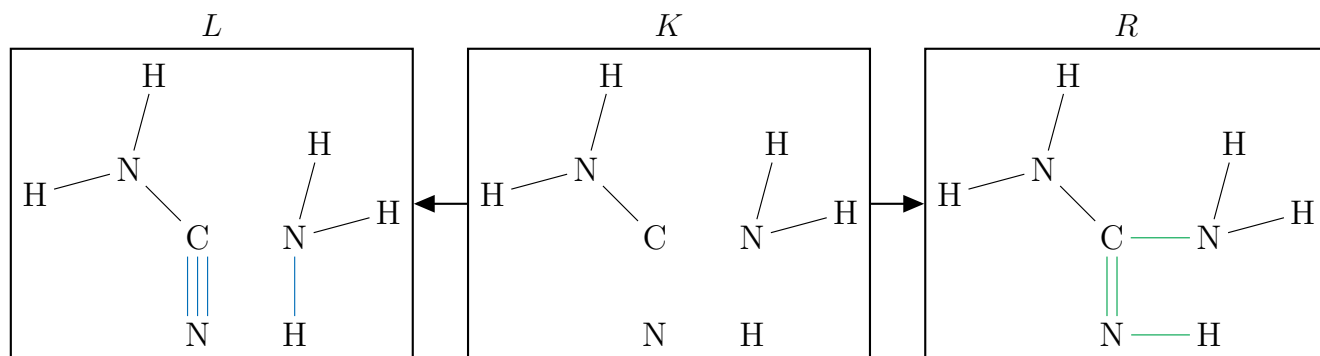


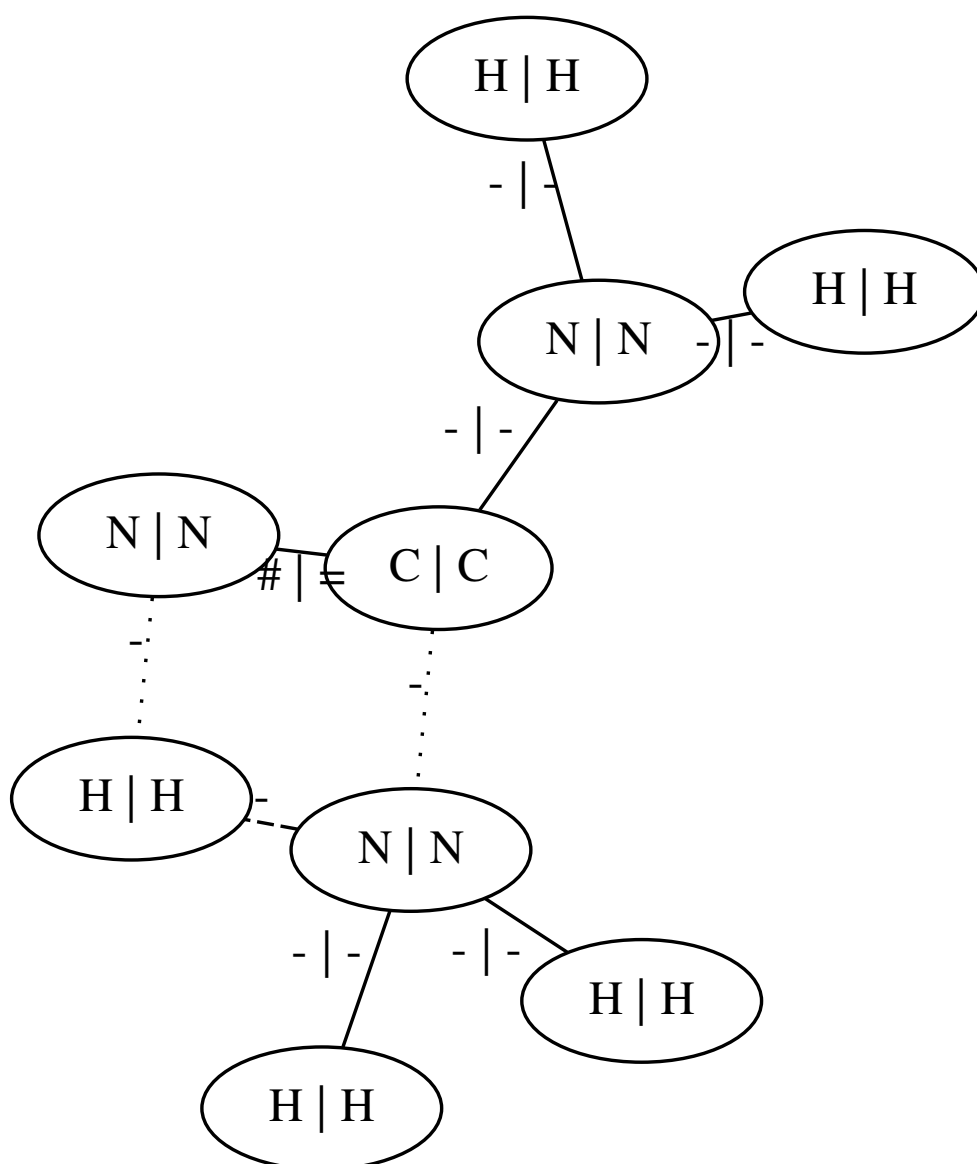
Files: out/396_r_79_10300000_{L, K, R}



File: out/398_r_79_combined

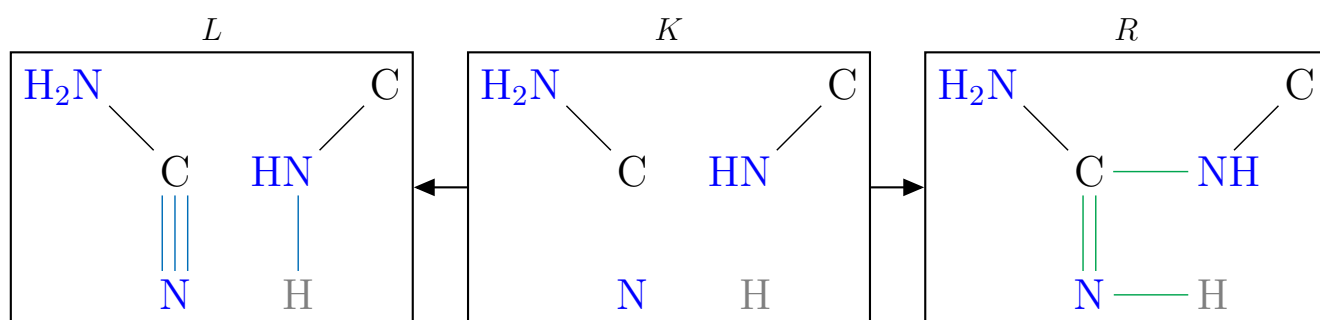
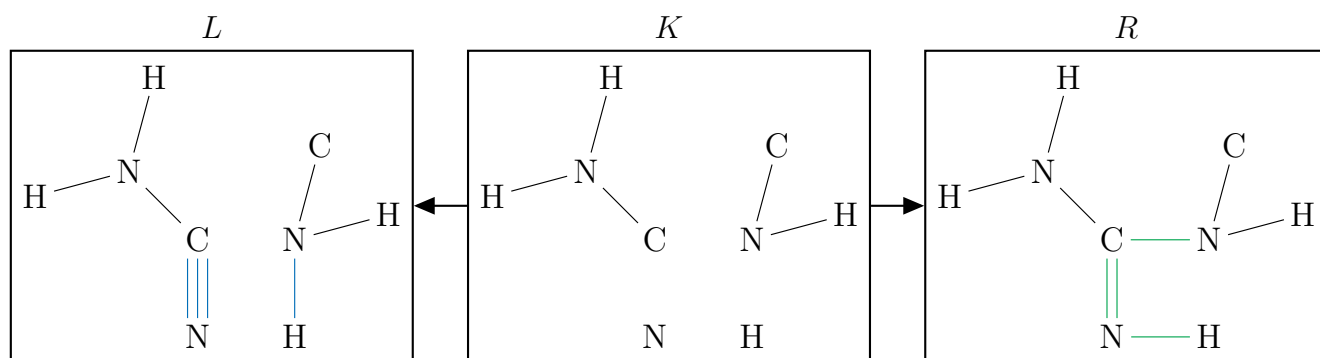
0.0.81 Cyanamidation, N, HH

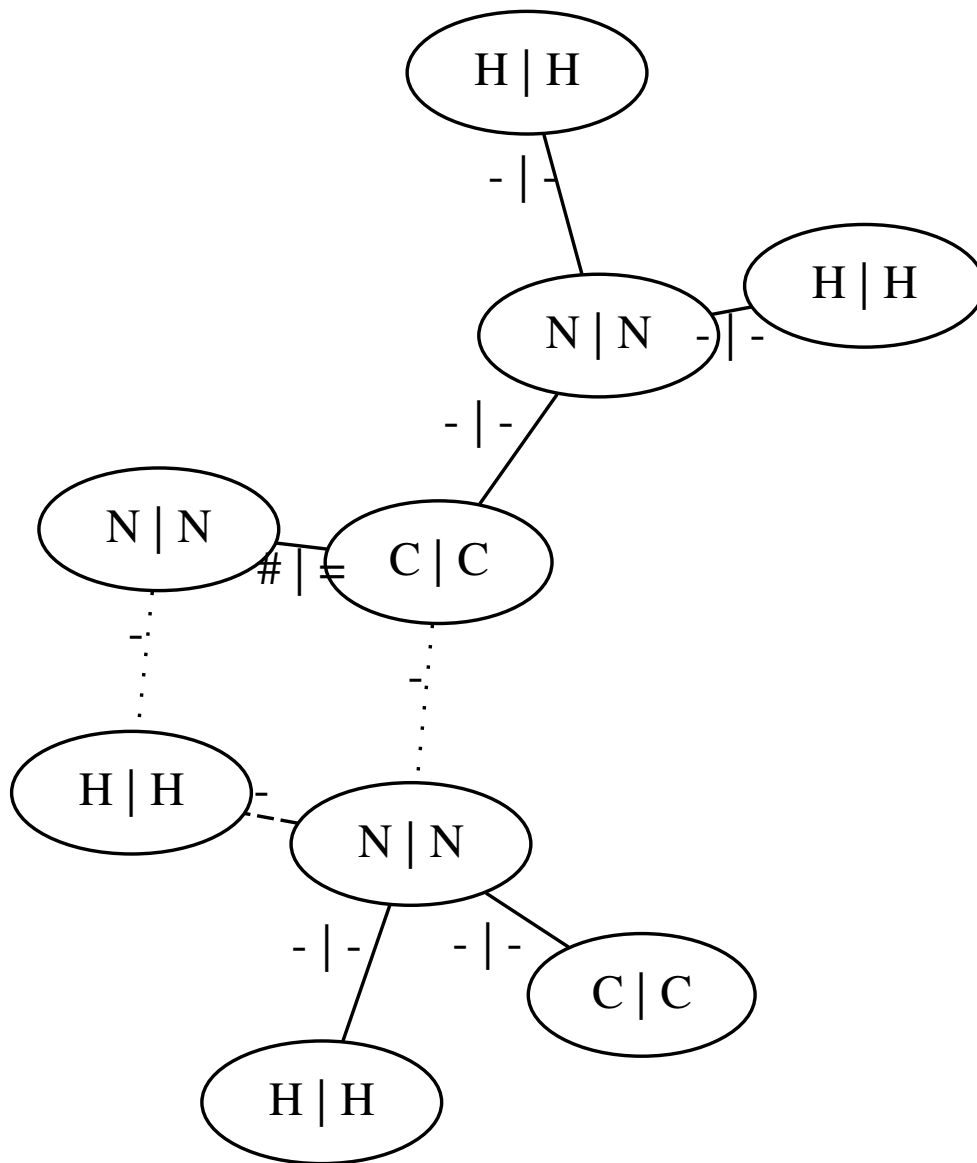




File: out/403_r_80_combined

0.0.82 Cyanamidation, N, HC

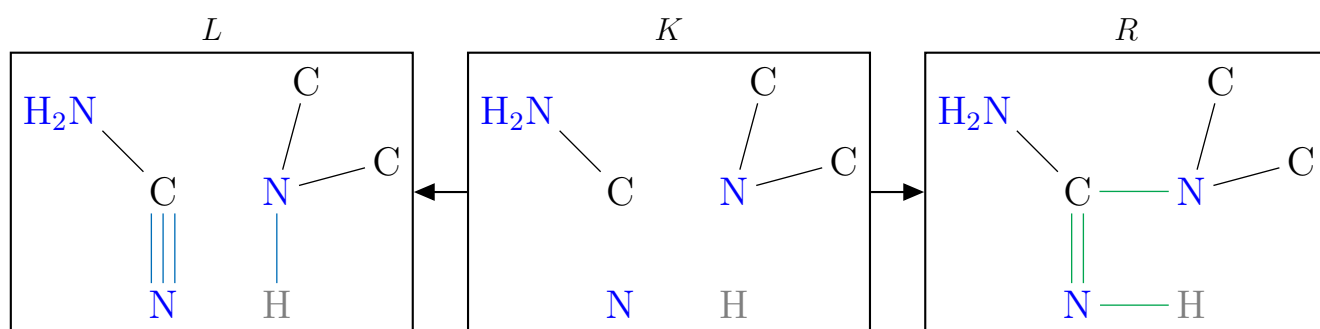
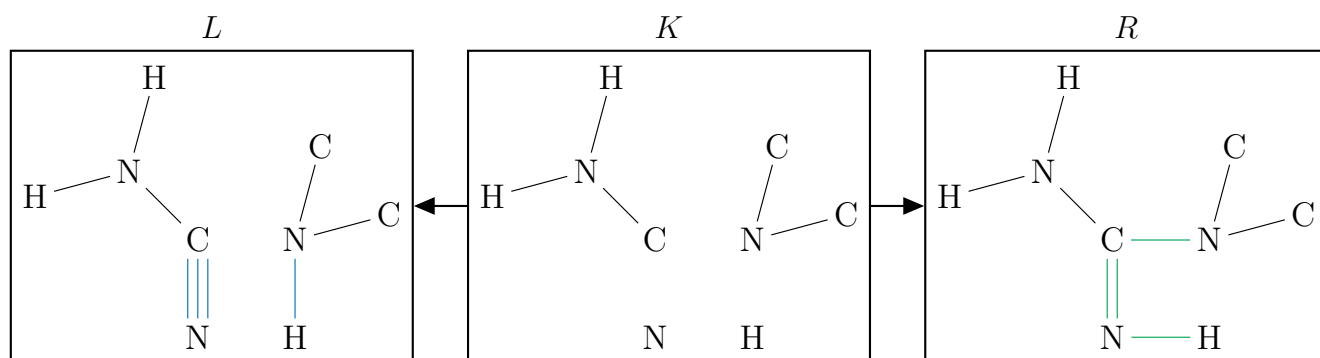




File: out/408_r_81_combined

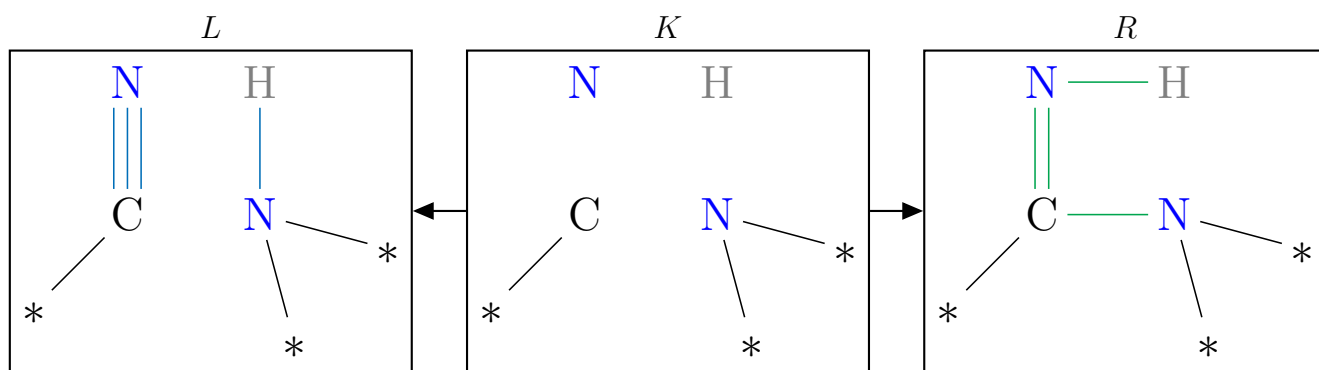
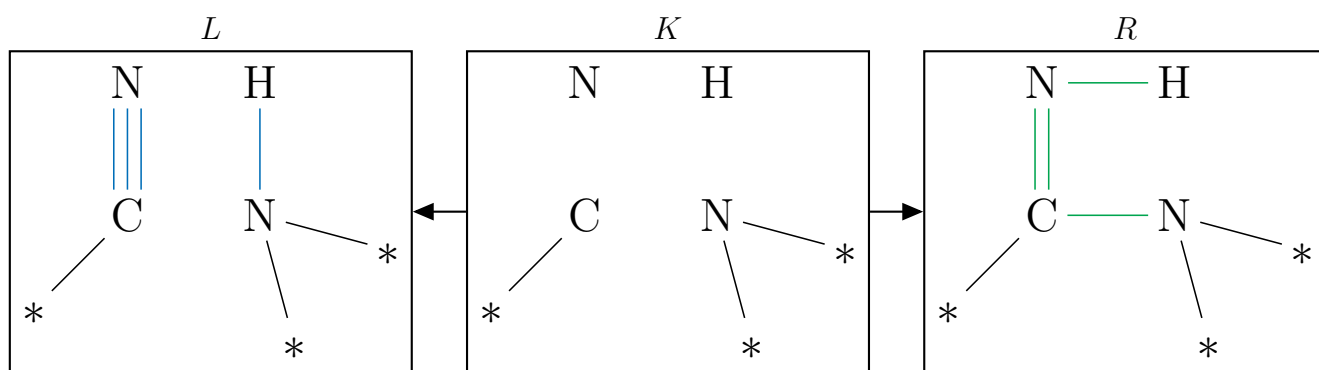
$$\begin{aligned}
 & |\{e \in \text{outEdges}(6) \mid \\
 & \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 & \quad \wedge \\
 & \quad \text{label}(e) \in \{'=\'} \\
 & \}\} = 0
 \end{aligned}$$

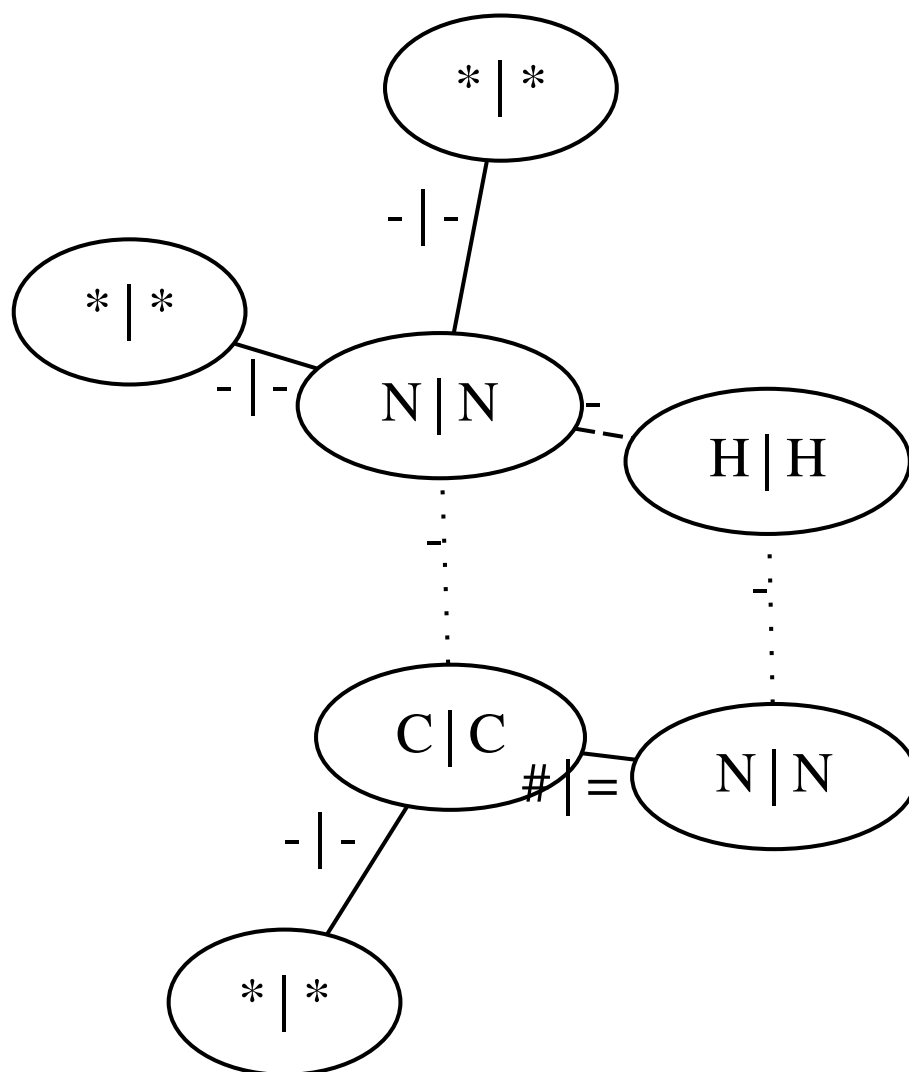
0.0.83 Cyanamidation, N, CC



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

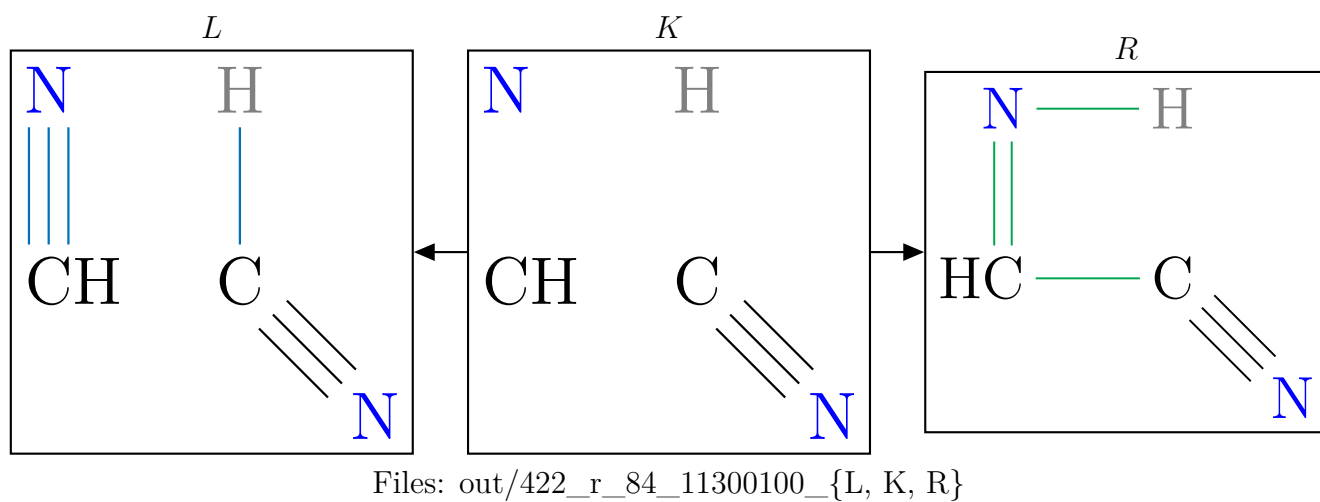
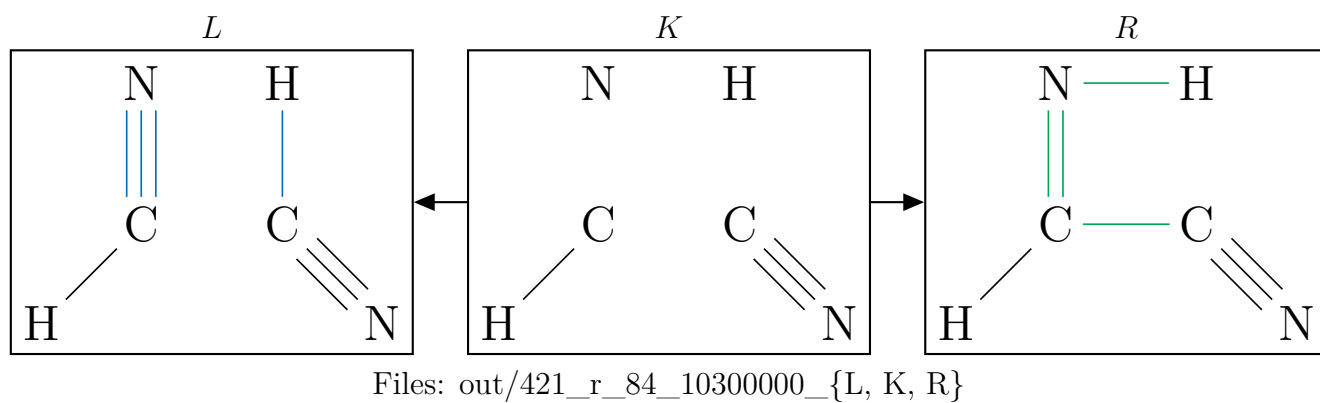
0.0.84 Nitrile Amination

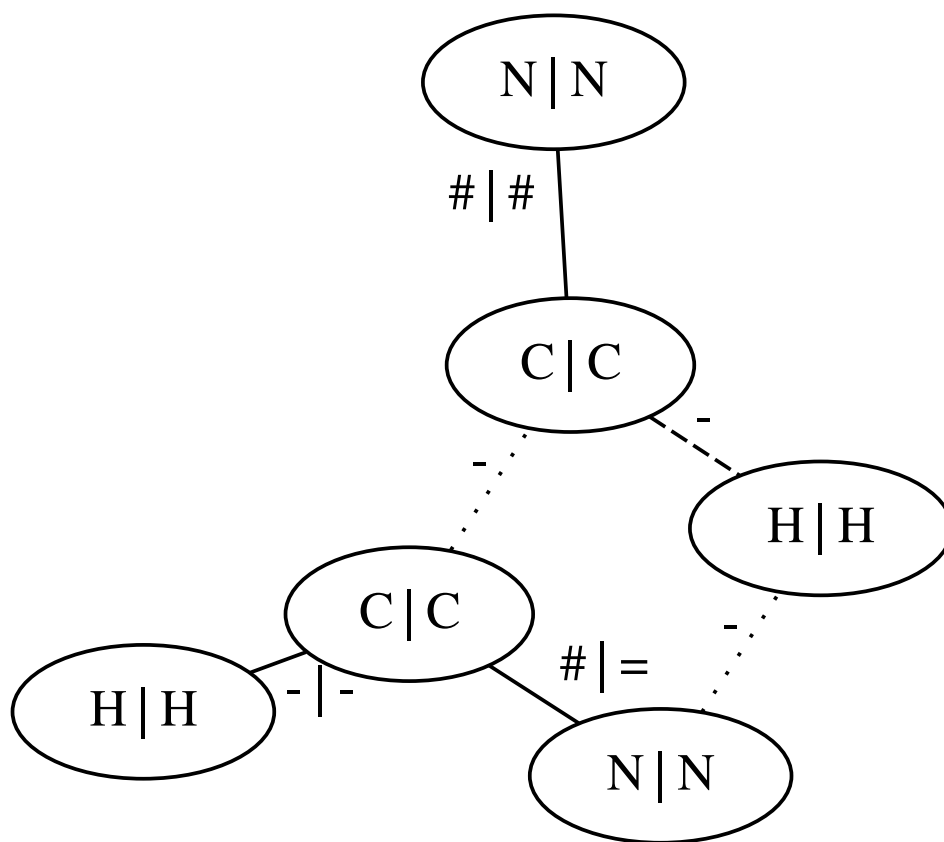




File: out/418_r_83_combined

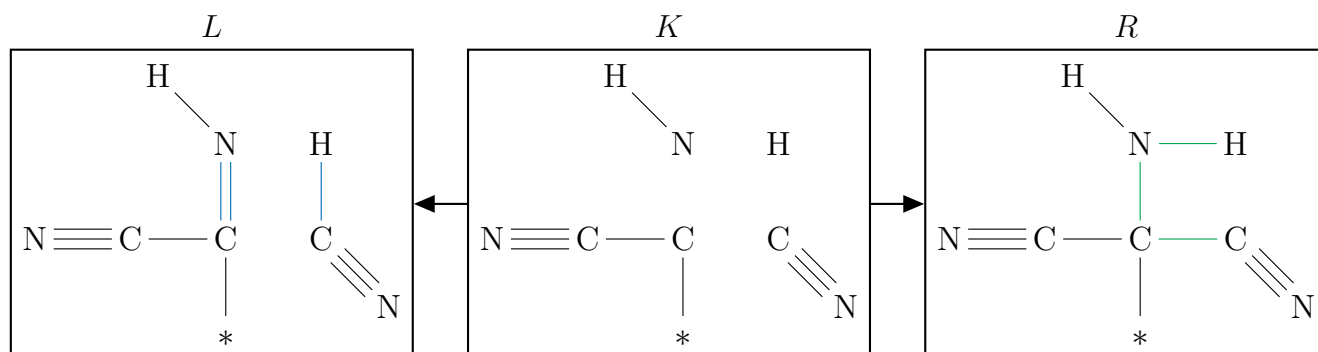
0.0.85 HCN Addition to Nitriles



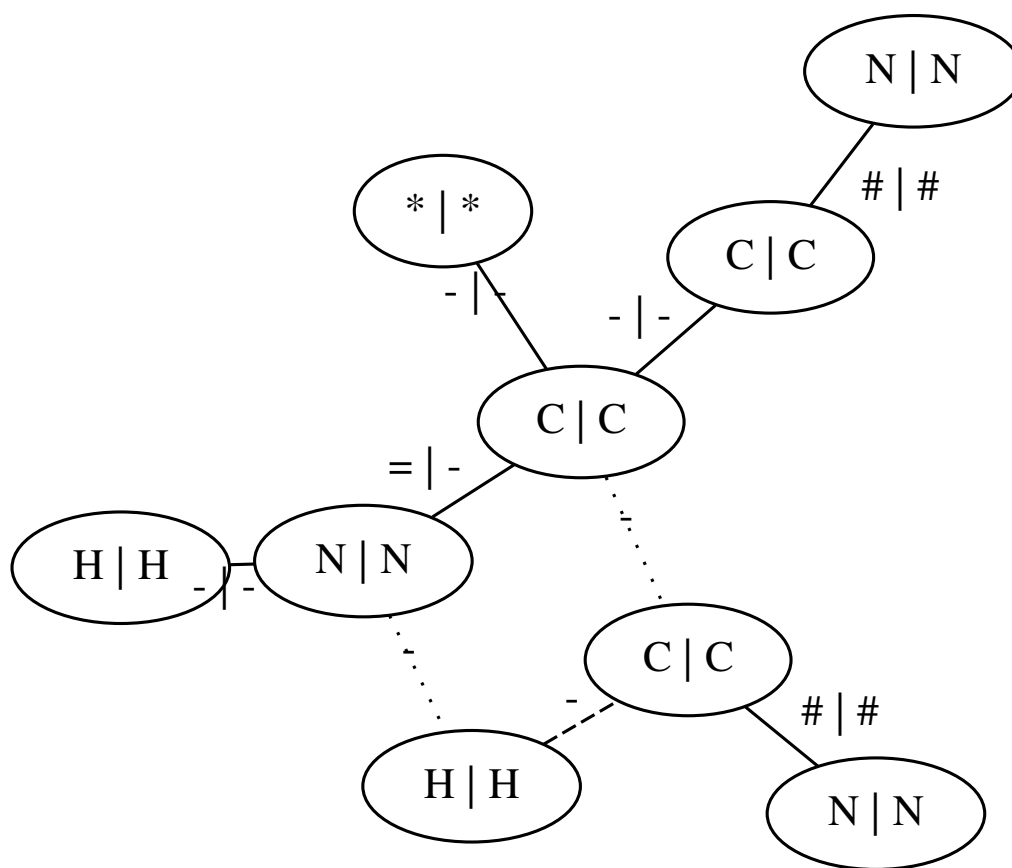
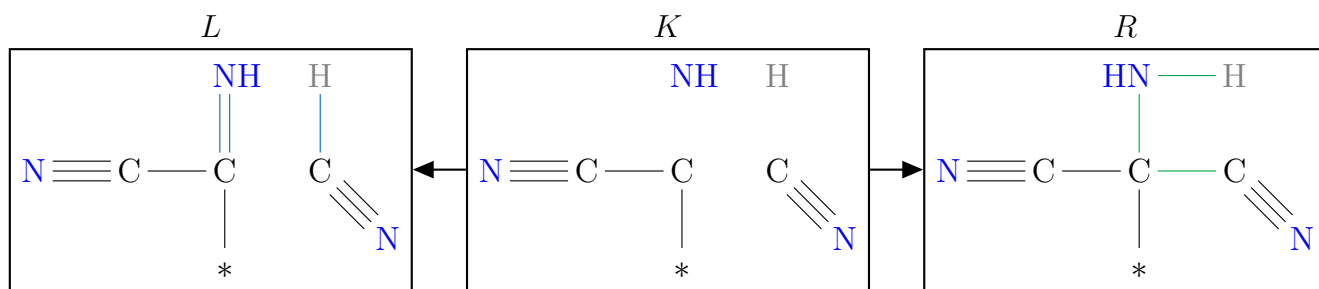


File: out/423_r_84_combined

0.0.86 CN addition to iminonitriles

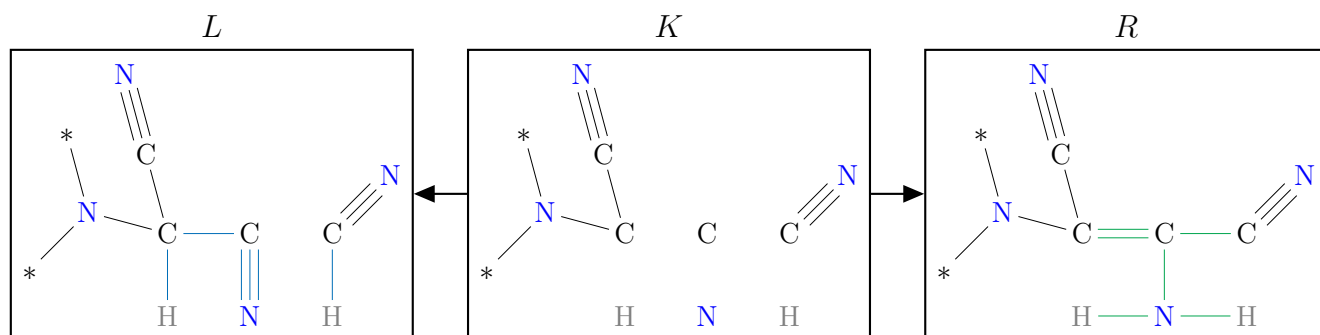
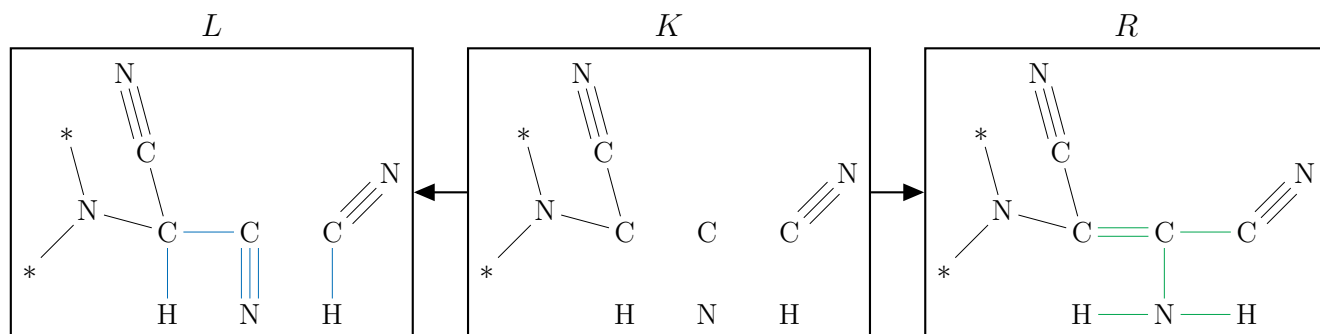


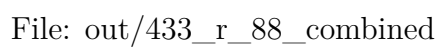
Files: out/426_r_86_10300000_{L, K, R}



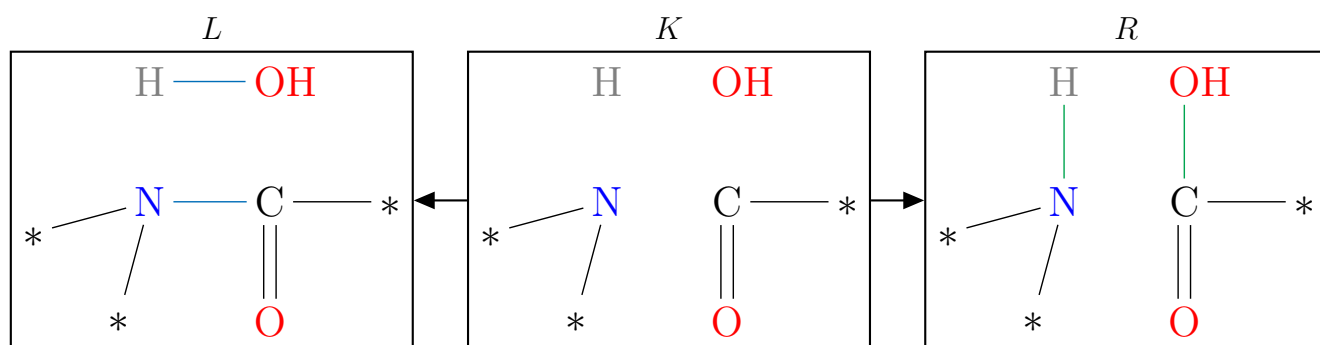
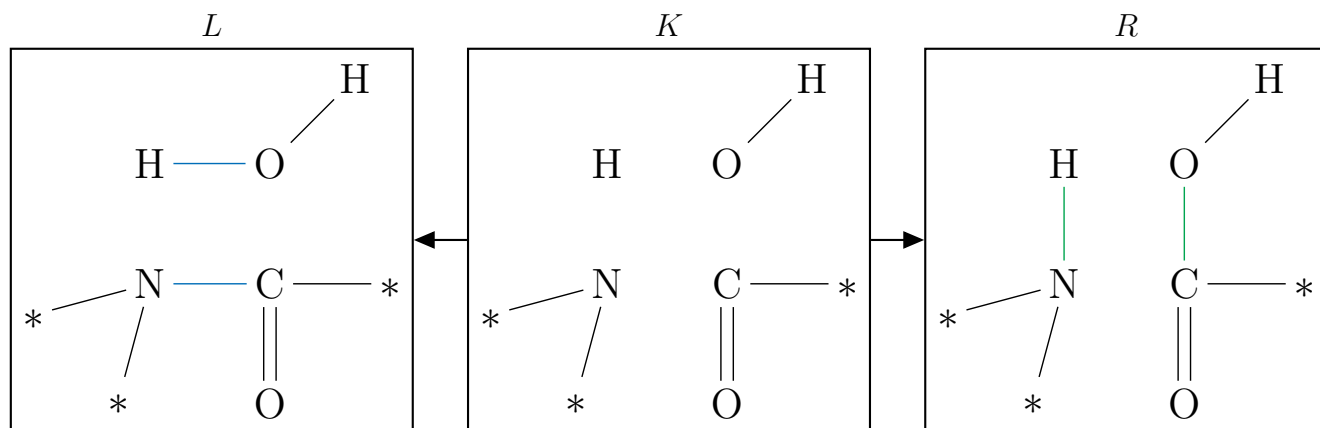
File: out/428_r_86_combined

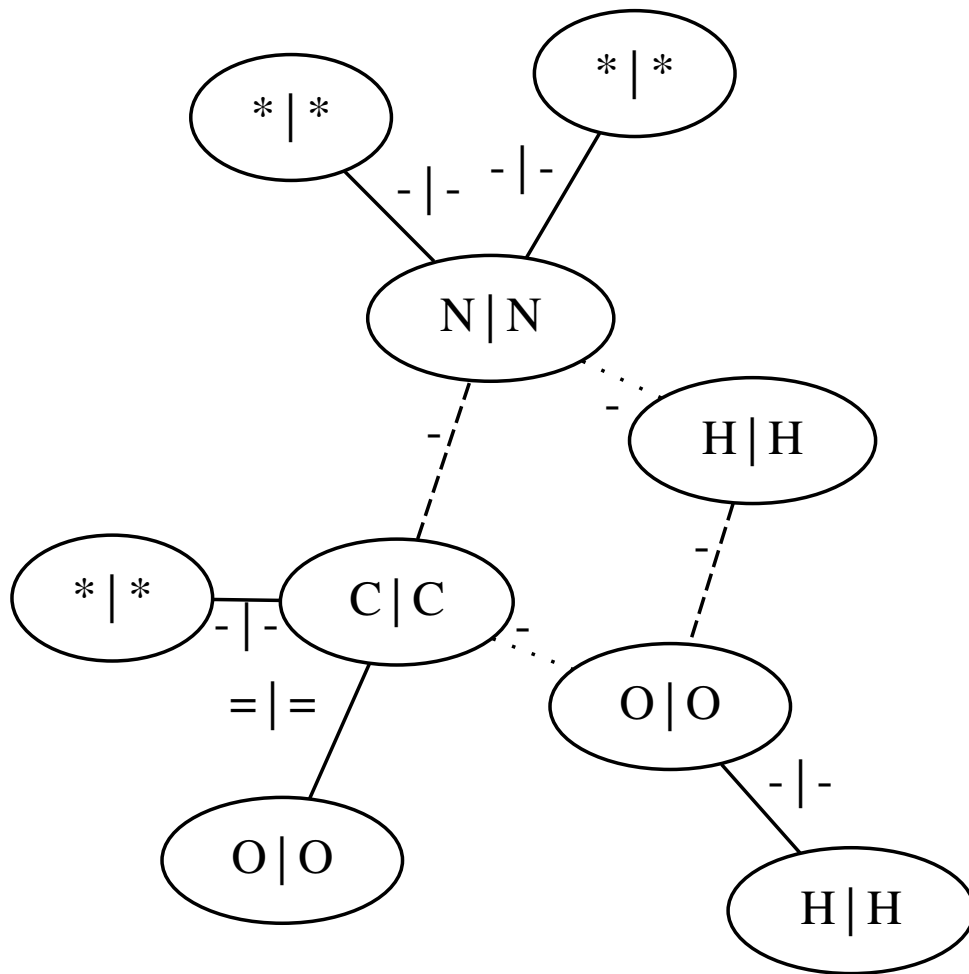
0.0.87 CN addition to aminodinitriles





0.0.88 Amide Hydrolysis





File: out/438_r_90_combined

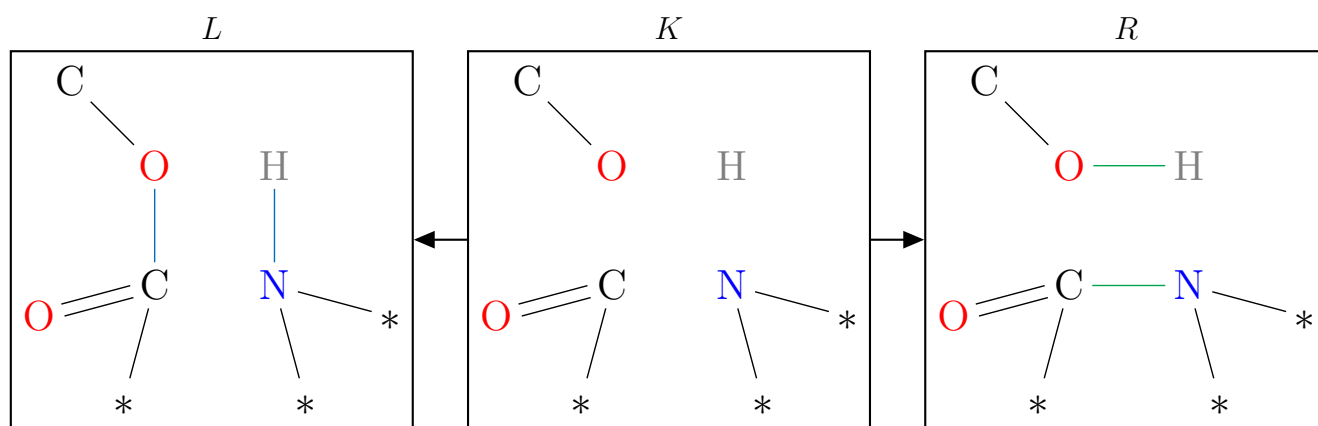
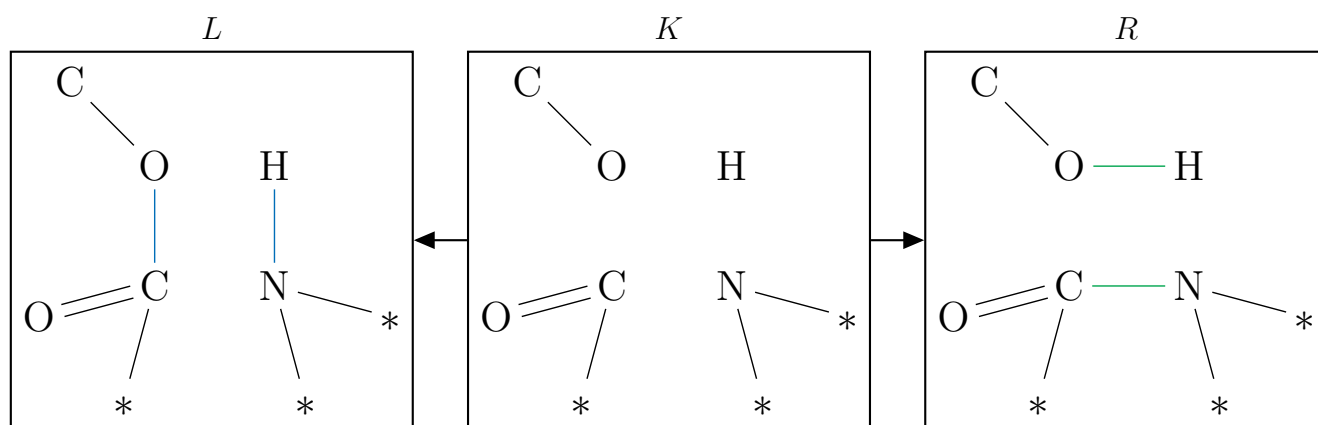
```

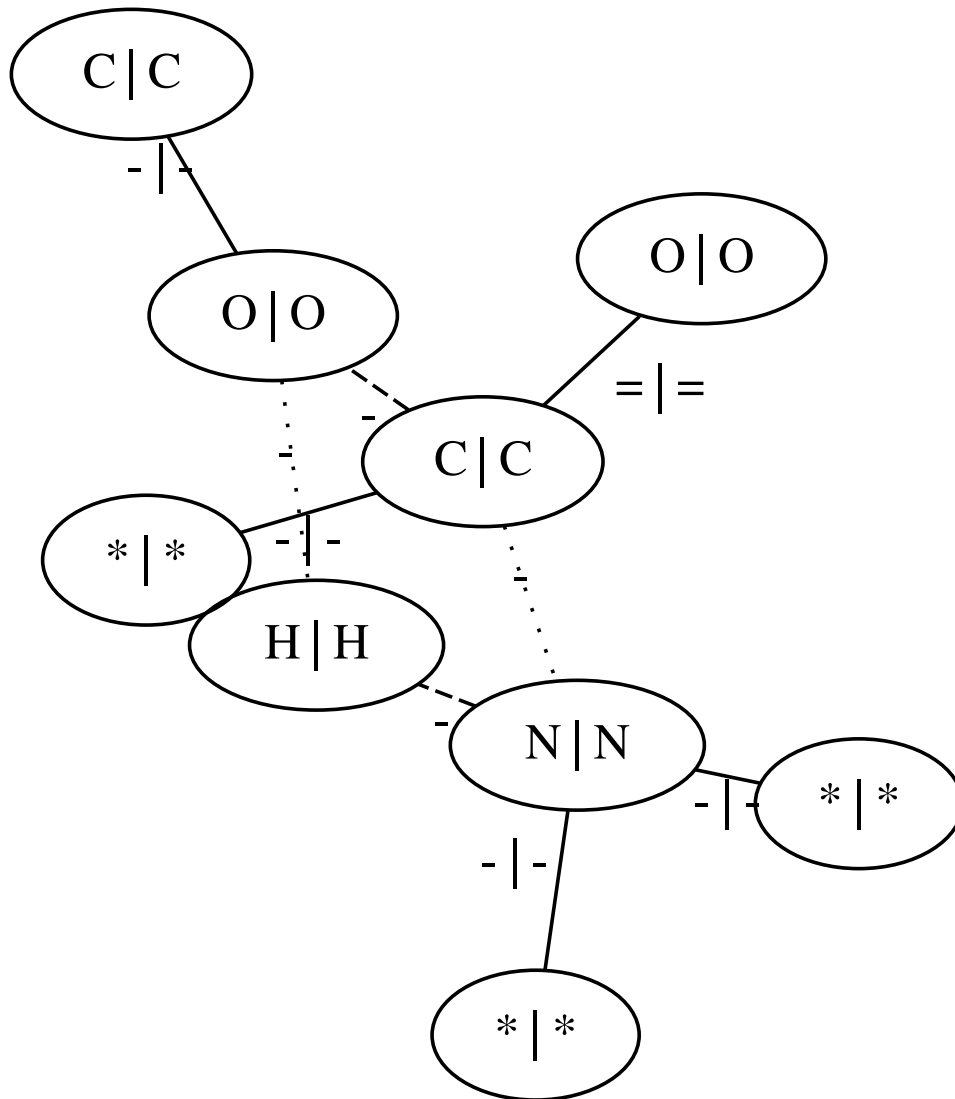
|{e ∈ outEdges(4) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

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

0.0.89 Amide Formation Hydrolysis, C



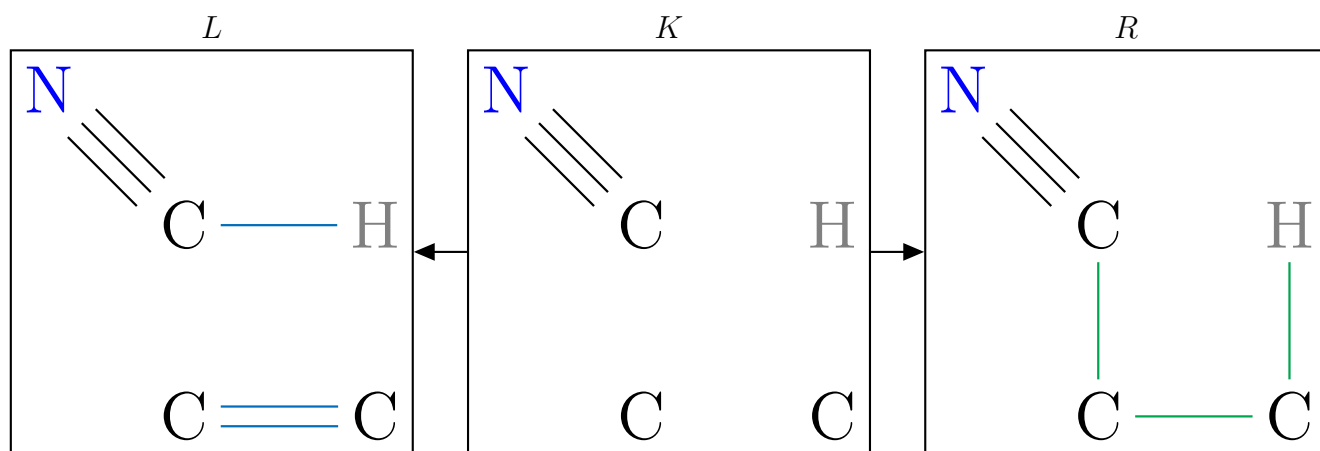
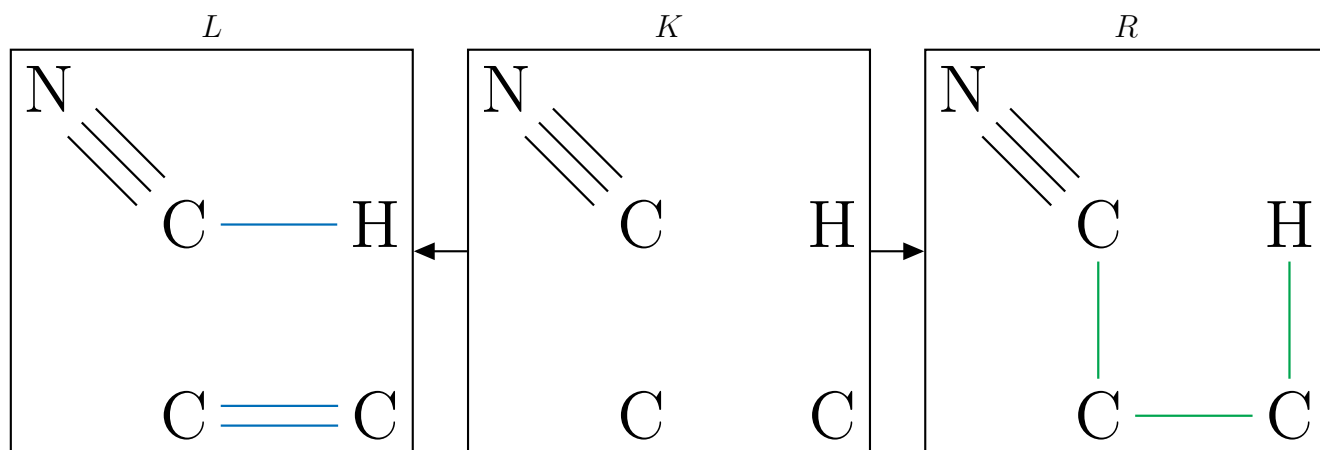


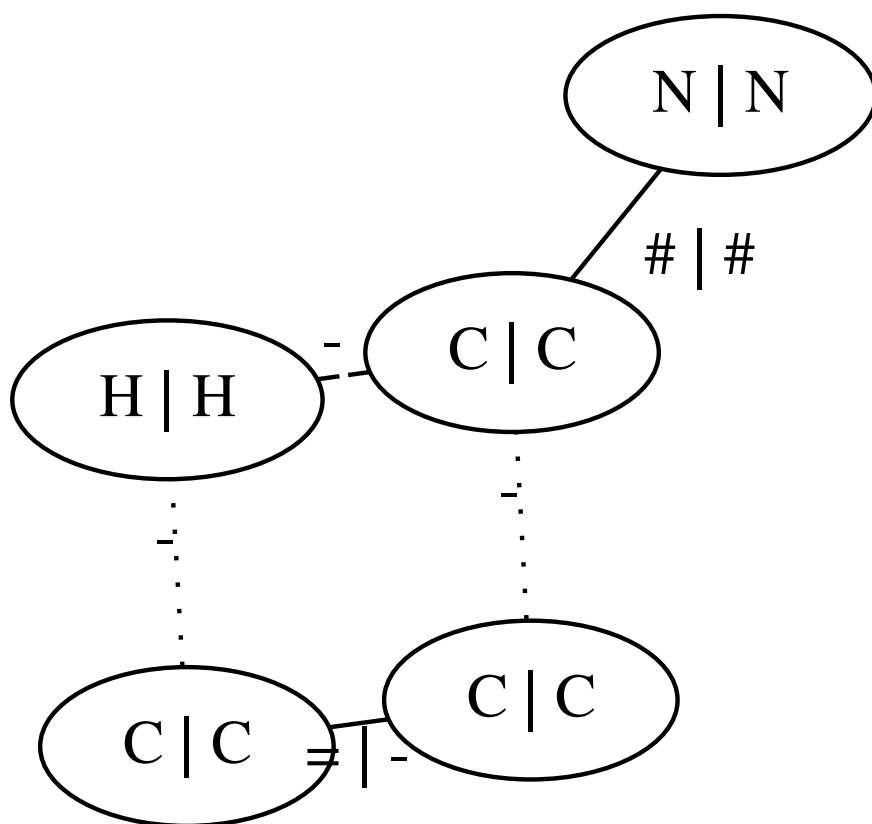
File: out/443_r_91_combined

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

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

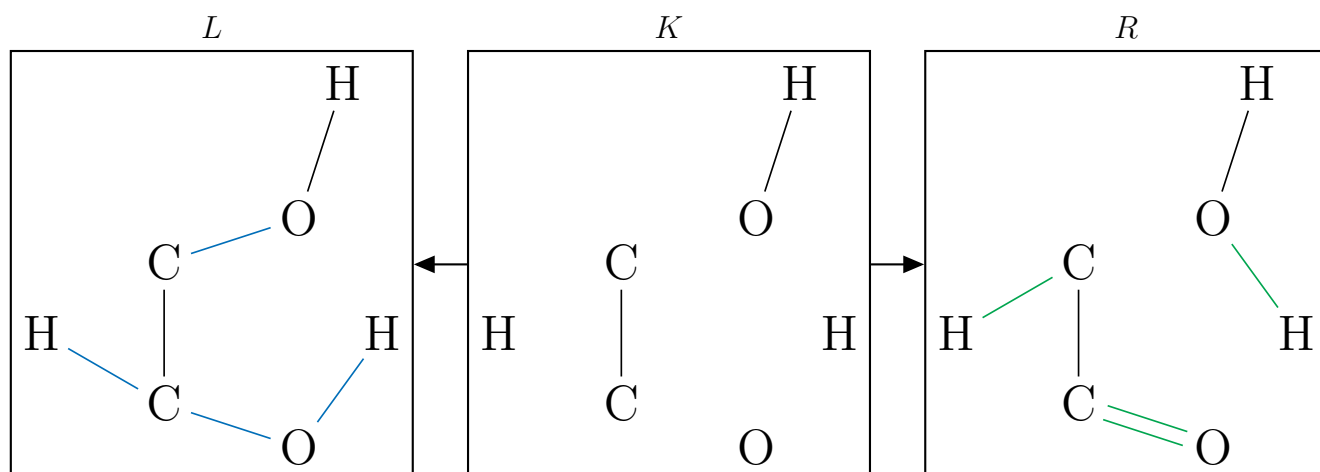
0.0.90 Alkene Addition, CN



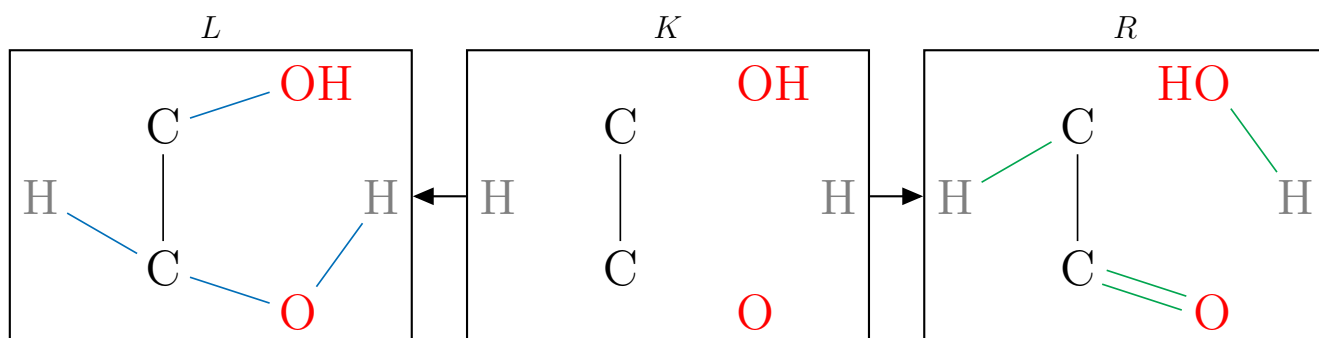


File: out/448_r_92_combined

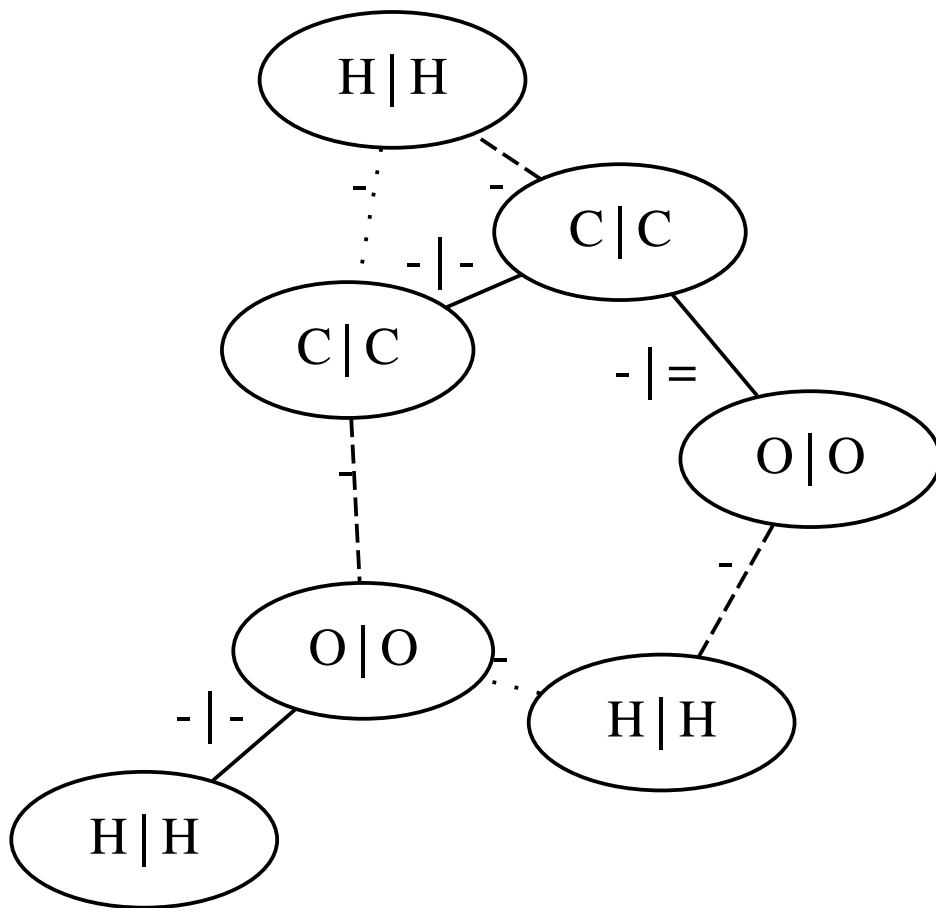
0.0.91 Elimination + enol to keto



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



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



File: out/453_r_93_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(4) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(0) \mid$$

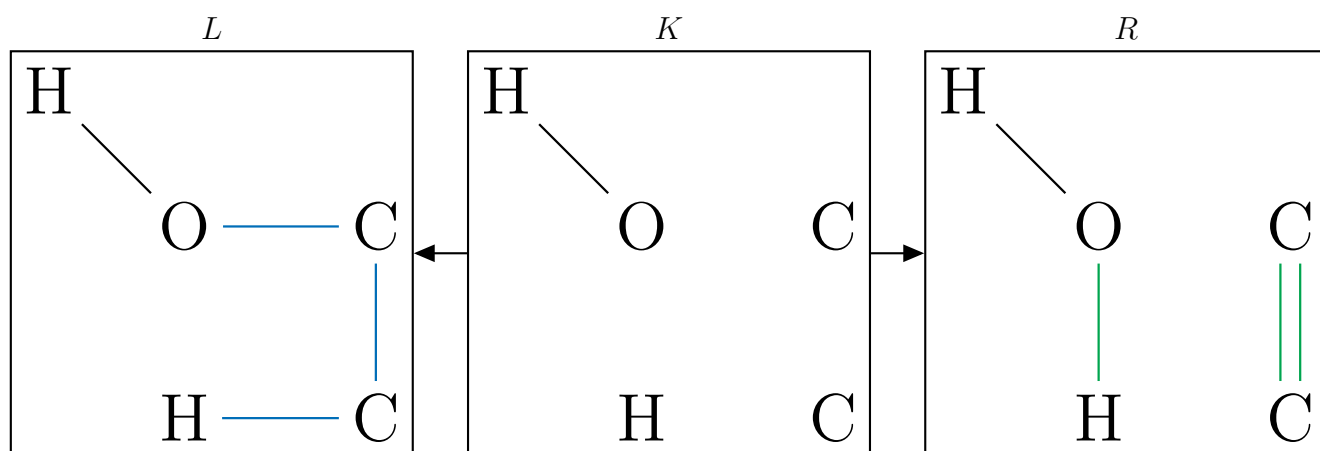
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'N'}\}$$

$$\wedge$$

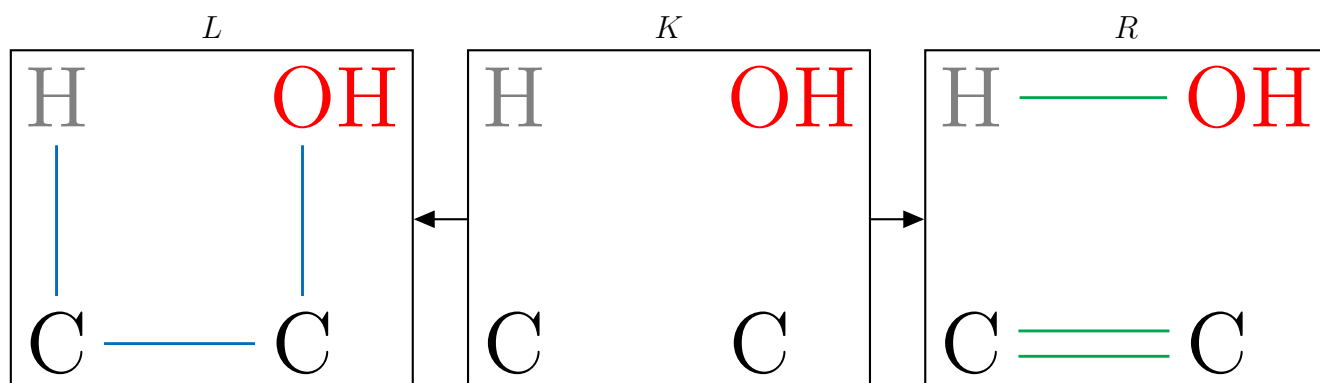
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

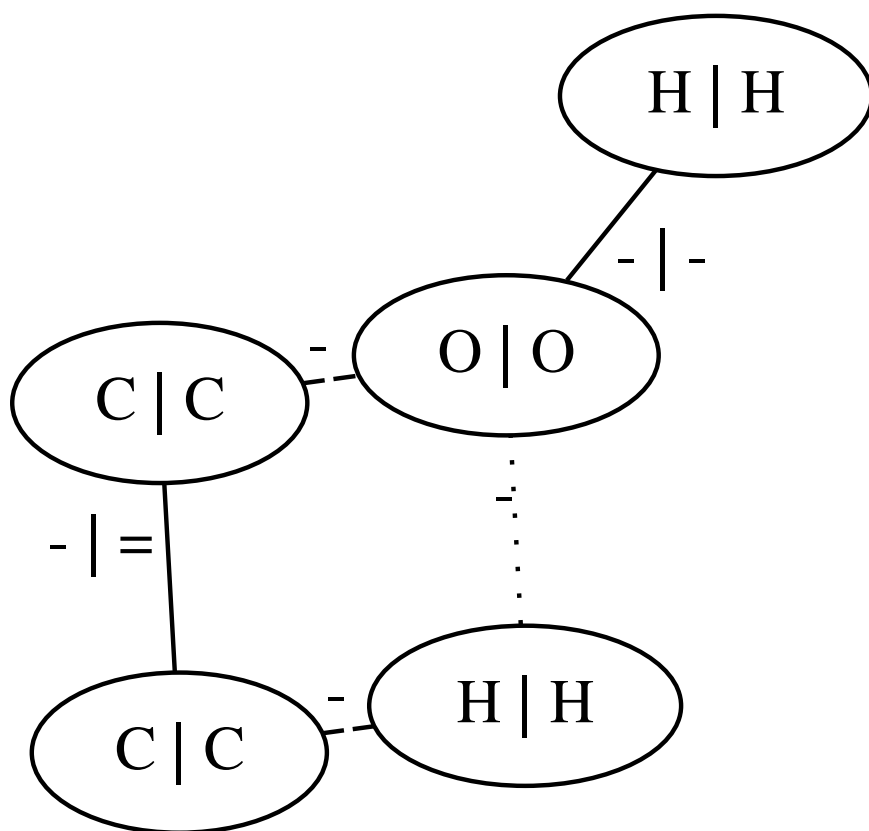
0.0.92 Elimination2



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



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



File: out/458_r_94_combined

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

$$|\{e \in \text{outEdges}(2) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'N'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}, \text{'-'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(2) \mid$$

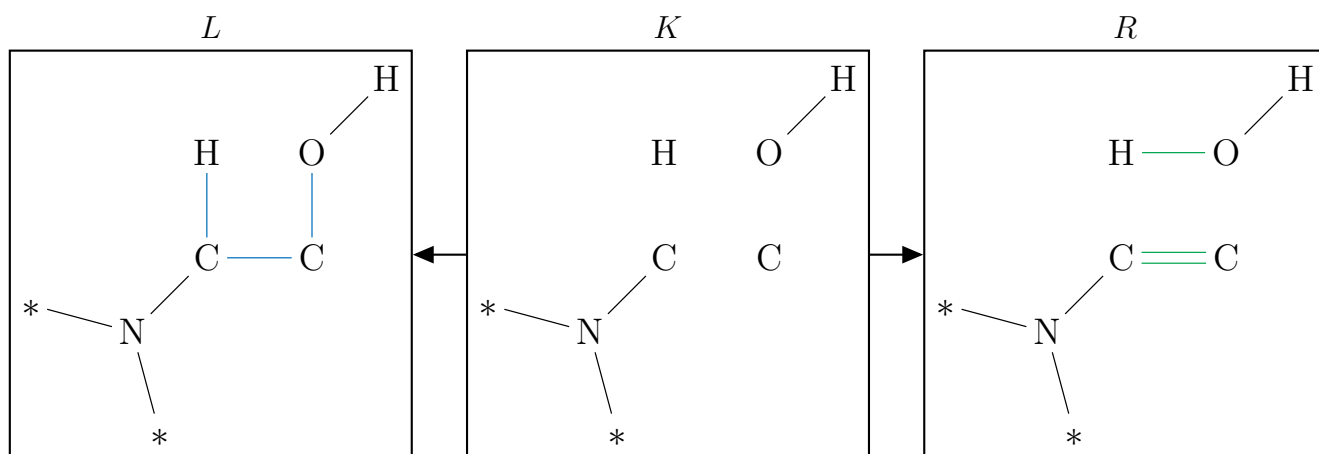
$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

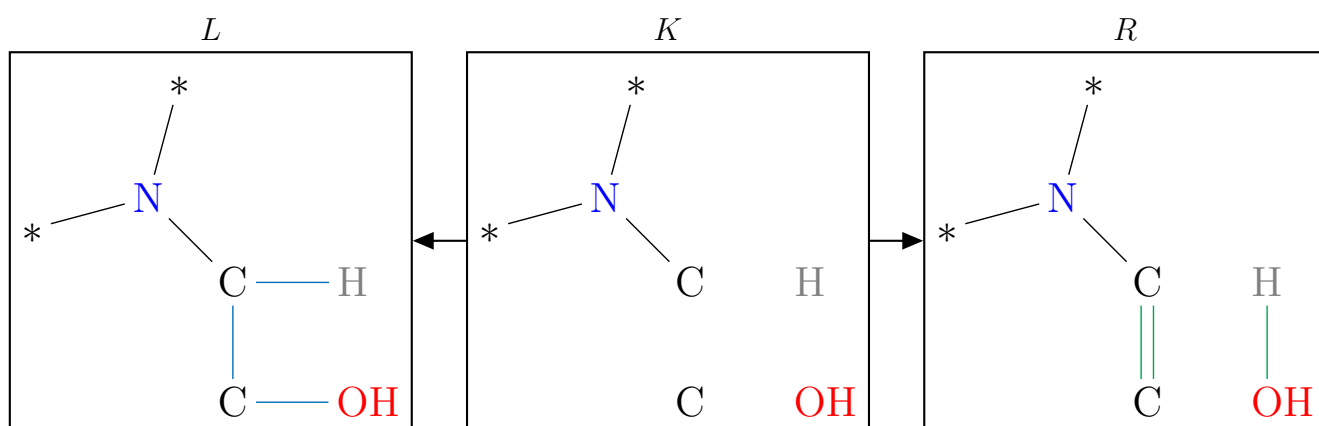
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

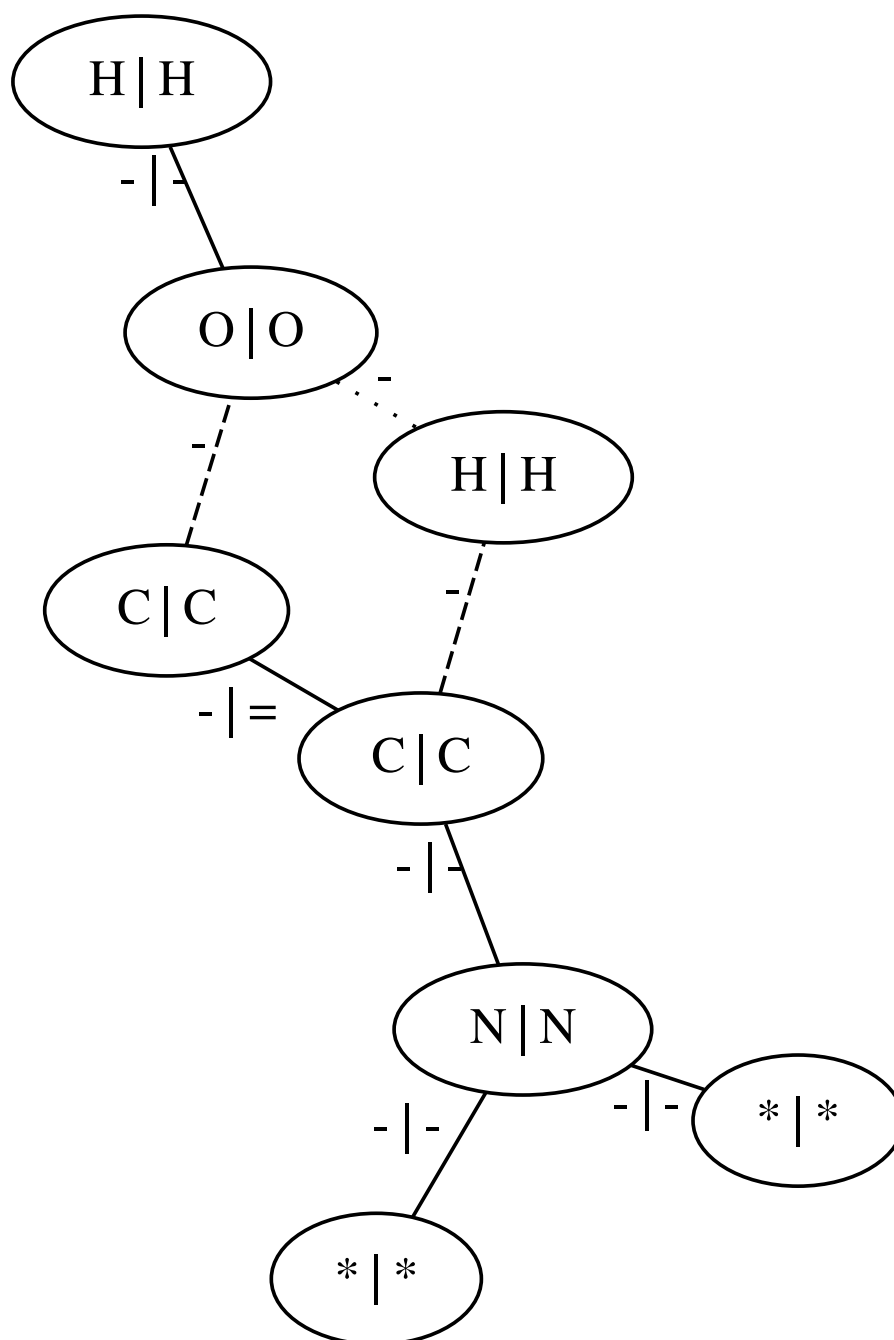
0.0.93 Dehydration of Amines



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



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



File: out/463_r_95_combined

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(7) \mid$$

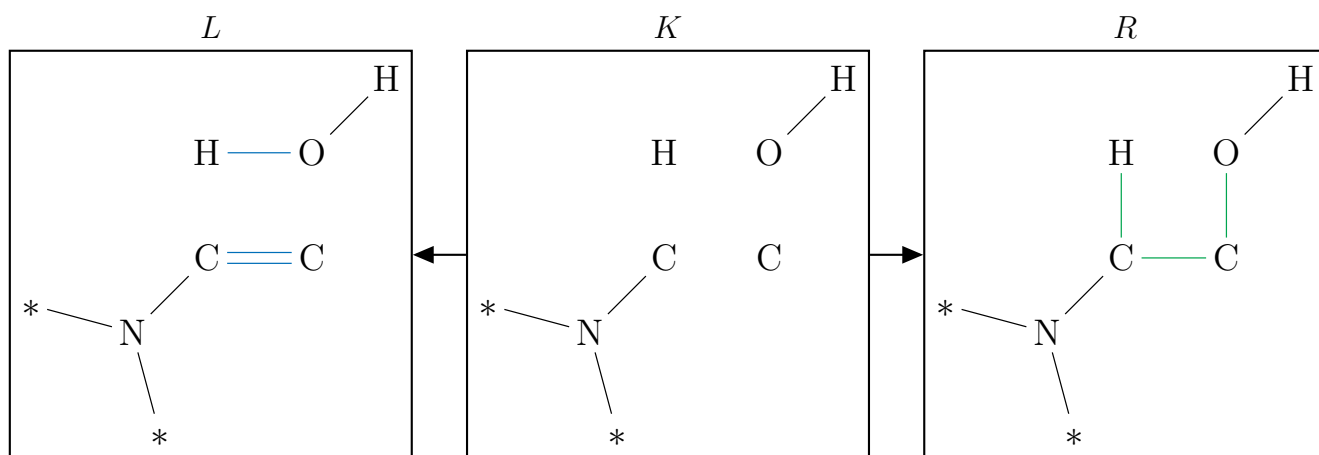
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

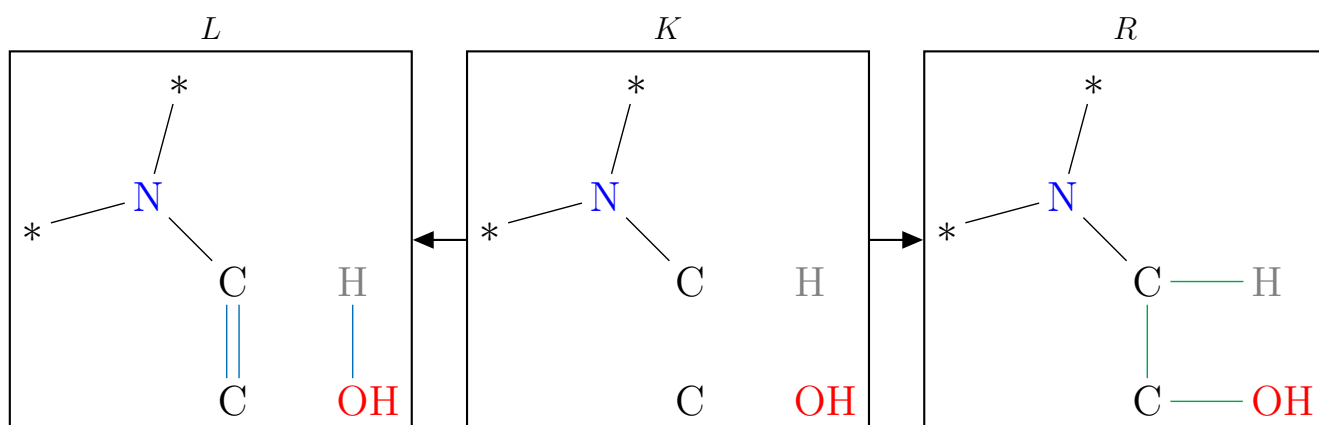
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

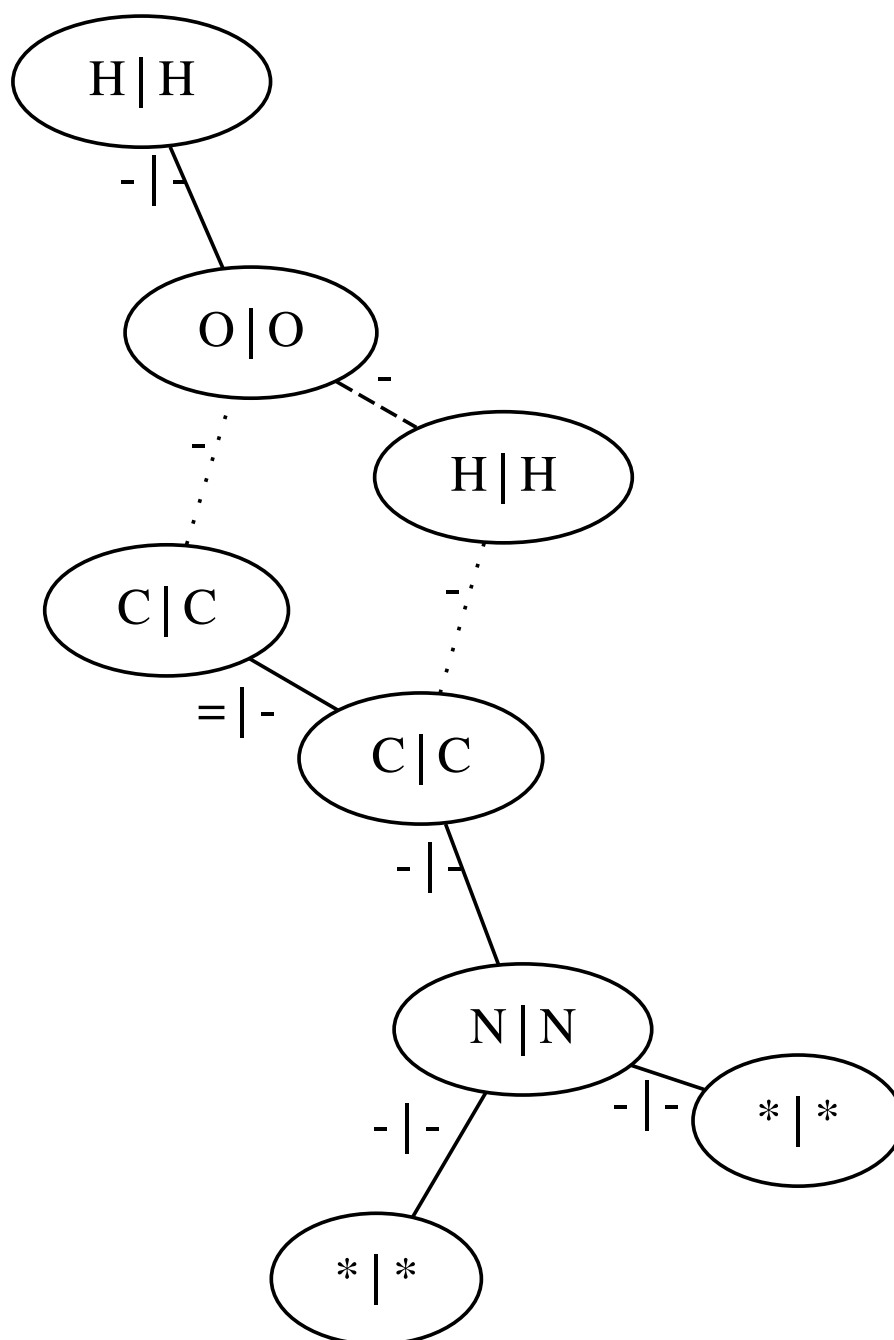
0.0.94 Deydration of Amines (inverse)



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



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



File: out/468_r_96_combined

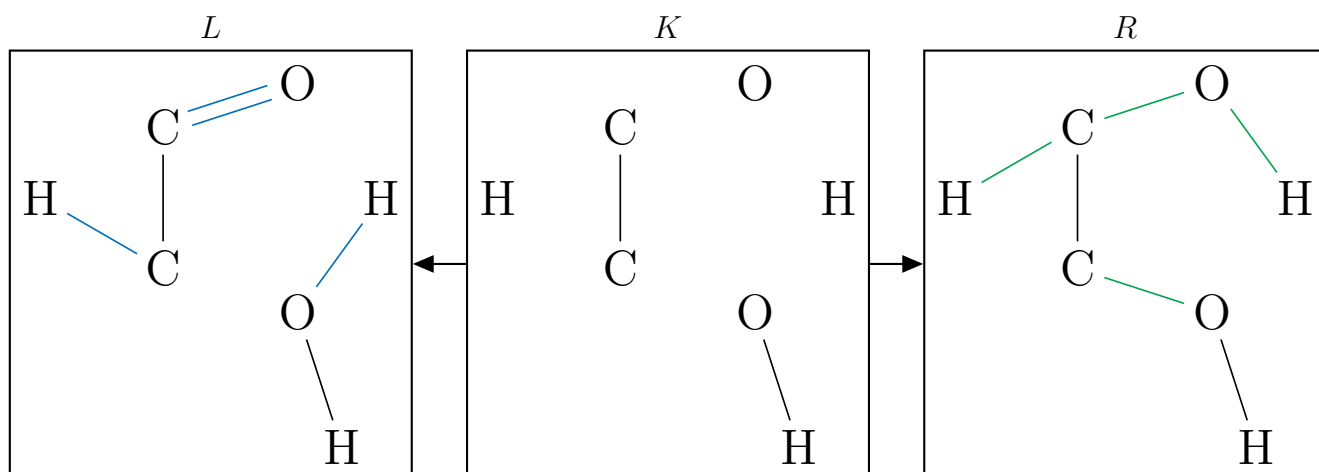
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \mid = 0
\end{aligned}$$

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

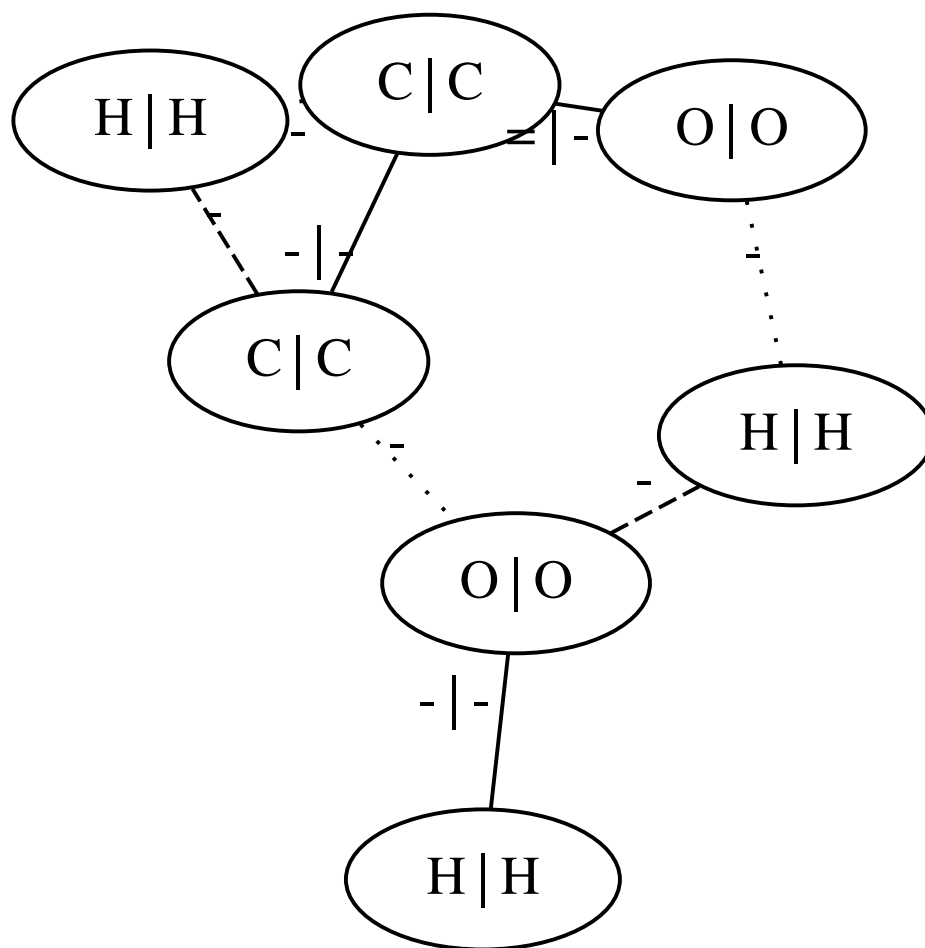
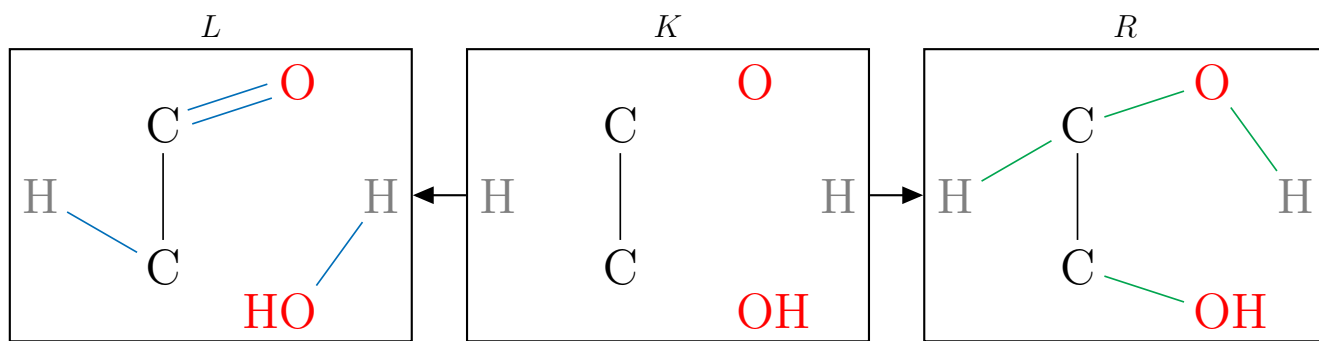
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \mid = 0
\end{aligned}$$

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

0.0.95 Hydration of C(=O)C



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



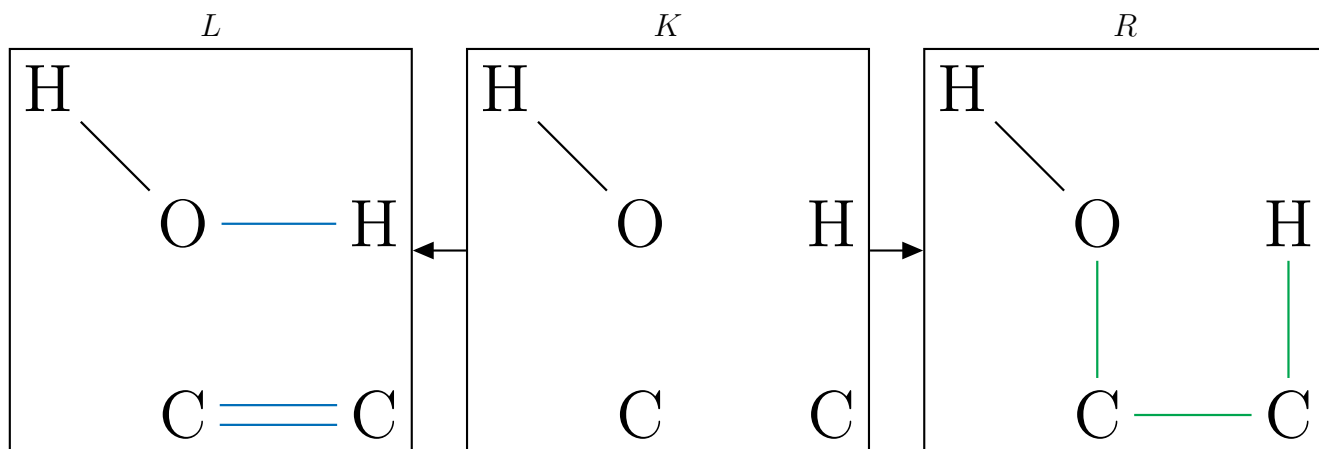
File: out/473_r_97_combined

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

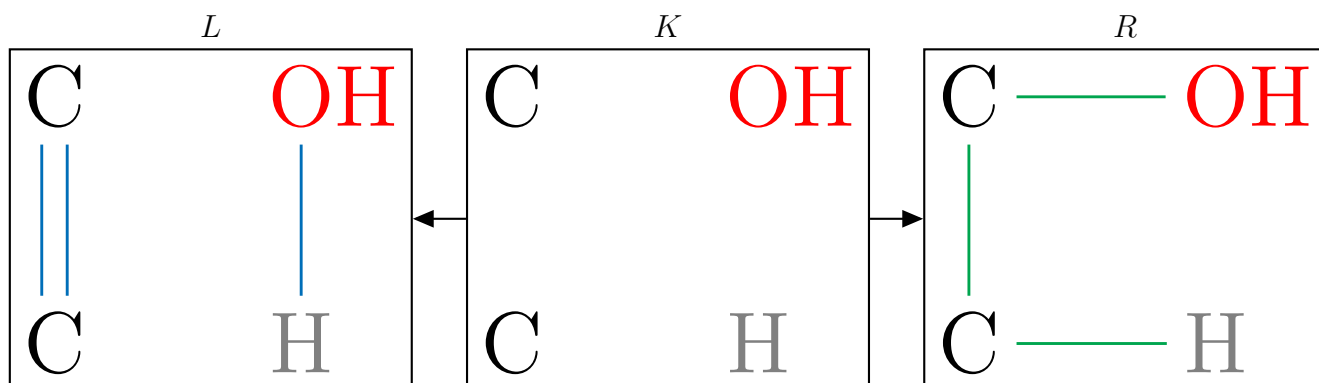
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}, \text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

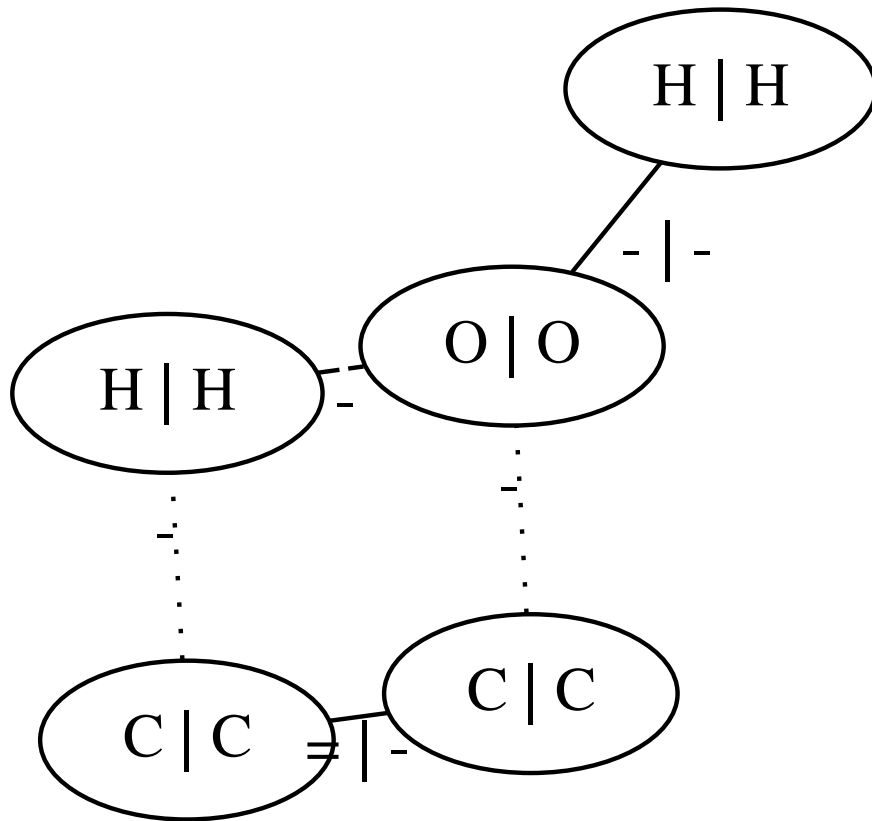
0.0.96 Hydration of C=C(O)



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



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

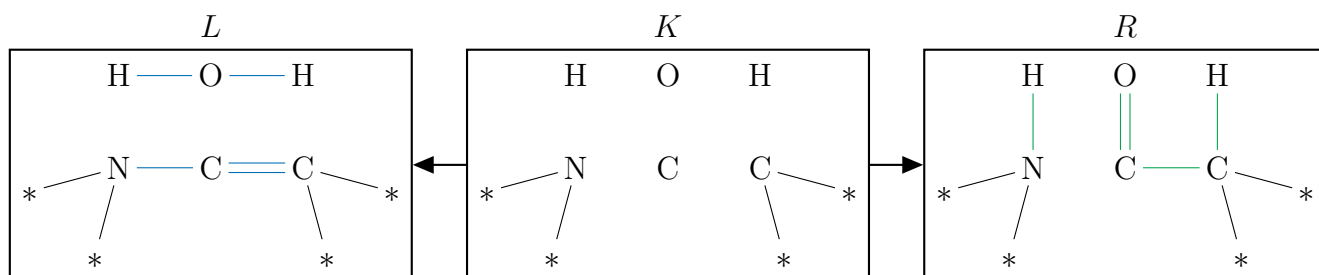


File: out/478_r_98_combined

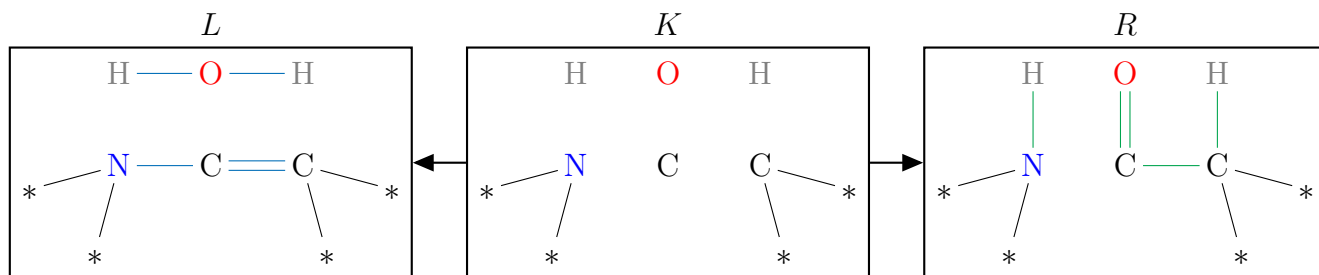
$$\begin{aligned}
 &|\{e \in \text{outEdges}(1) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
 &\} = 0
 \end{aligned}$$

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

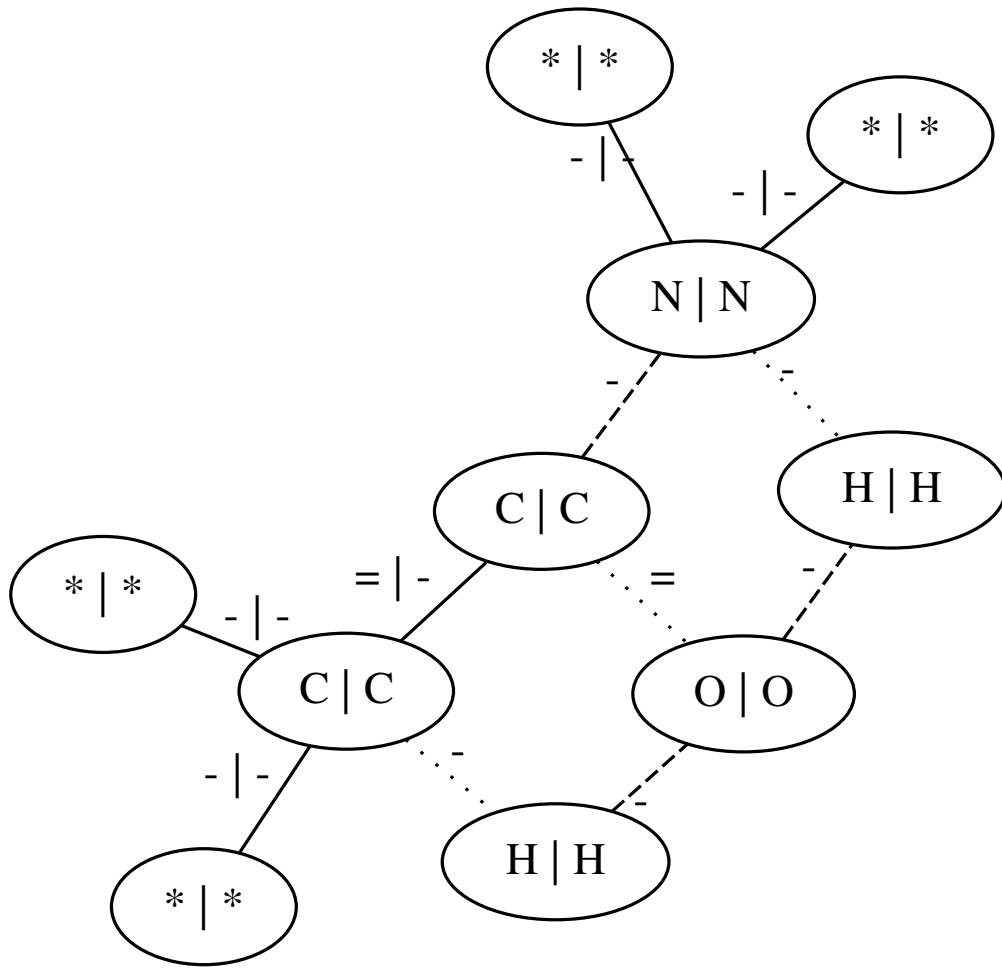
0.0.97 Enamine Hydration and Elimination



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 ∈ outEdges(3) |
  label(target(e)) ∈ {'N', 'O'}
  ∧
  label(e) ∈ {'='}
}| = 0

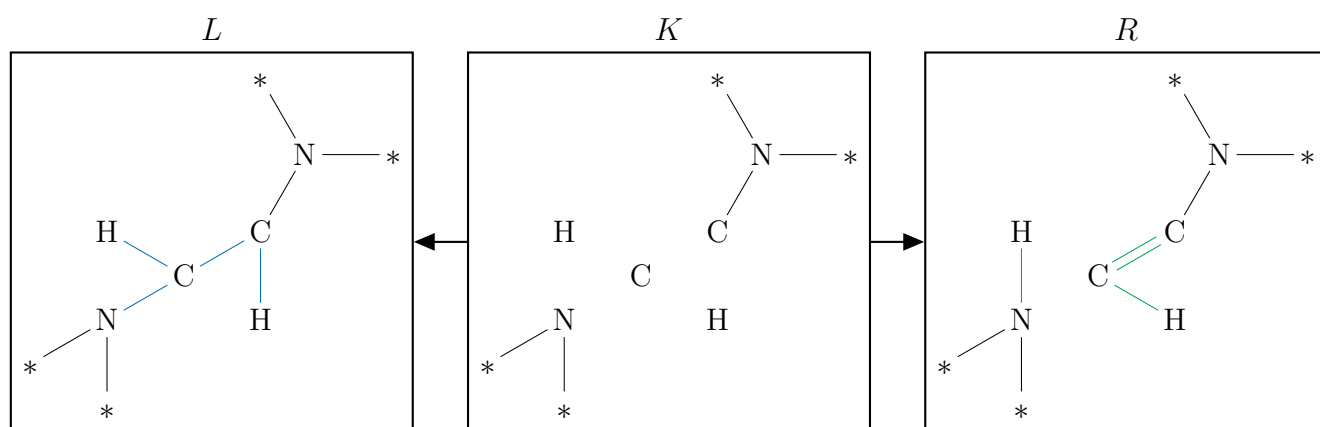
```

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

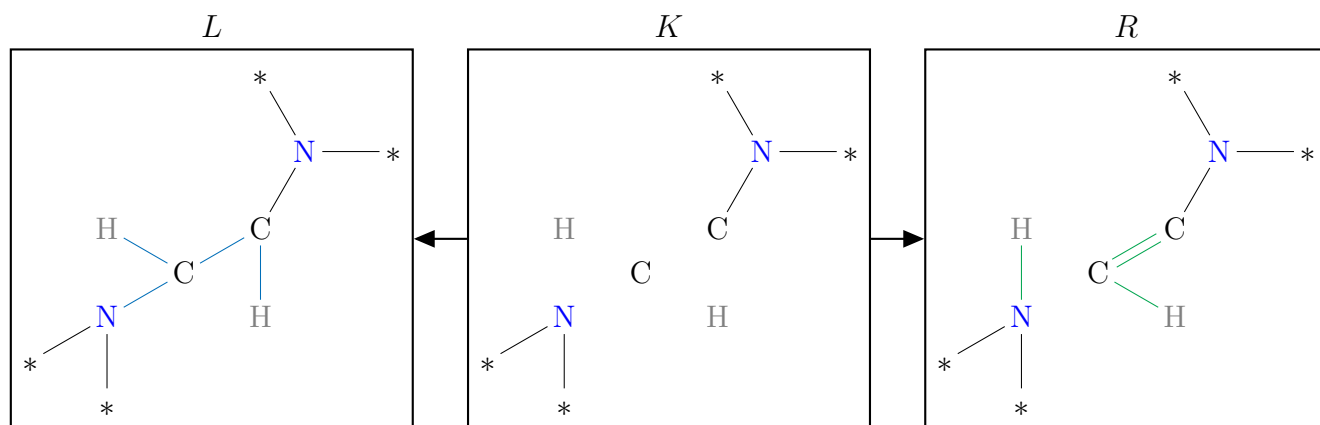
$$\begin{aligned}
 &|\{e \in \text{outEdges}(8) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}\}\} = 0
 \end{aligned}$$

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

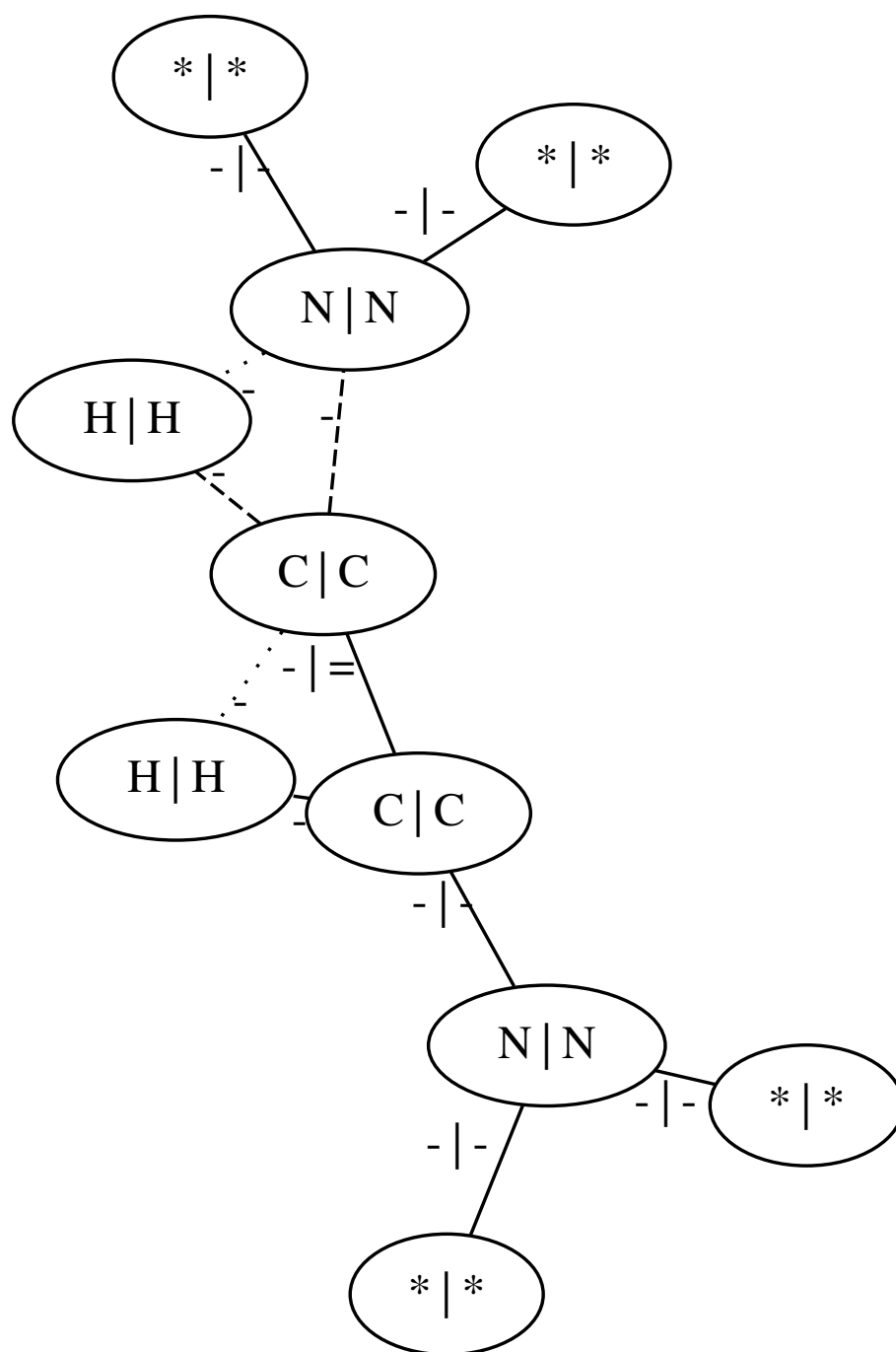
0.0.98 Deamination of Vicinal Diamine



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



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



File: out/488_r_100_combined

$$|\{e \in \text{outEdges}(3) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(4) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(8) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(9) \mid$$

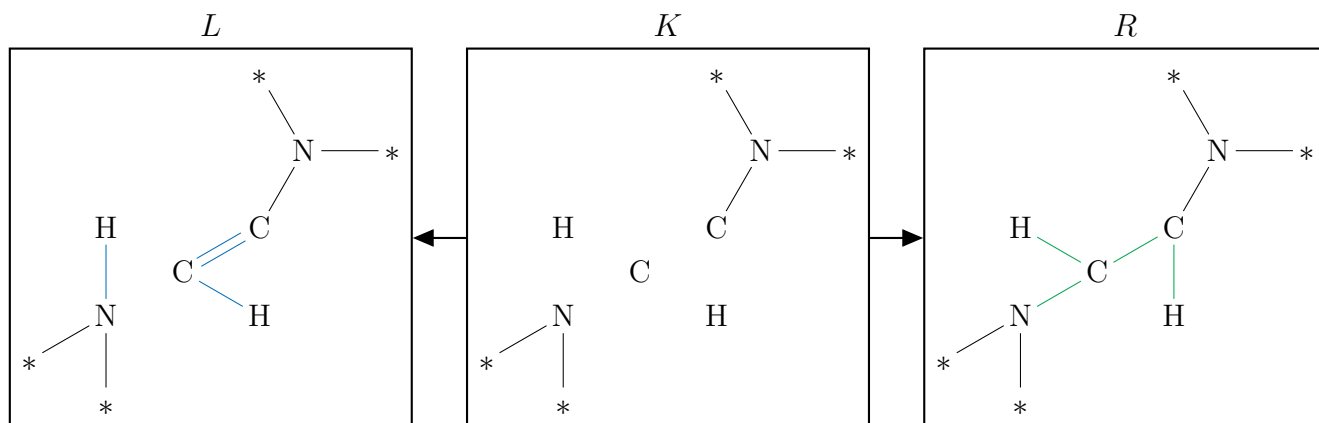
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

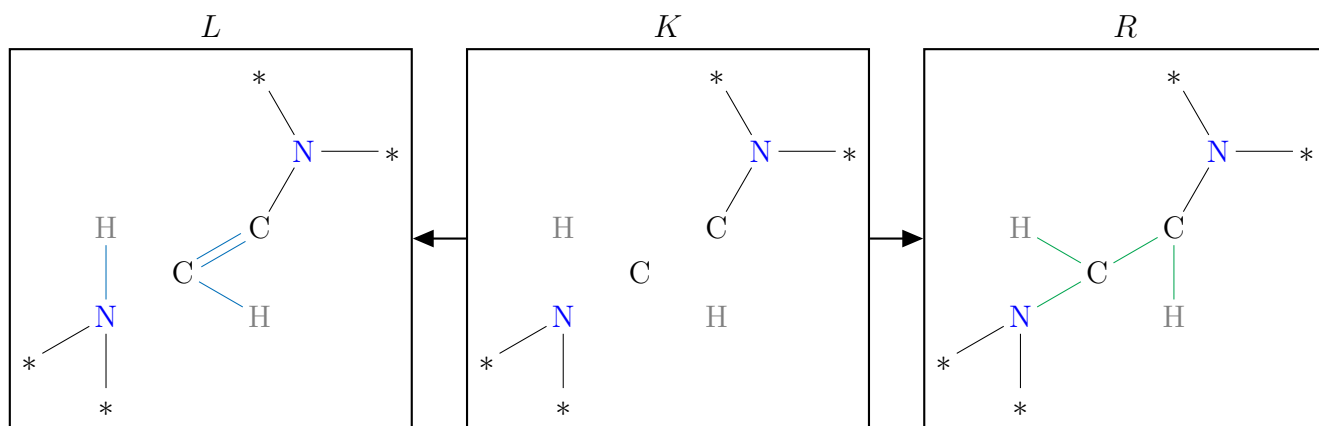
$$\text{label}(e) \in \{\text{'='}\}$$

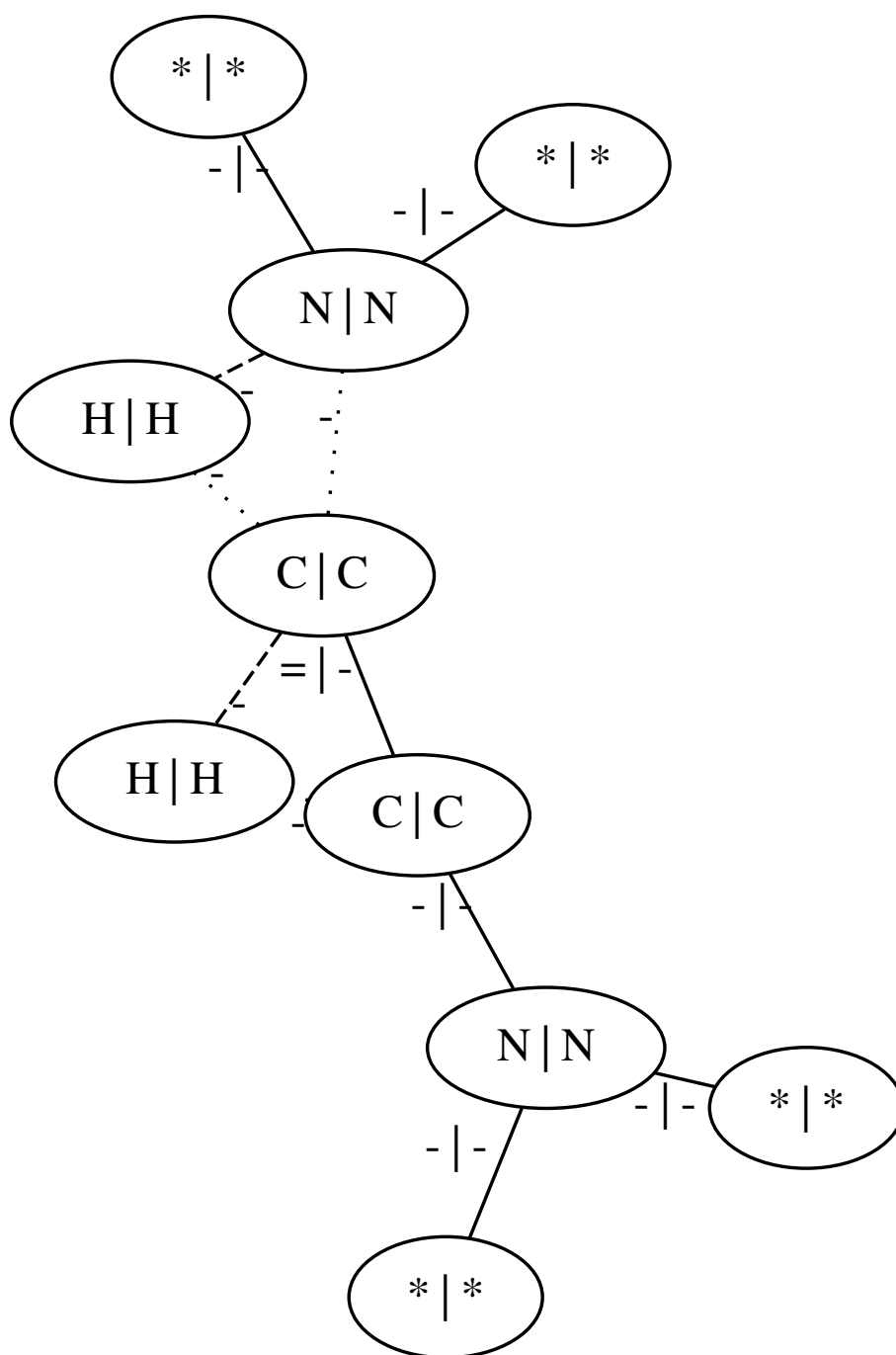
$$\}| = 0$$

0.0.99 Deamination of Vicinal Diamine, (inverse)



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





File: out/493_r_101_combined

$$|\{e \in \text{outEdges}(3) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(4) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(8) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(9) \mid$$

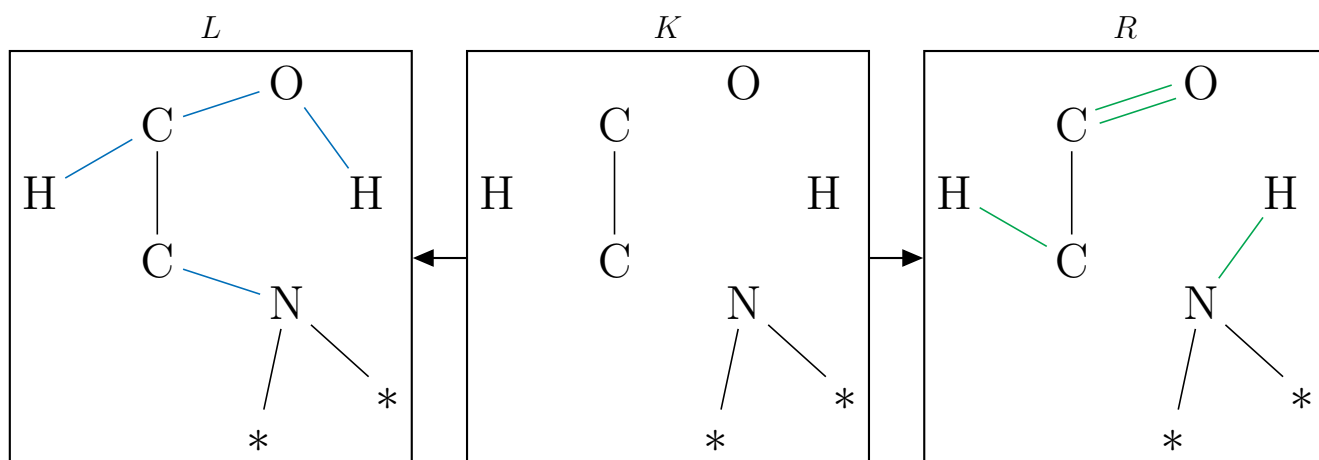
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

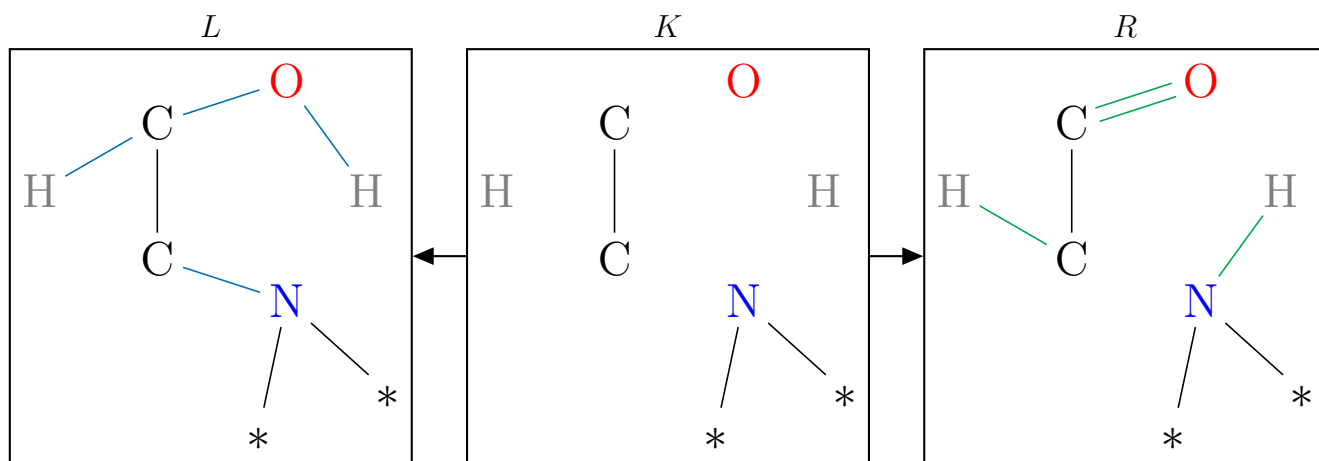
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

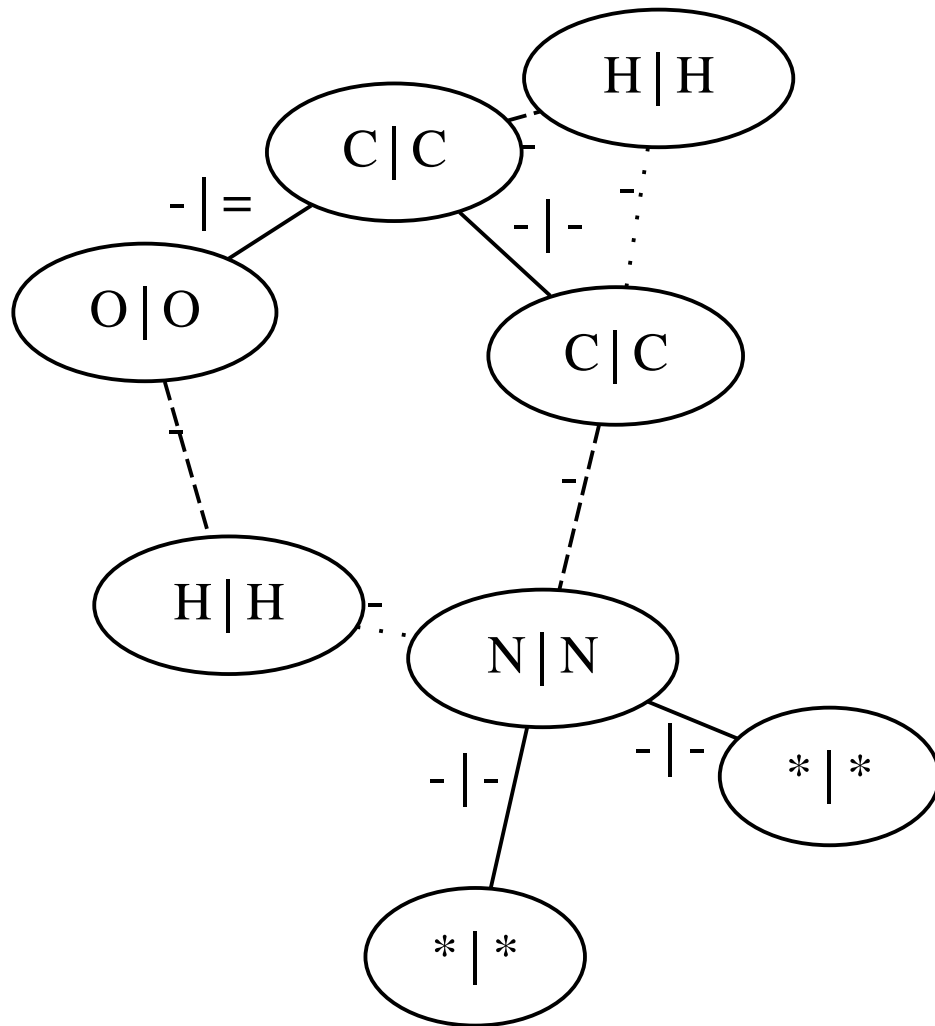
0.0.100 Deamination 2



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



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



File: out/498_r_102_combined

```

|{e ∈ outEdges(6) |
  label(target(e)) ∈ {'N', 'O'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

$$|\{e \in \text{outEdges}(7) \mid$$

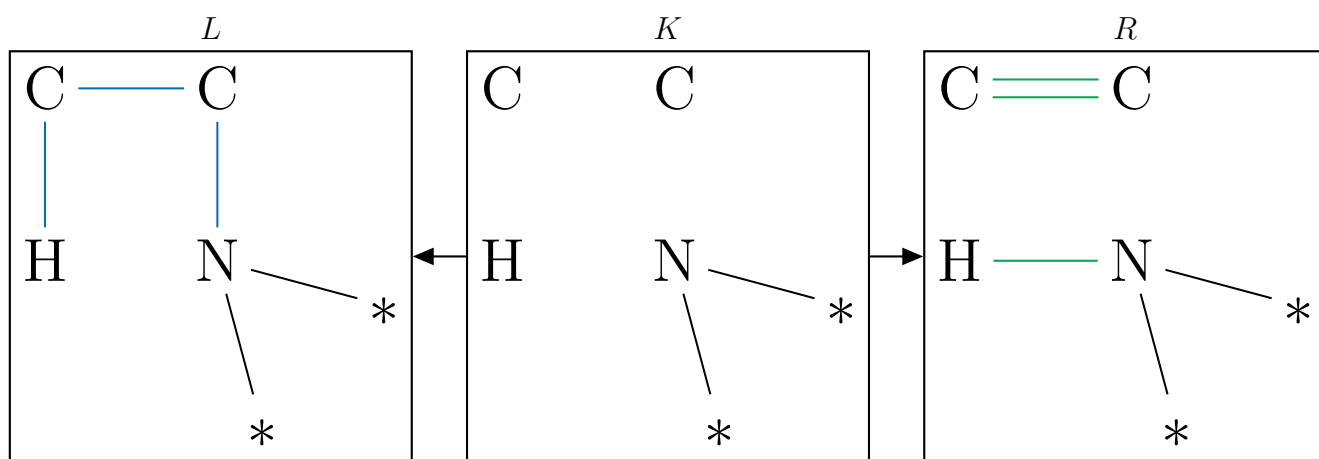
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\}$$

$$\wedge$$

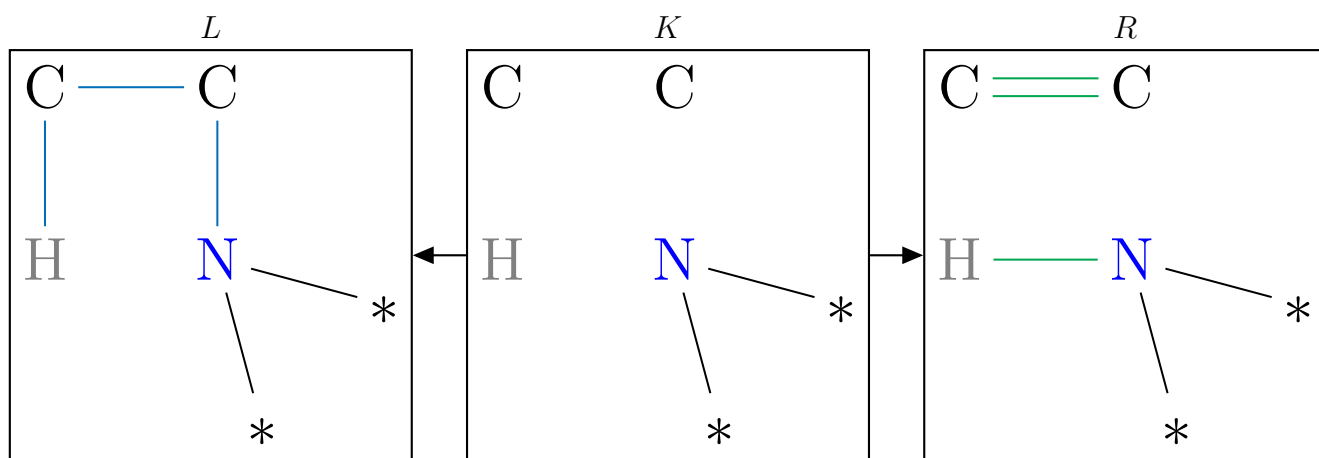
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

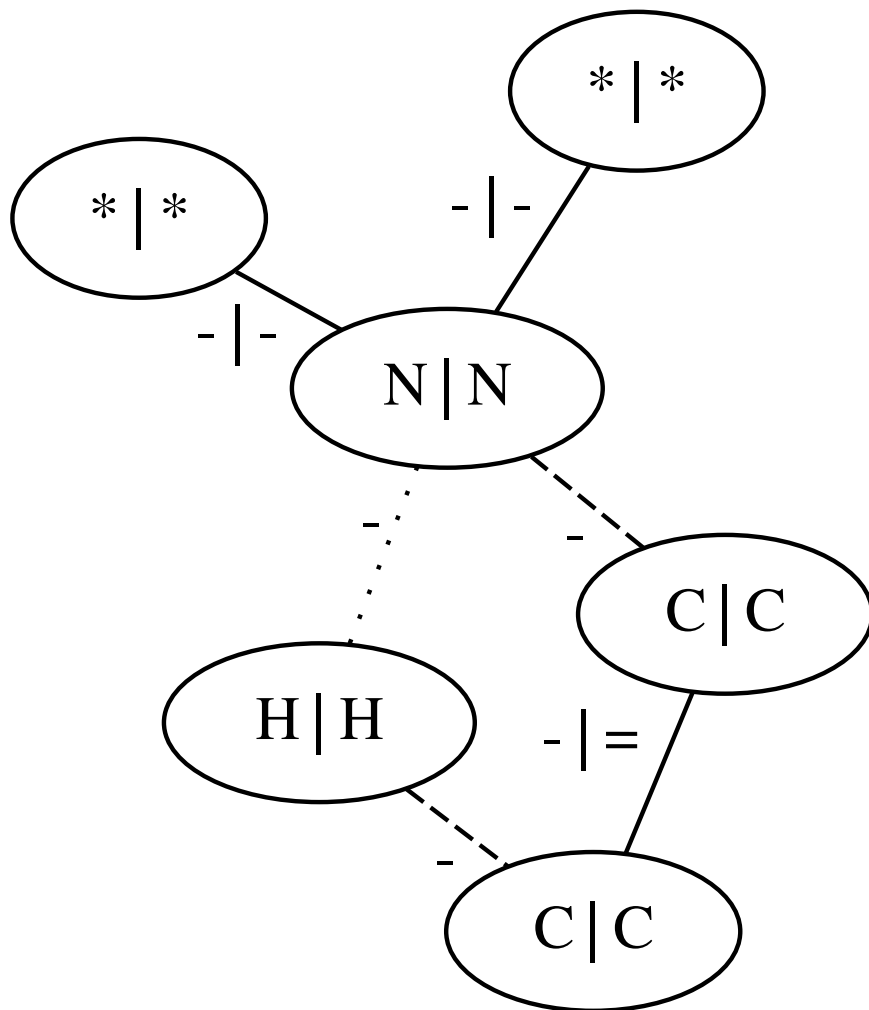
0.0.101 Deamination 3



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



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



File: out/503_r_103_combined

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

$$|\{e \in \text{outEdges}(2) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}, \text{'-'}\}$$

$$\}| = 1$$

$$|\{e \in \text{outEdges}(4) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

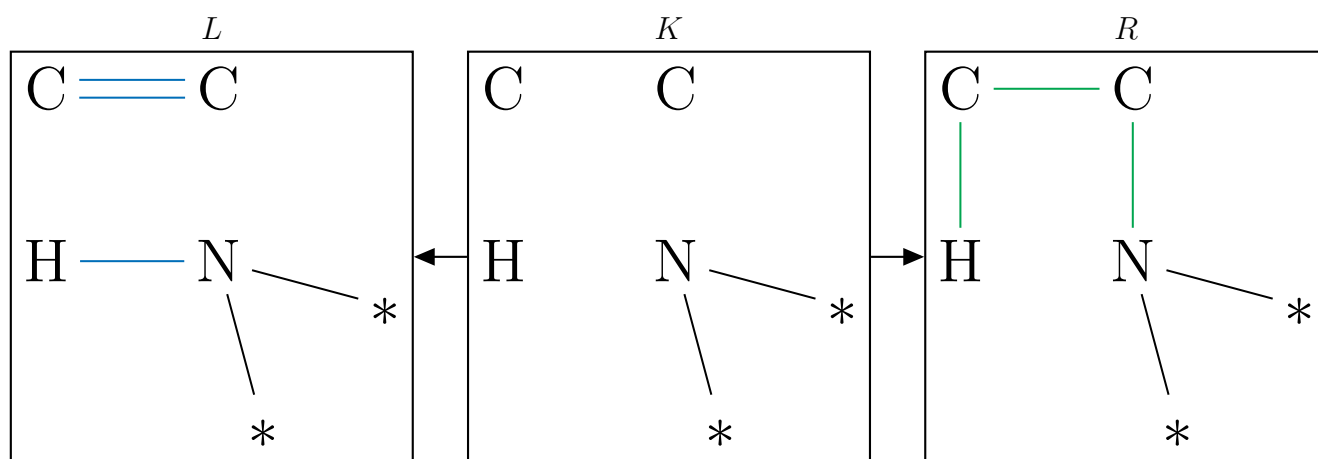
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

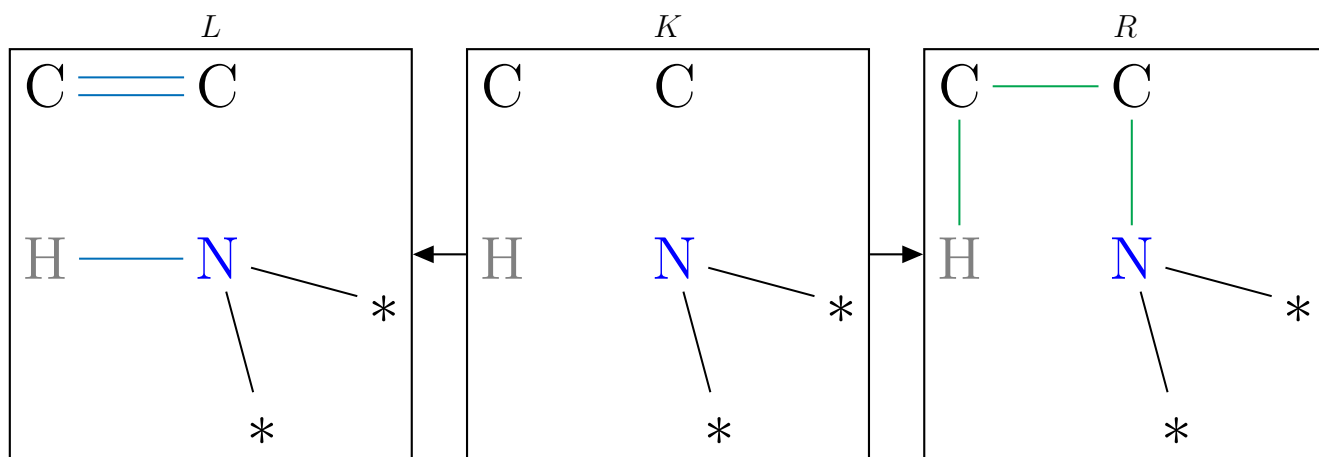
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

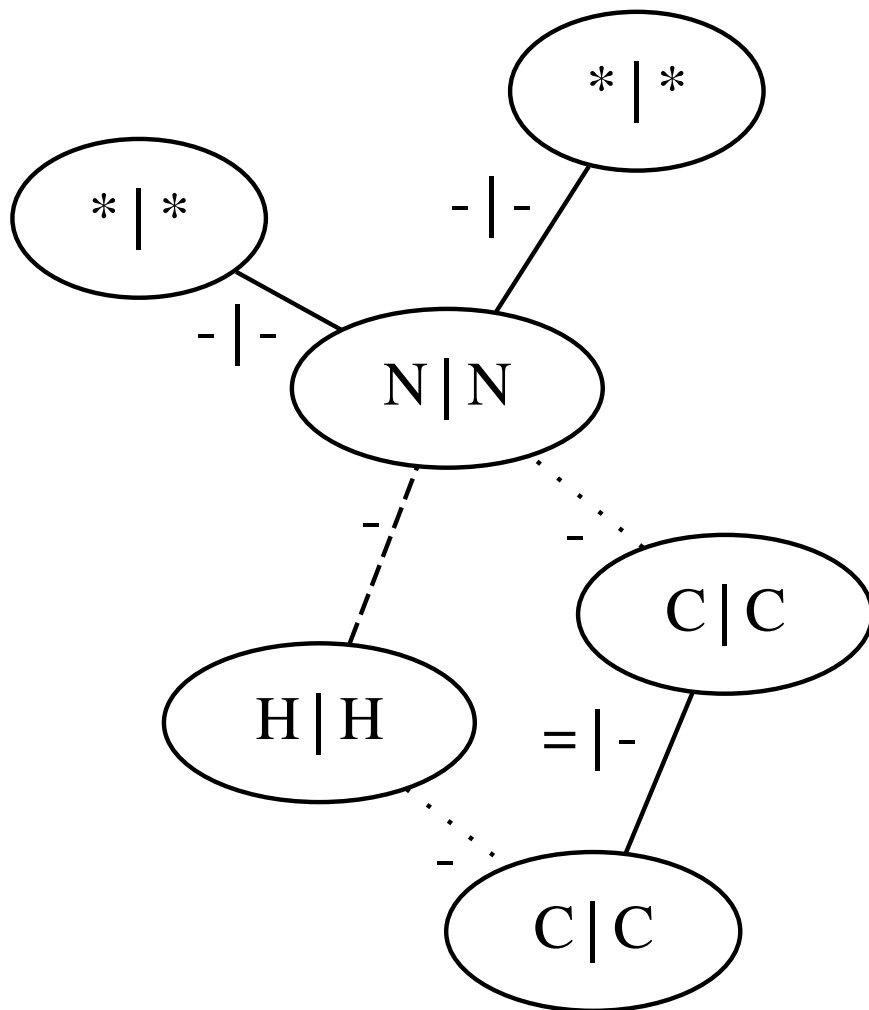
0.0.102 Deamination 3 (inverse)



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



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



File: out/508_r_104_combined

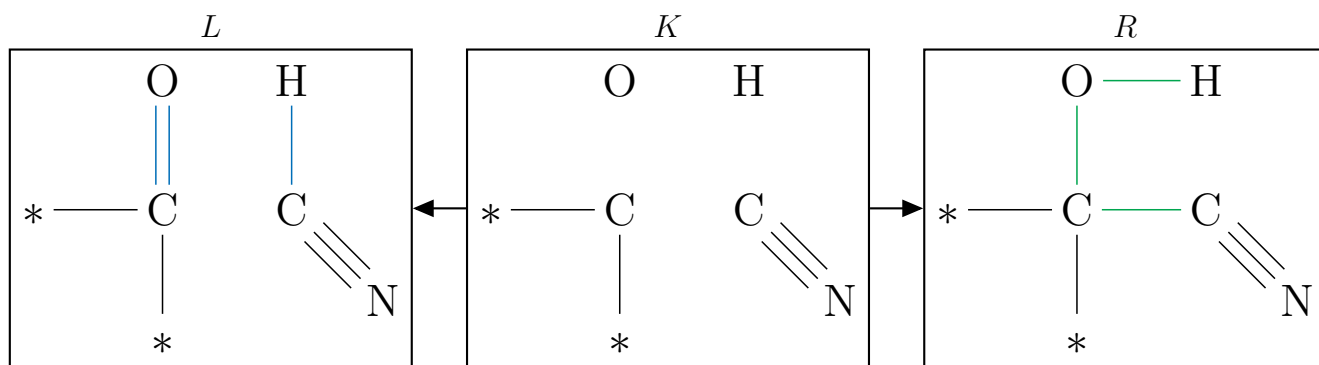
$$\begin{aligned}
 &|\{e \in \text{outEdges}(1) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
 &\quad \} = 0
 \end{aligned}$$

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

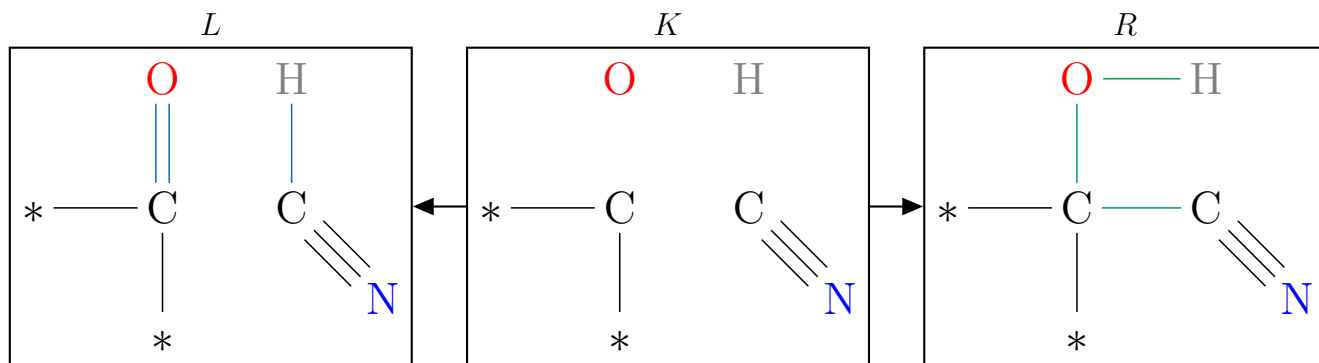
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\} = 0
\end{aligned}$$

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

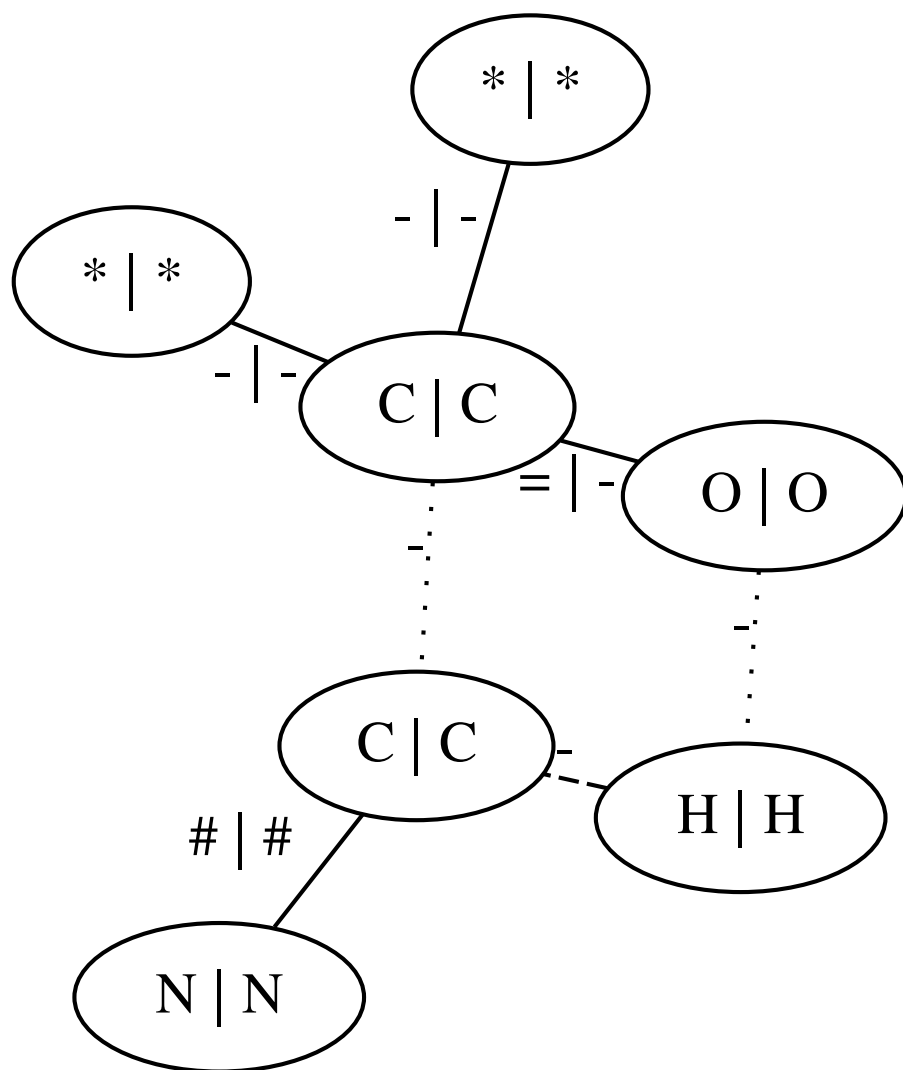
0.0.103 Cyanohydrin Formation



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



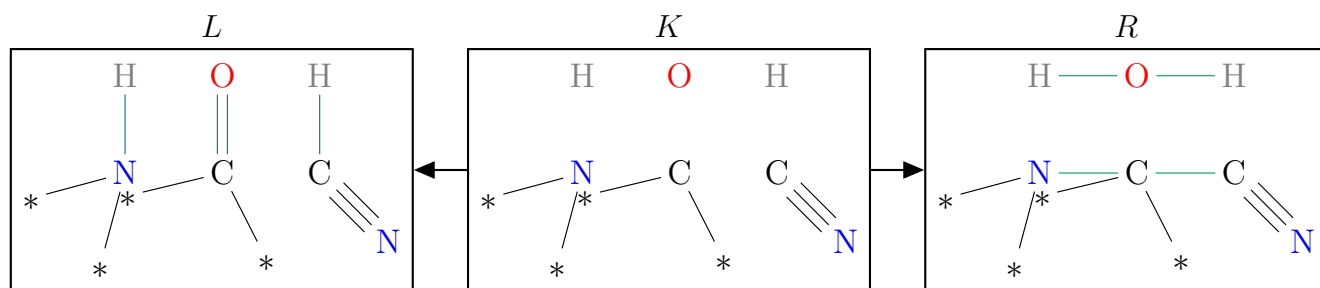
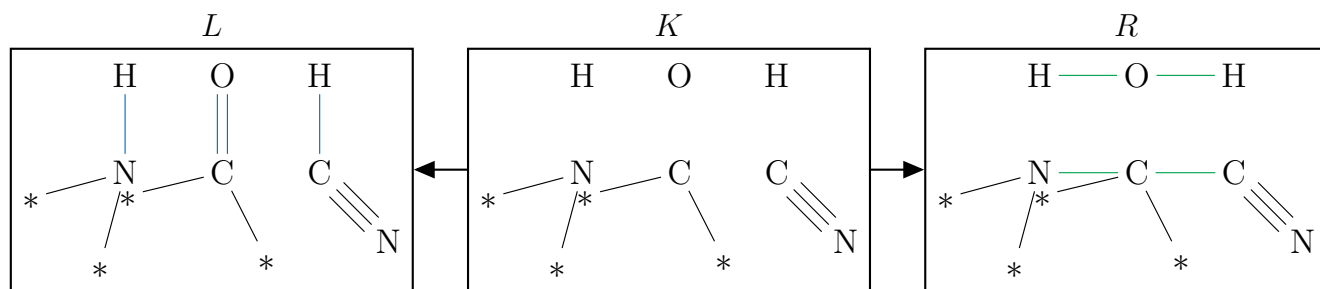
Files: out/512_r_105_11300100_{L, K, R}

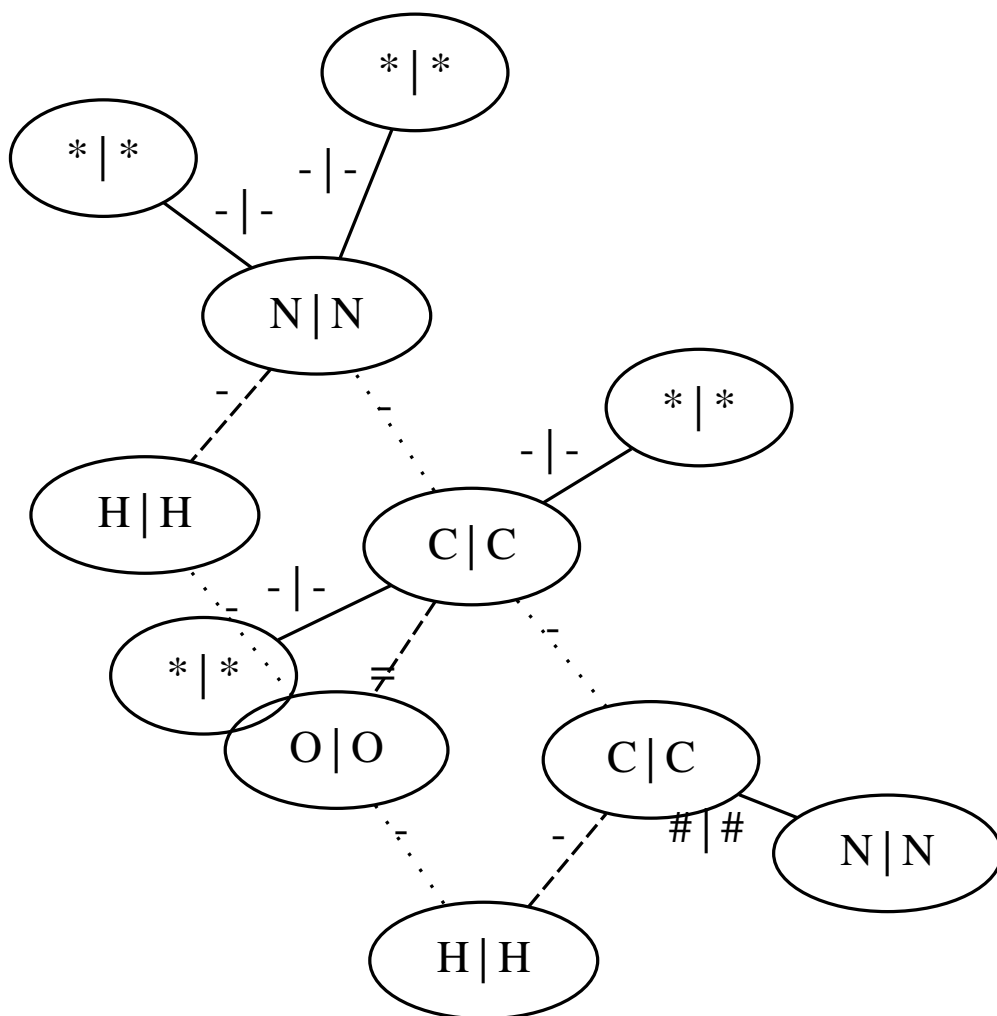


File: out/513_r_105_combined

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

0.0.104 Strecker Synthesis





File: out/517_r_106_combined

```

|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

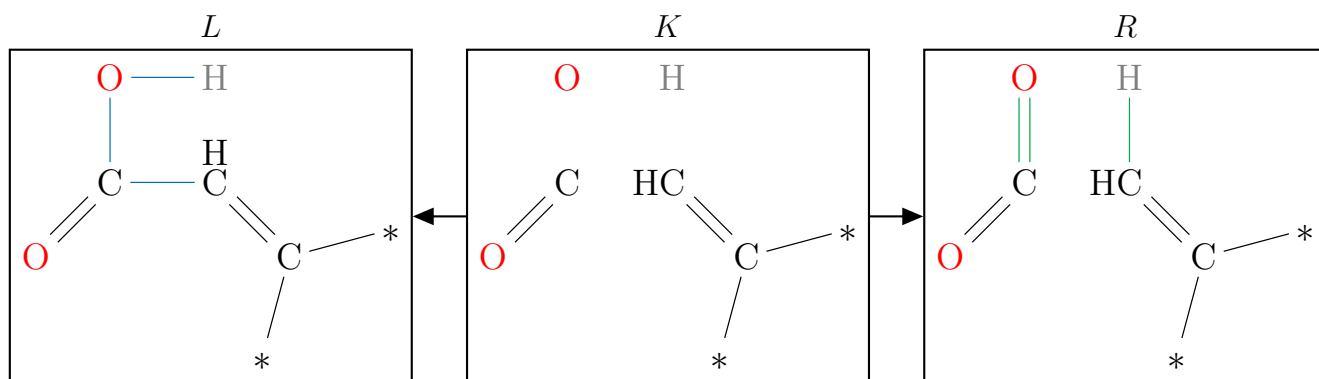
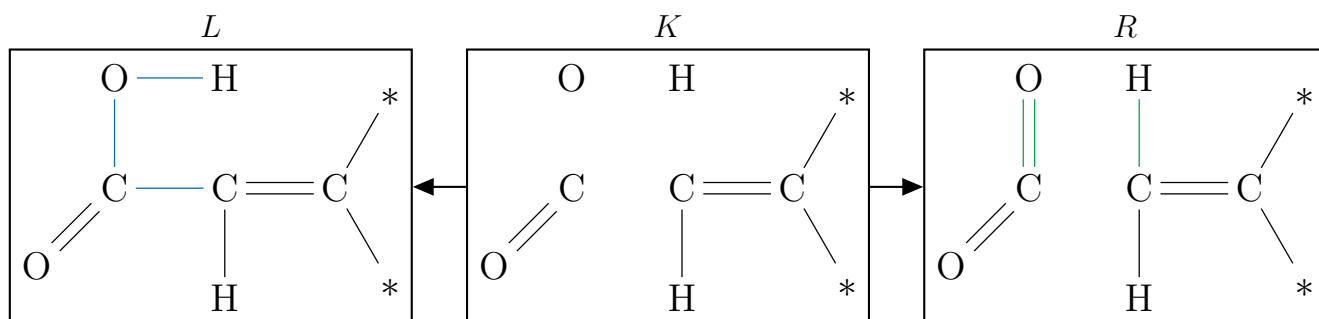
```

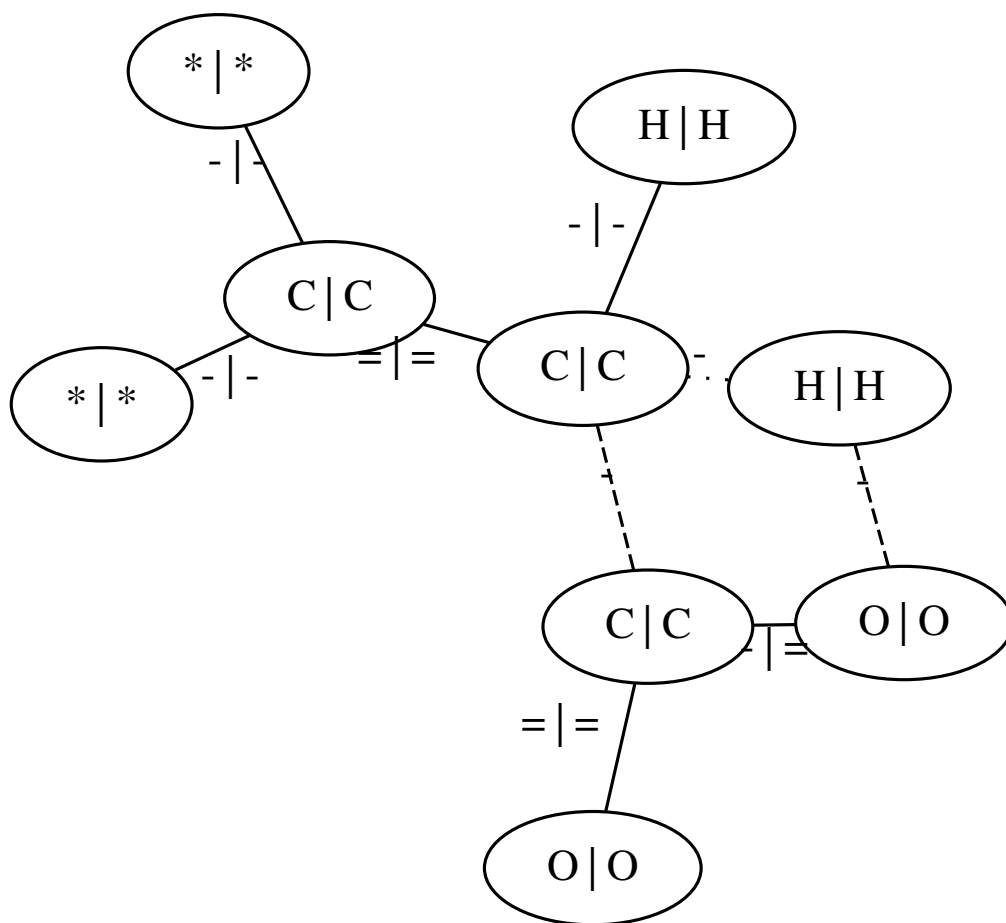
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

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

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

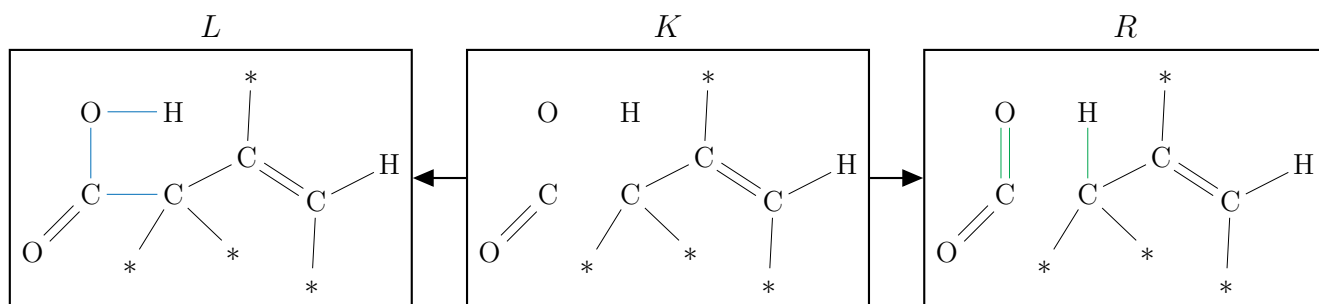
0.0.105 Alpha-Beta Unsaturated Acid Decarboxylation



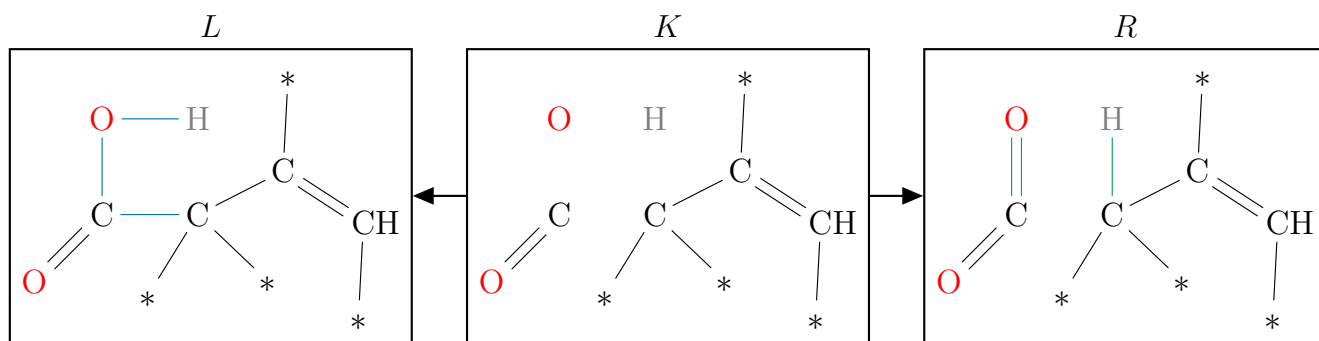


File: out/522_r_107_combined

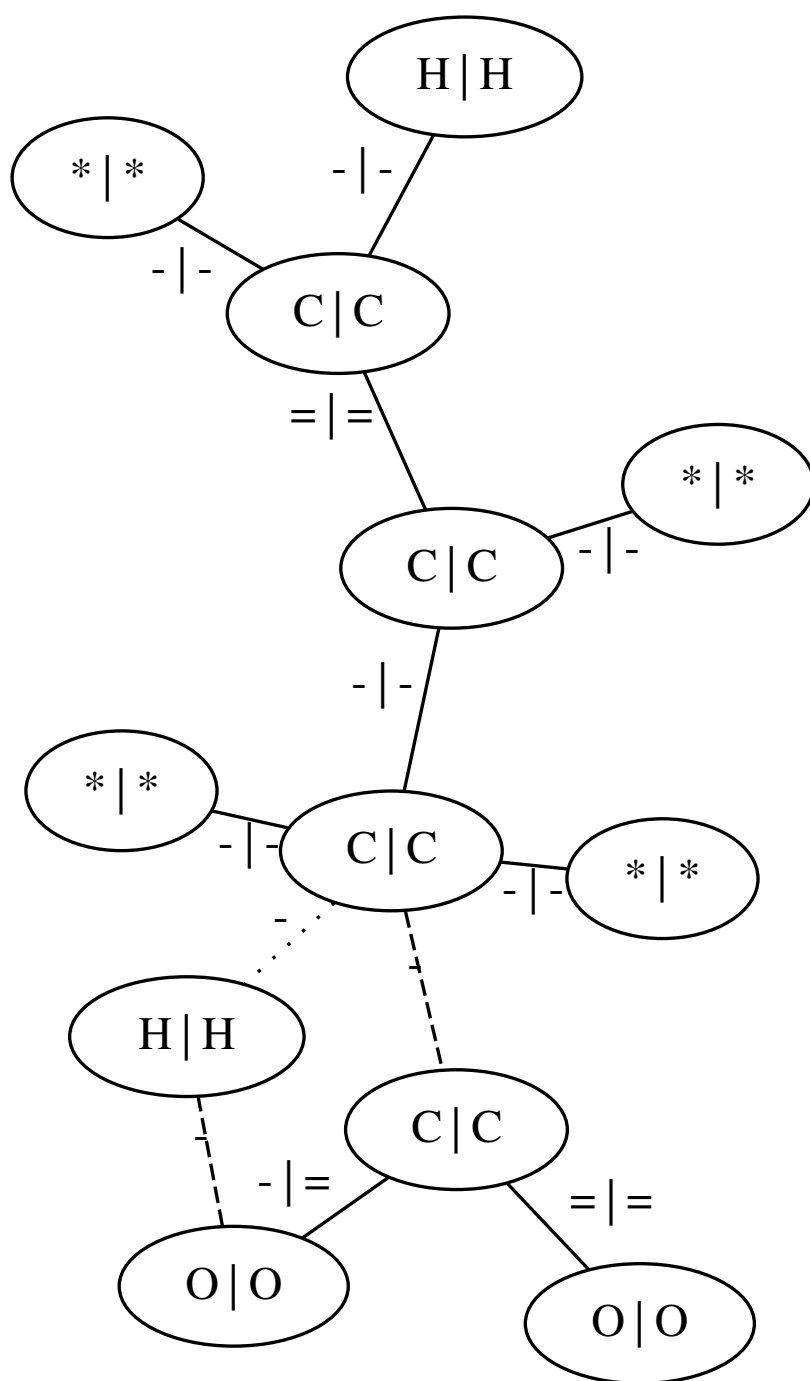
0.0.106 Beta-gamma Unsaturated Acid Decarboxylation



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

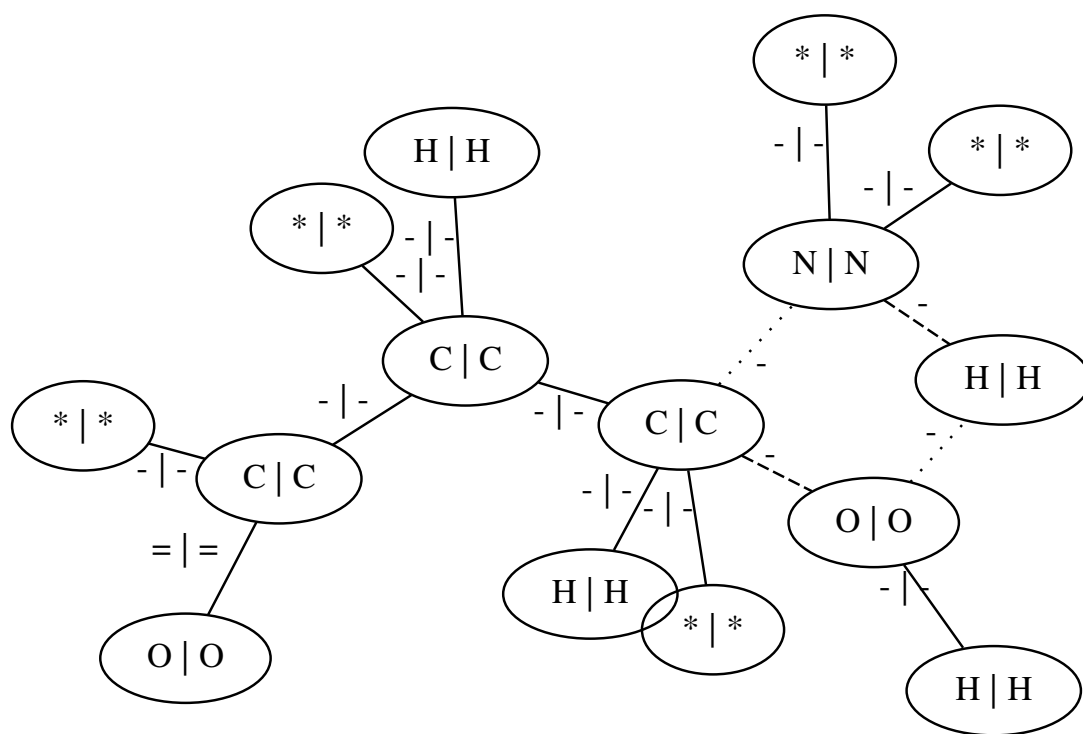
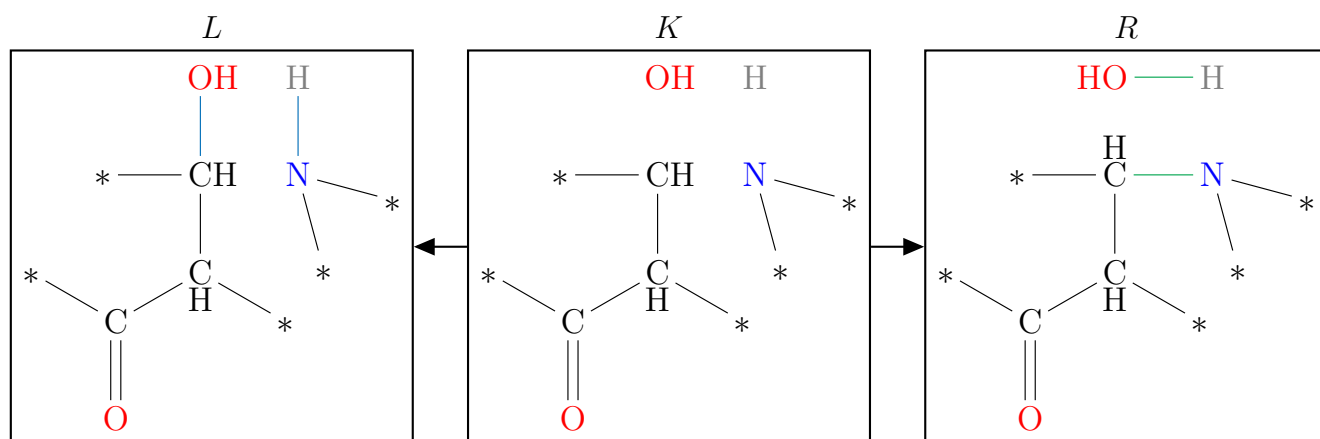
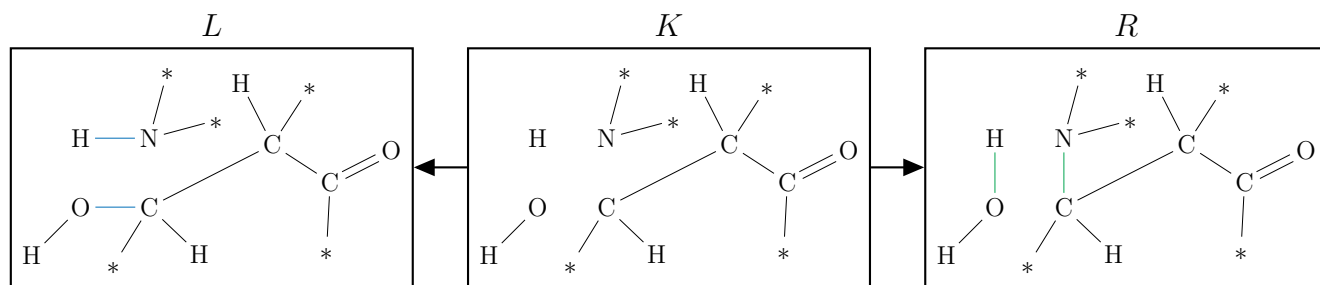


Files: out/526_r_108_11300100_{L, K, R}



File: out/527_r_108_combined

0.0.107 Mannich Addition



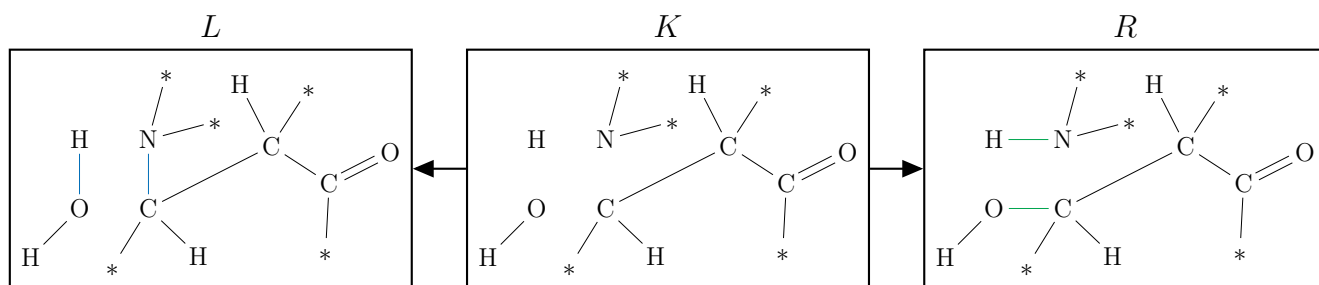
$$\begin{aligned}
 &|\{e \in \text{outEdges}(12) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\quad \}| = 1
 \end{aligned}$$

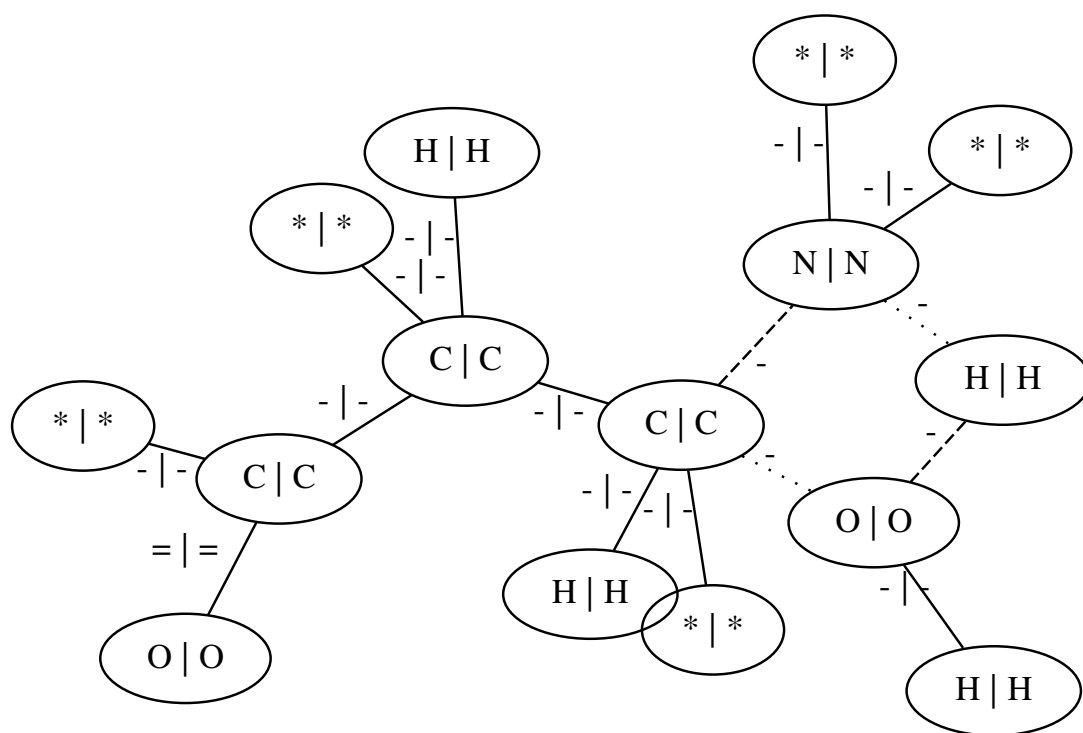
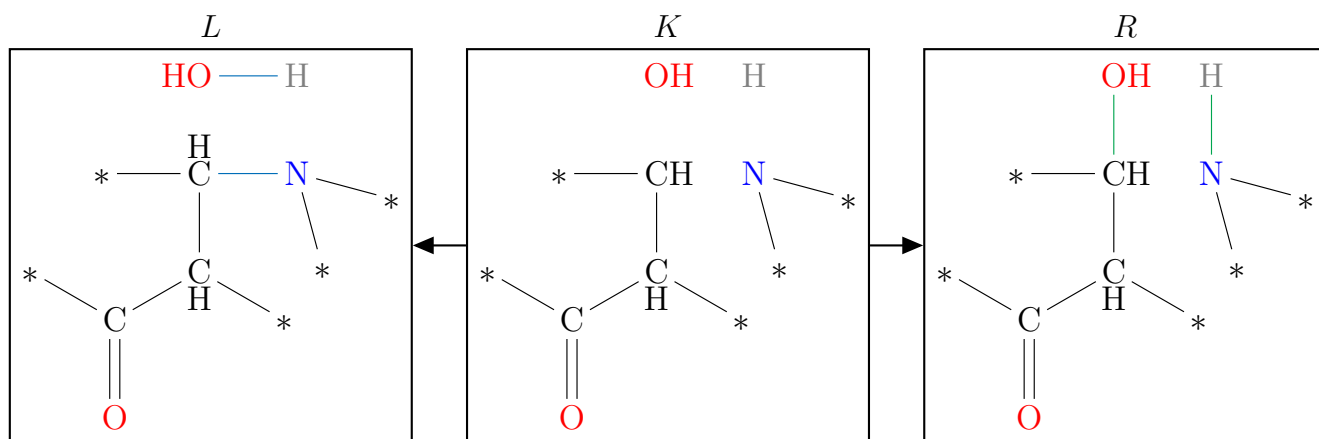
$$\begin{aligned}
 &|\{e \in \text{outEdges}(12) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}\} \\
 &\quad \}| = 0
 \end{aligned}$$

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

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

0.0.108 Mannich Addition (reverse)





File: out/537_r_110_combined

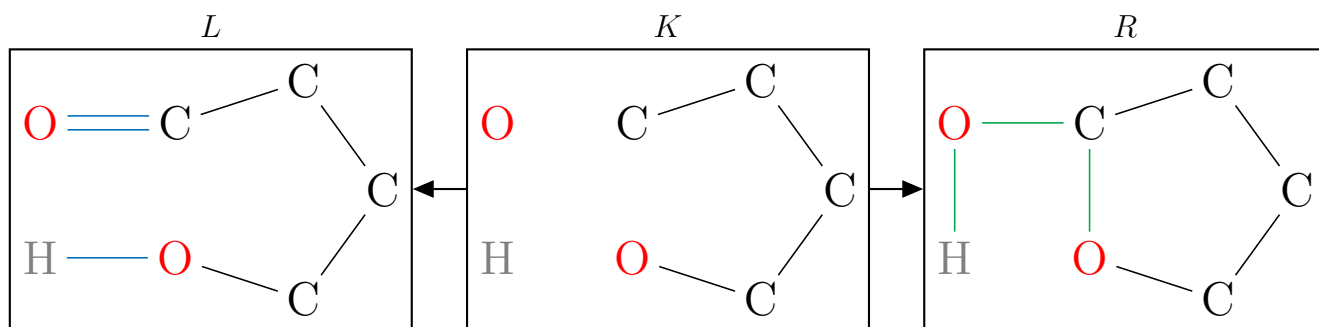
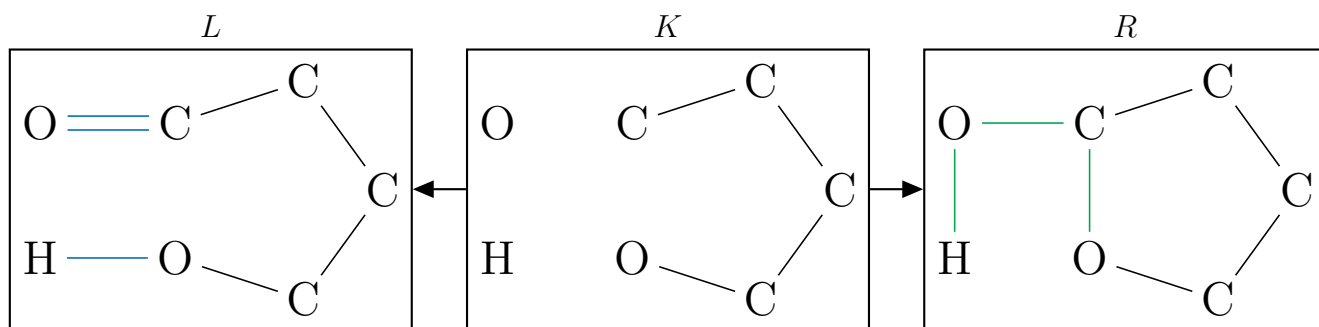
$$\begin{aligned}
 &|\{e \in \text{outEdges}(12) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\quad \}| = 1
 \end{aligned}$$

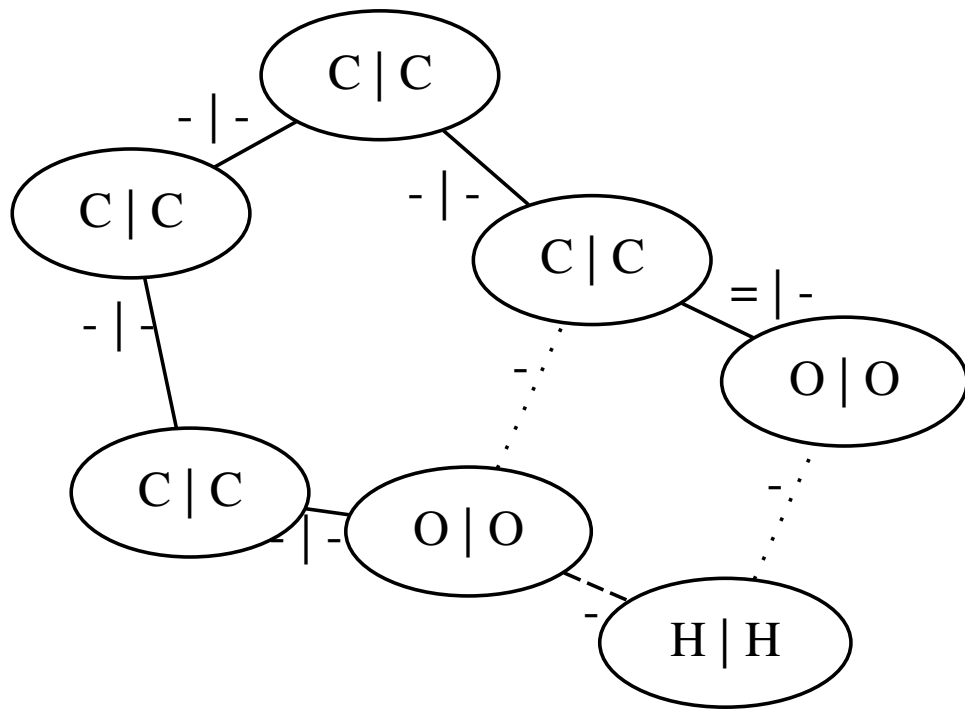
$$\begin{aligned}
& |\{e \in \text{outEdges}(12) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

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

0.0.109 Hemiacetal Formation for 5 membered rings

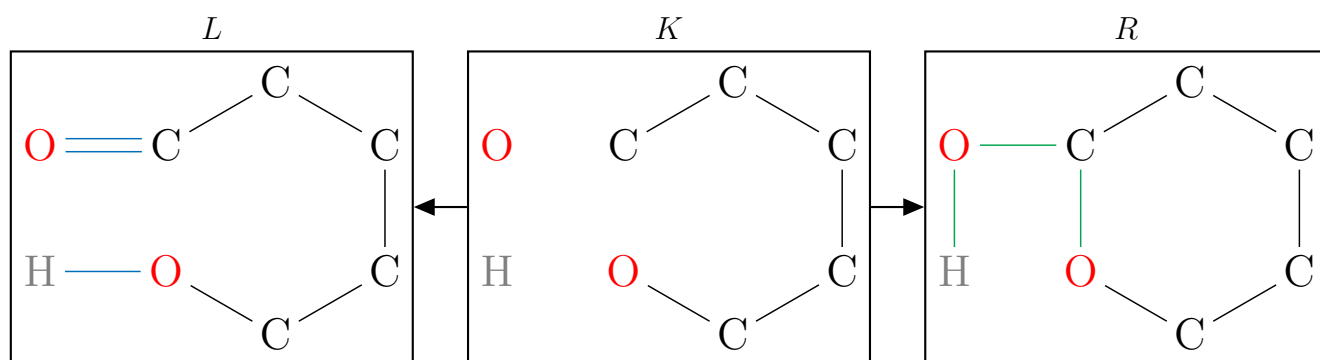
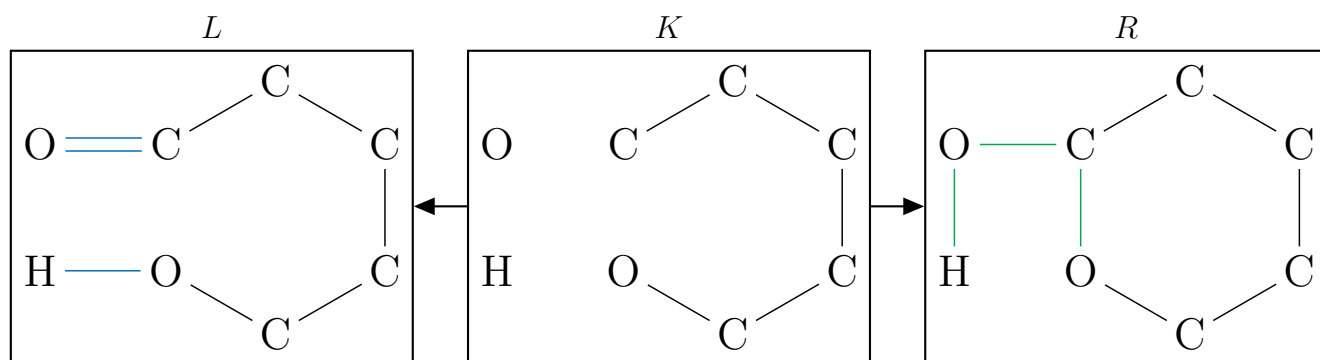


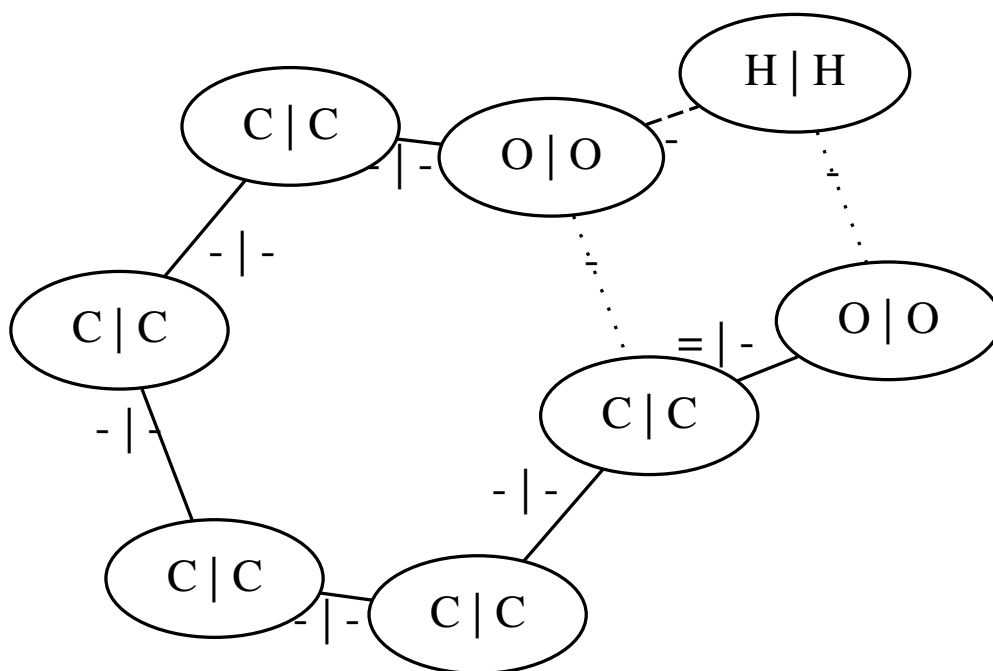


File: out/542_r_111_combined

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

0.0.110 Hemiacetal Formation for 6 membered rings

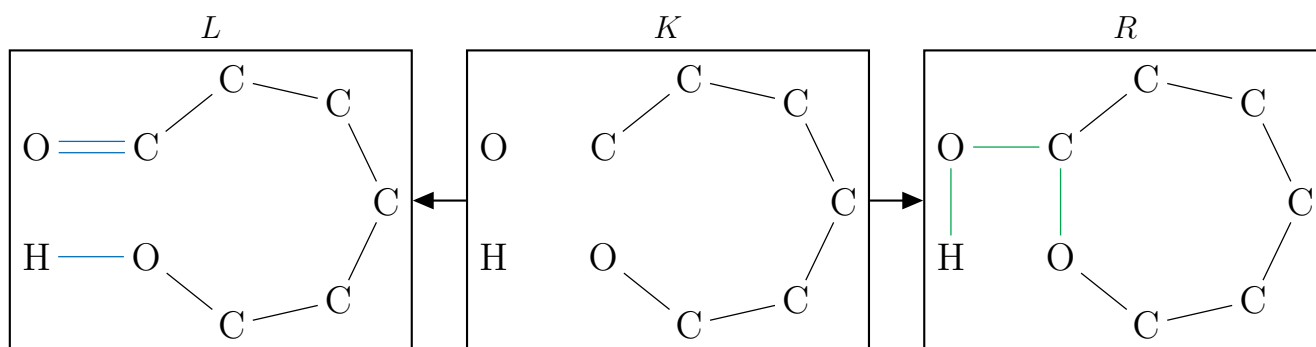




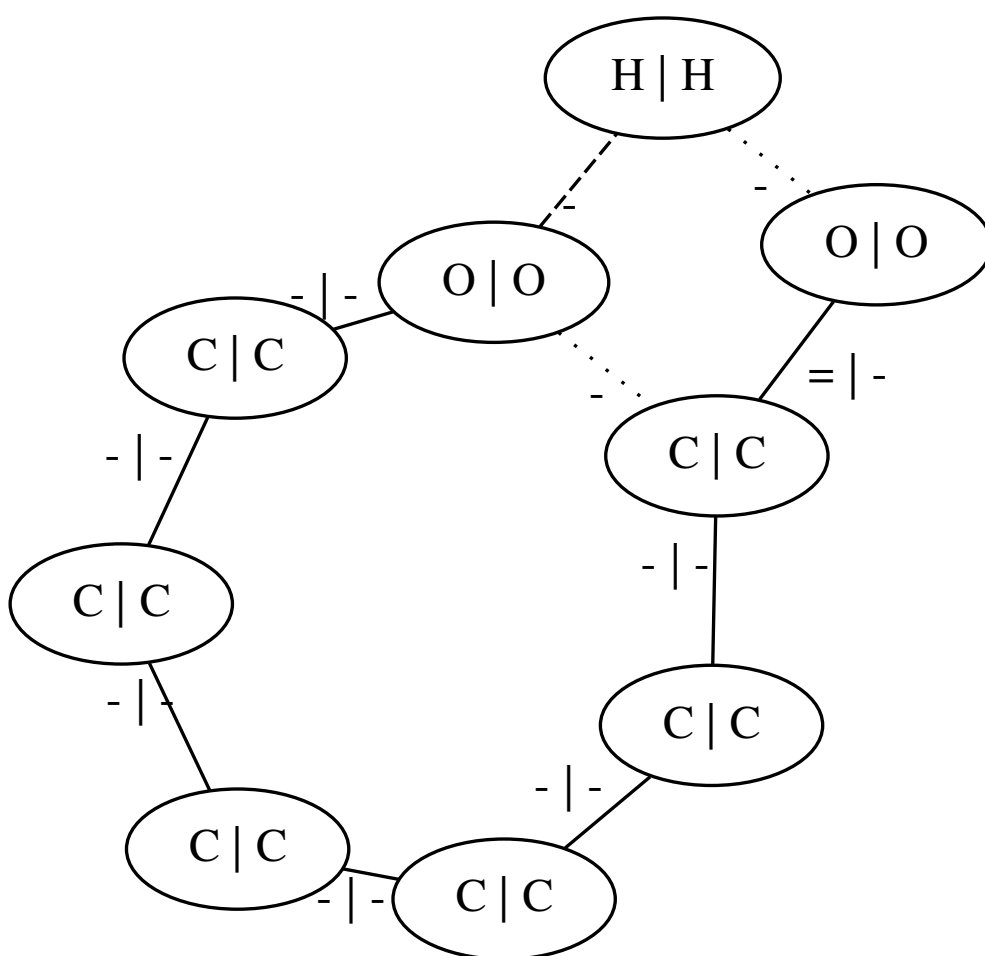
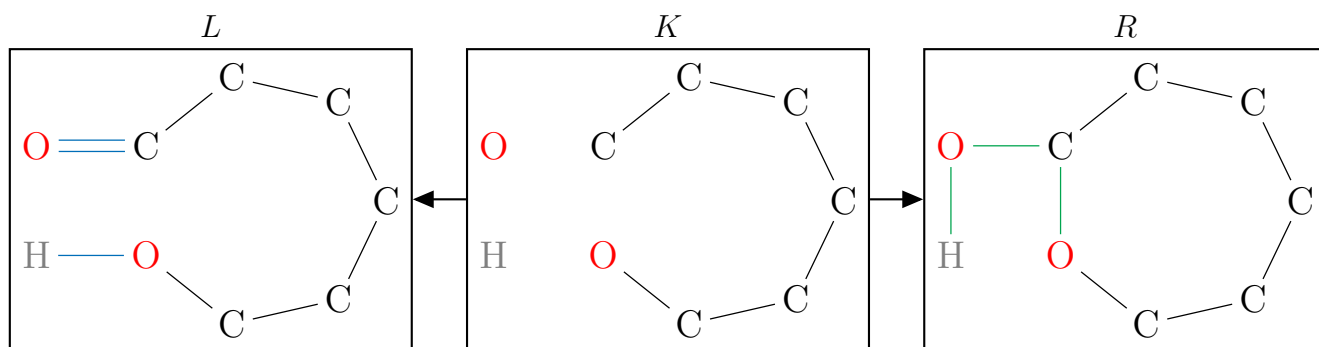
File: out/547_r_112_combined

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

0.0.111 Hemiacetal Formation for 7 membered rings



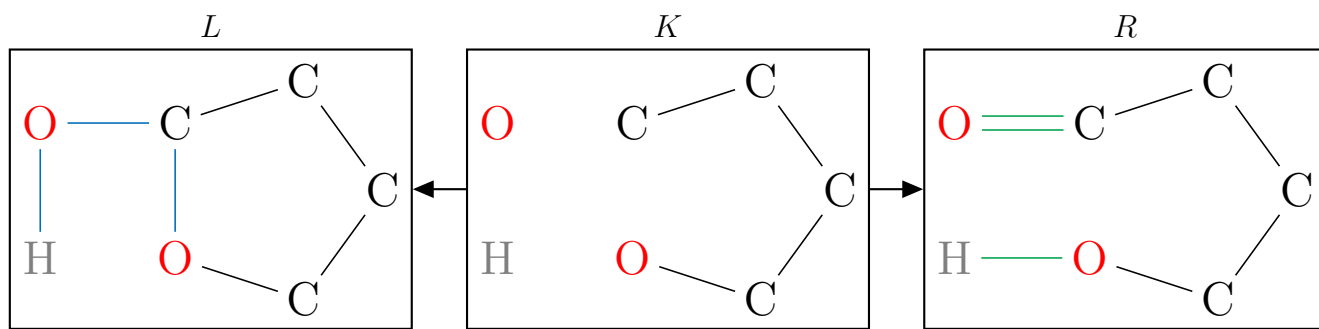
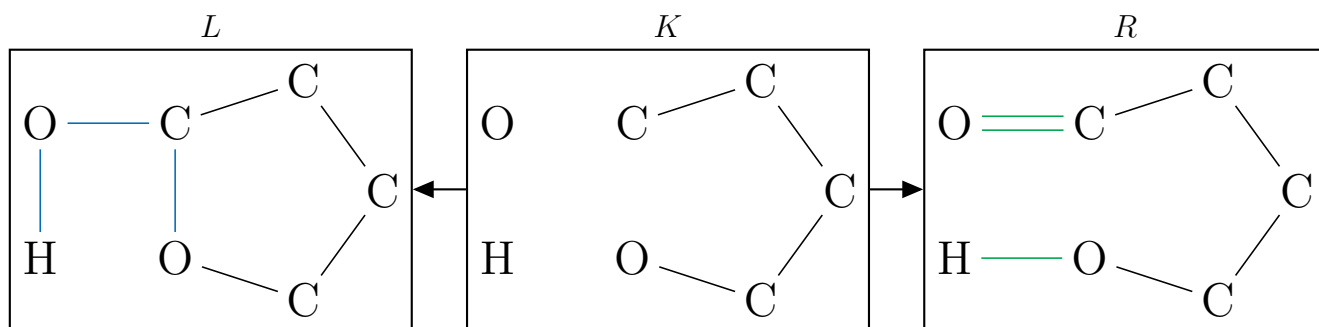
Files: out/550_r_113_10300000_{L, K, R}

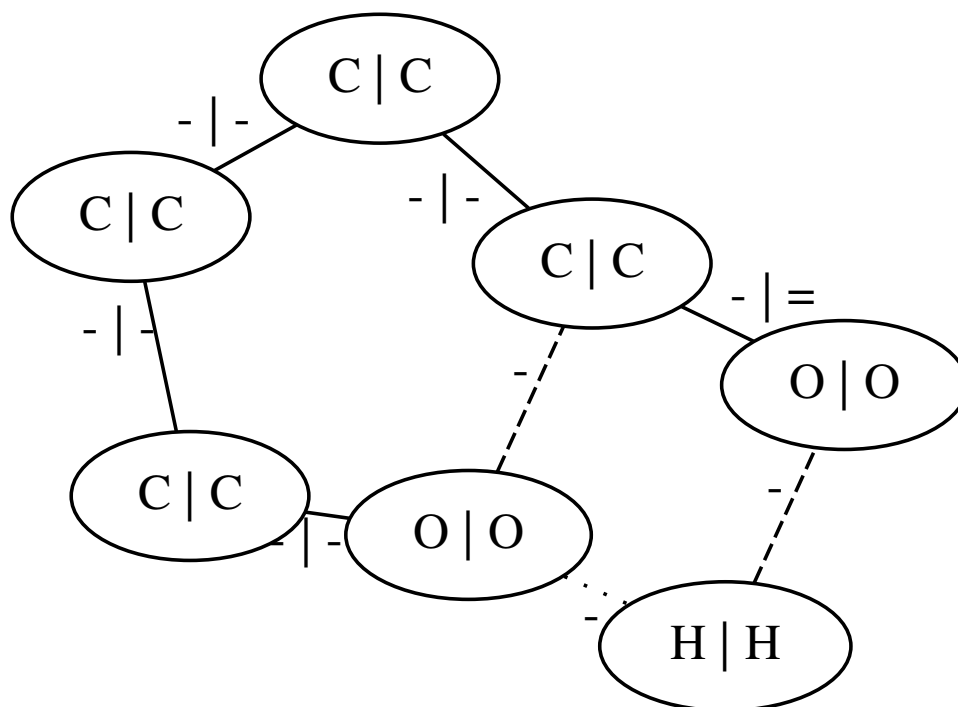


File: out/552_r_113_combined

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

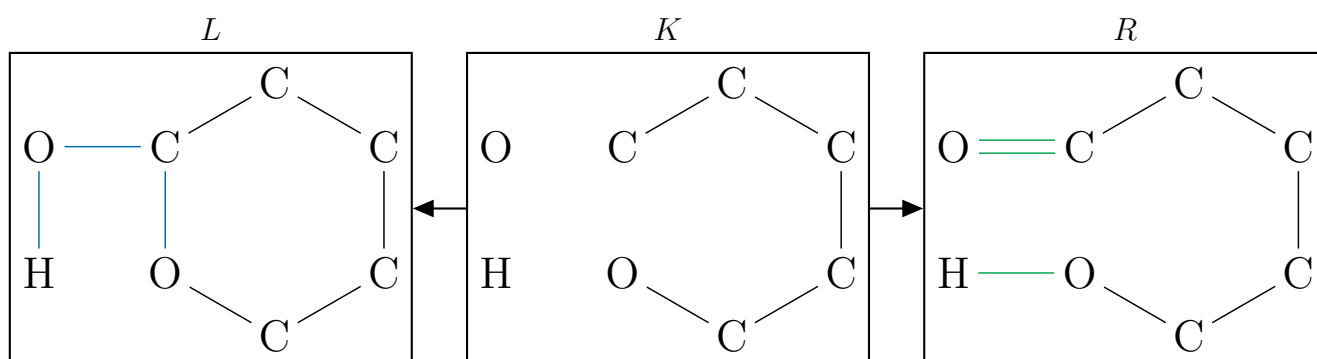
0.0.112 Hemiacetal Formation for 5 membered rings, inverse



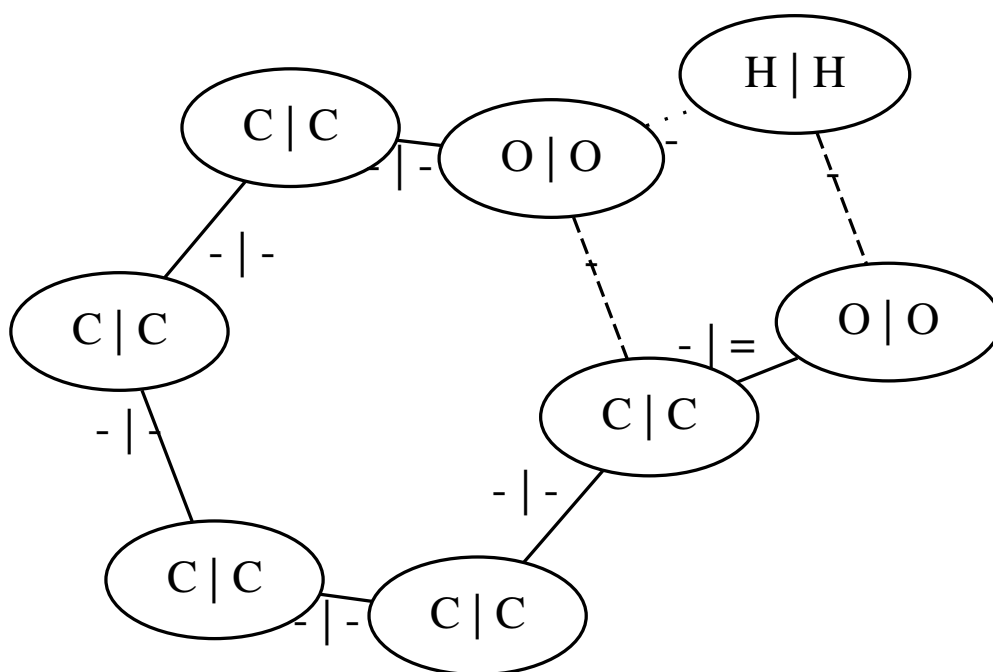
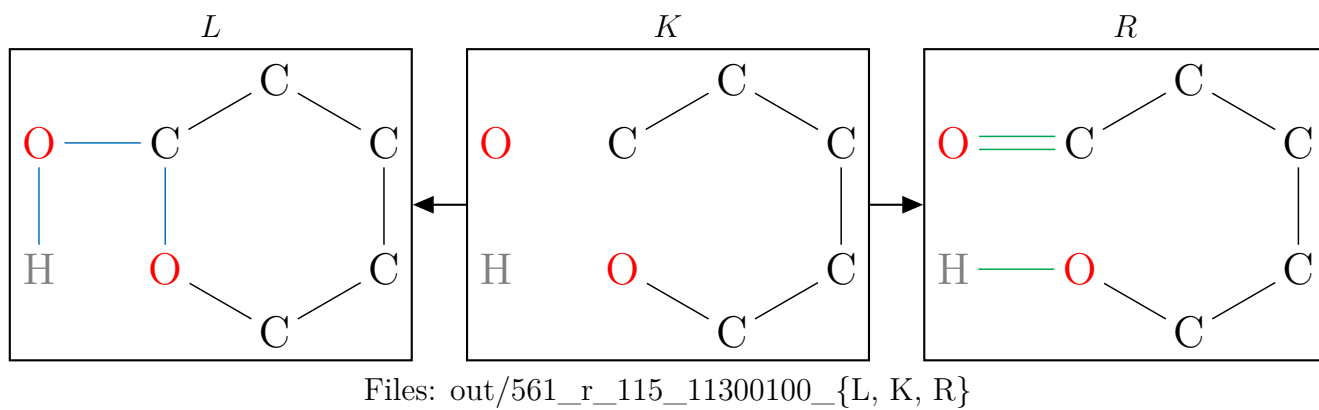


File: out/557_r_114_combined

0.0.113 Hemiacetal Formation for 6 membered rings, inverse

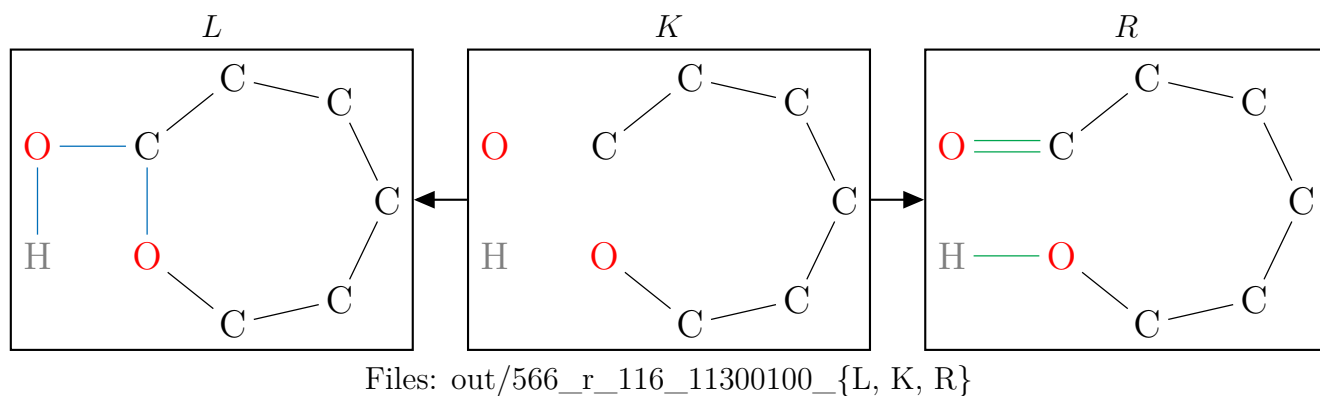
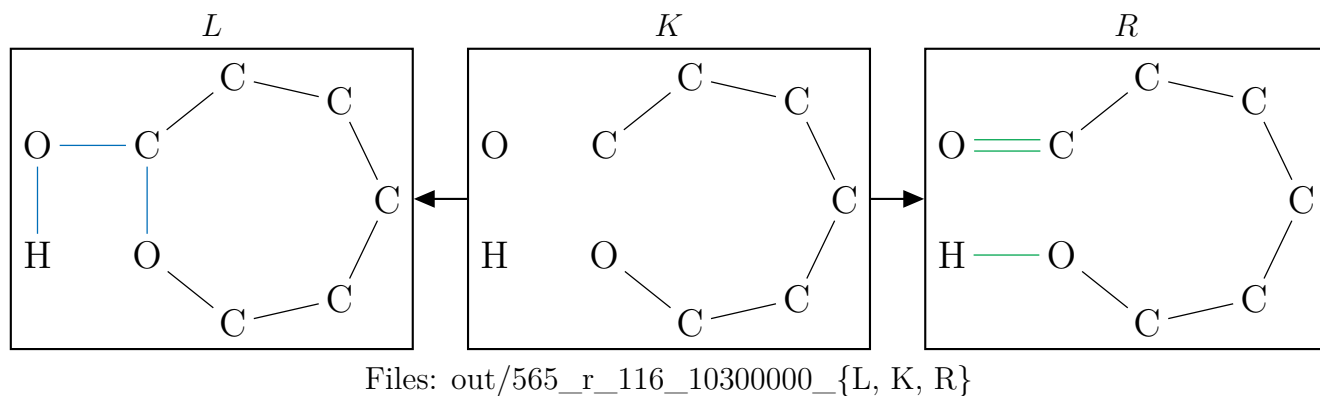


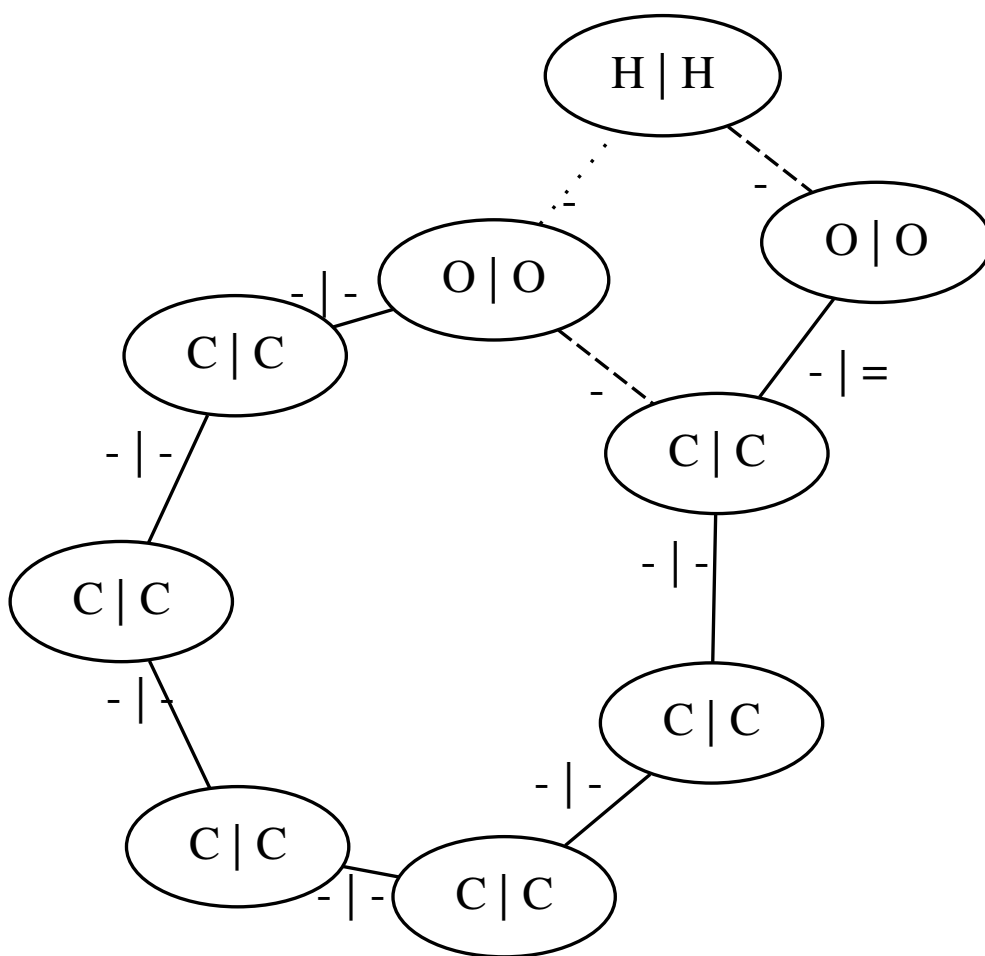
Files: out/560_r_115_10300000_{L, K, R}



File: out/562_r_115_combined

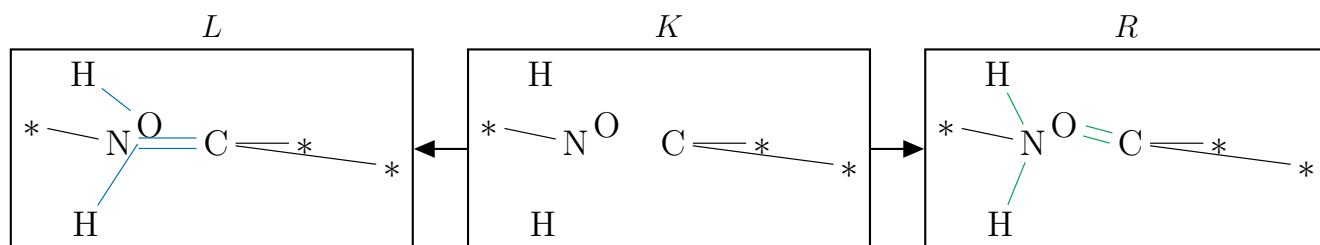
0.0.114 Hemiacetal Formation for 7 membered rings, inverse



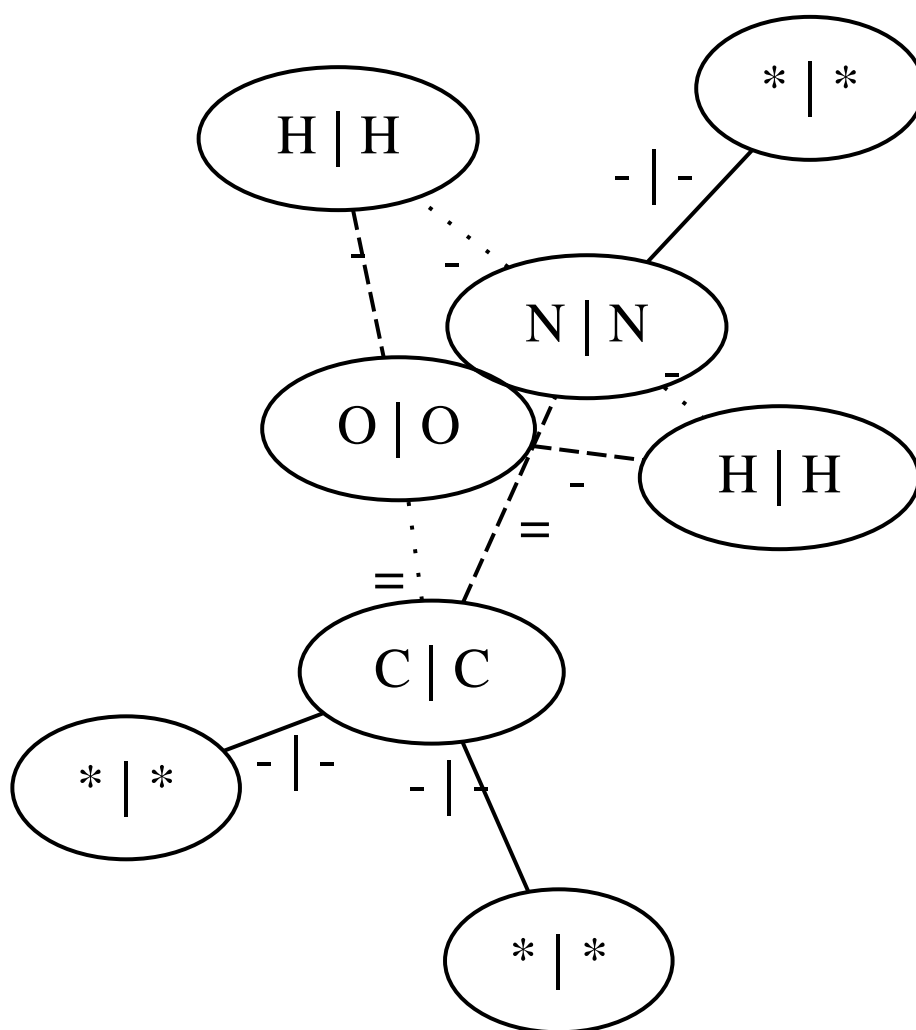
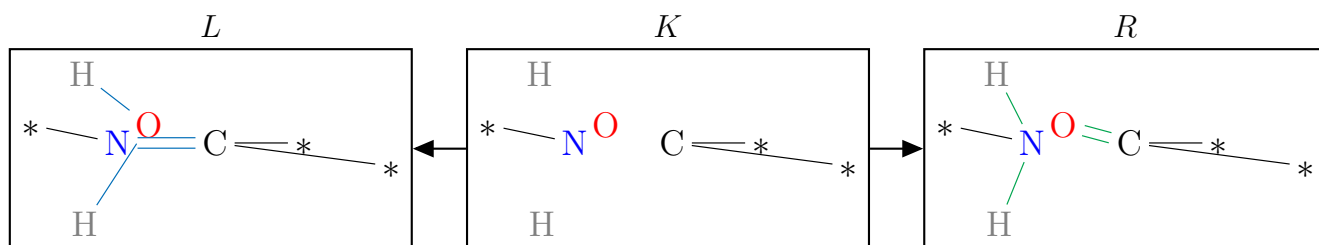


File: out/567_r_116_combined

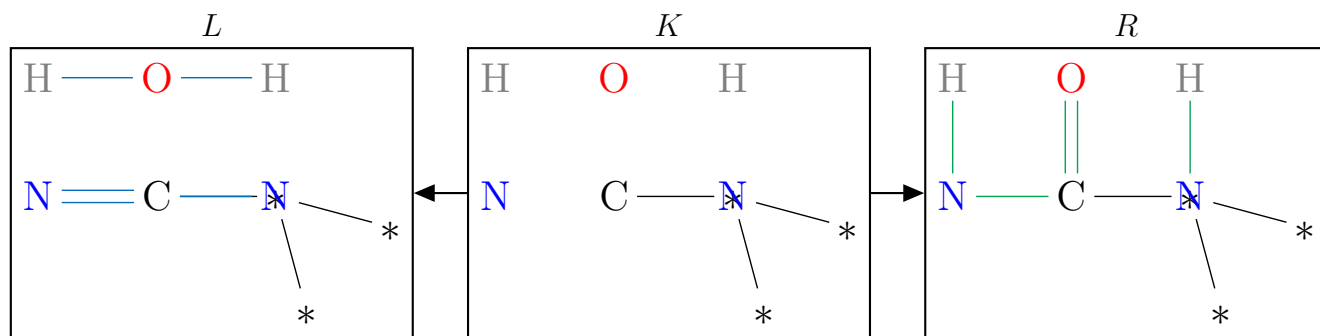
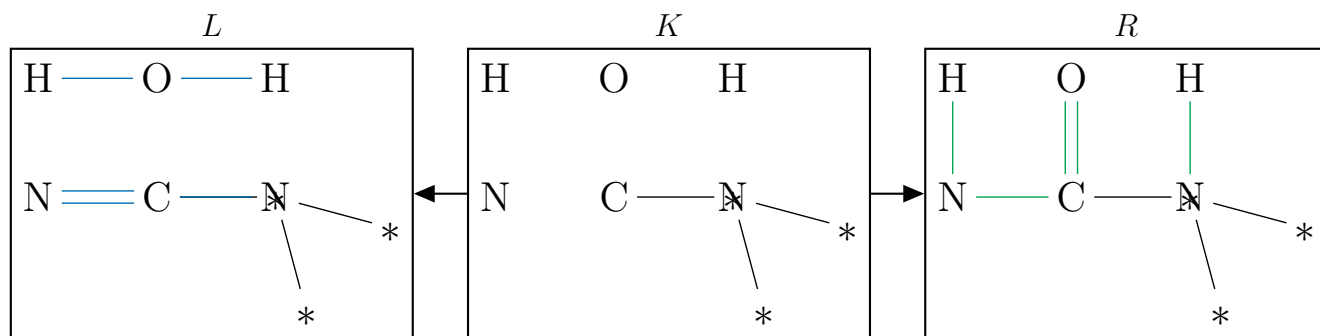
0.0.115 Imine to Carbonyl

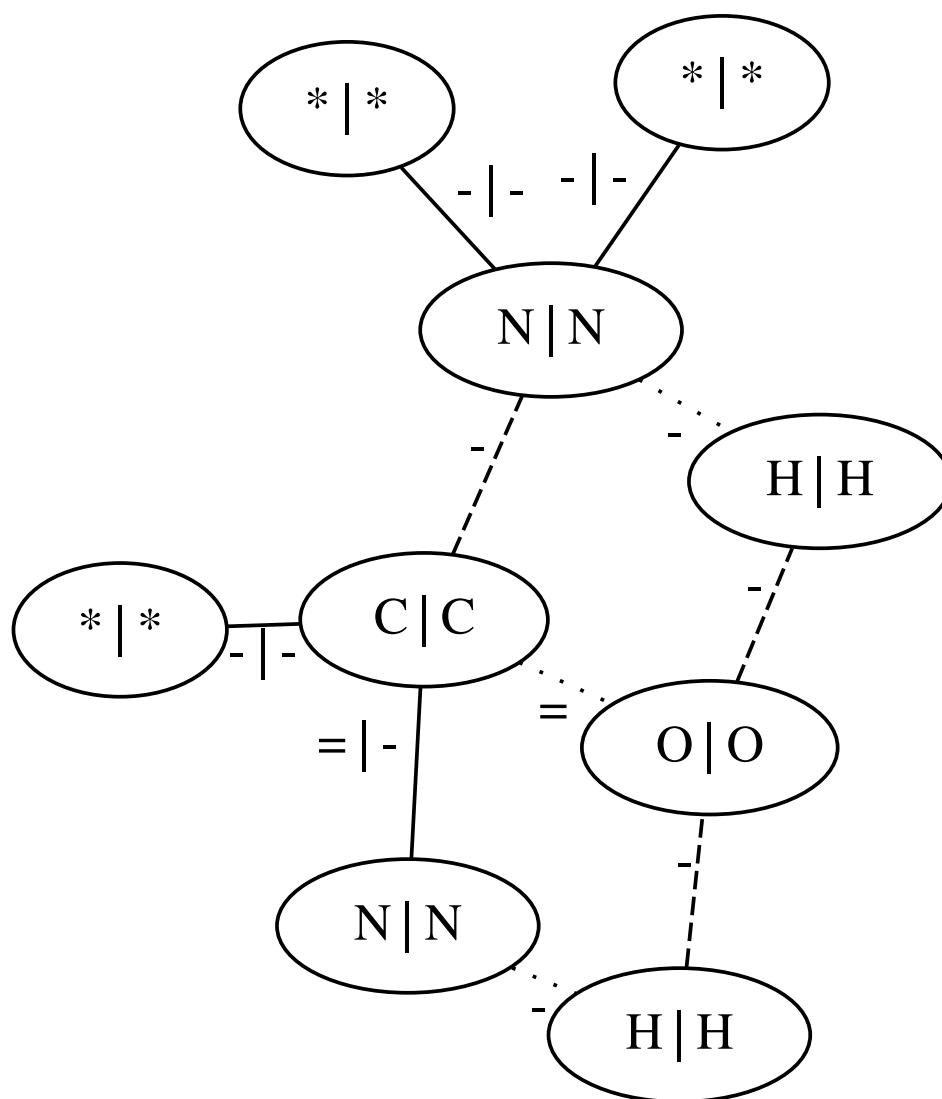


Files: out/570_r_117_10300000_{L, K, R}



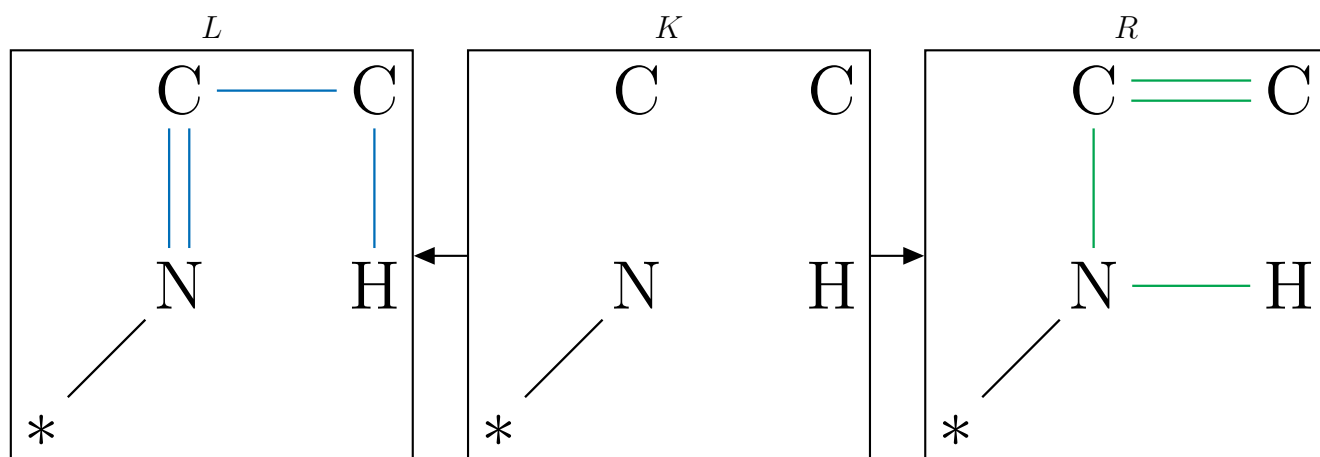
0.0.116 Amidine to Amide Hydrolysis



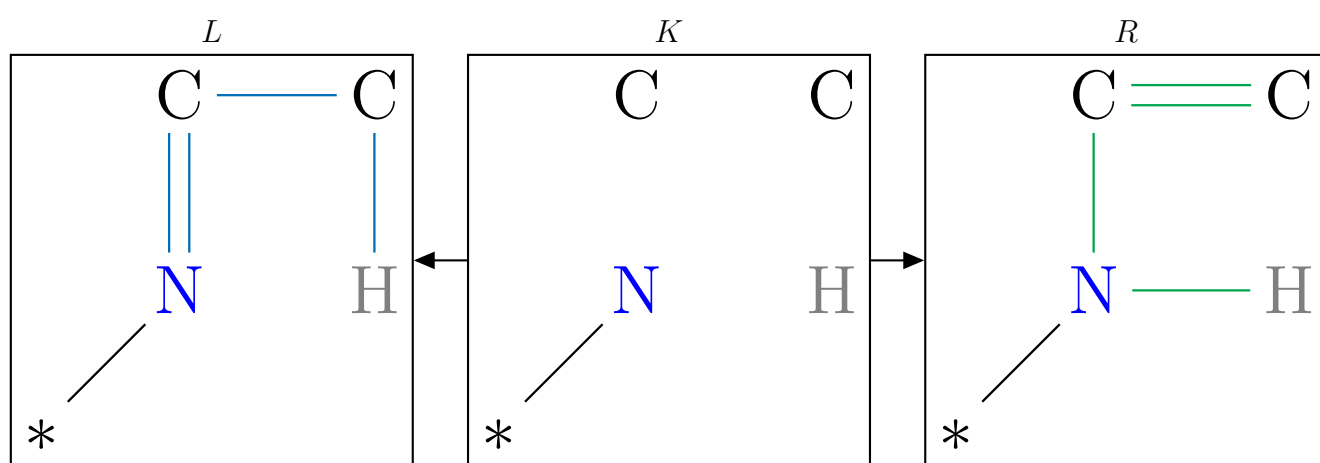


File: out/577_r_118_combined

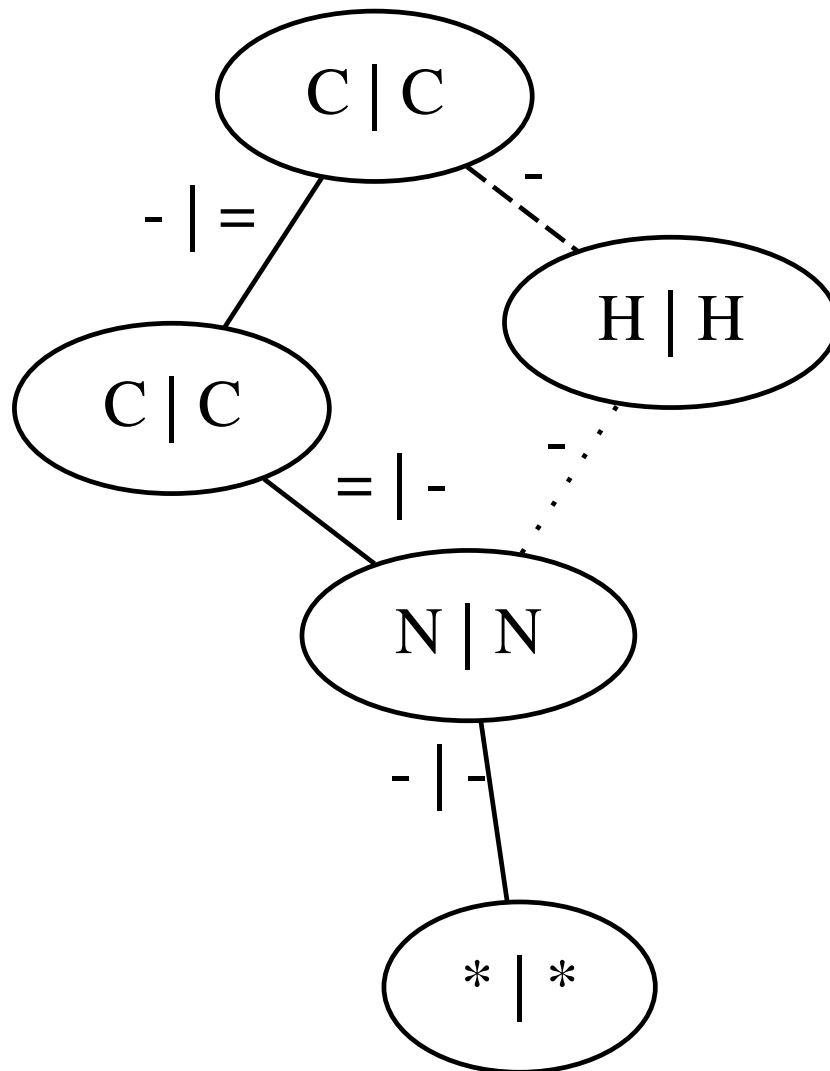
0.0.117 Imine to Enamine



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



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



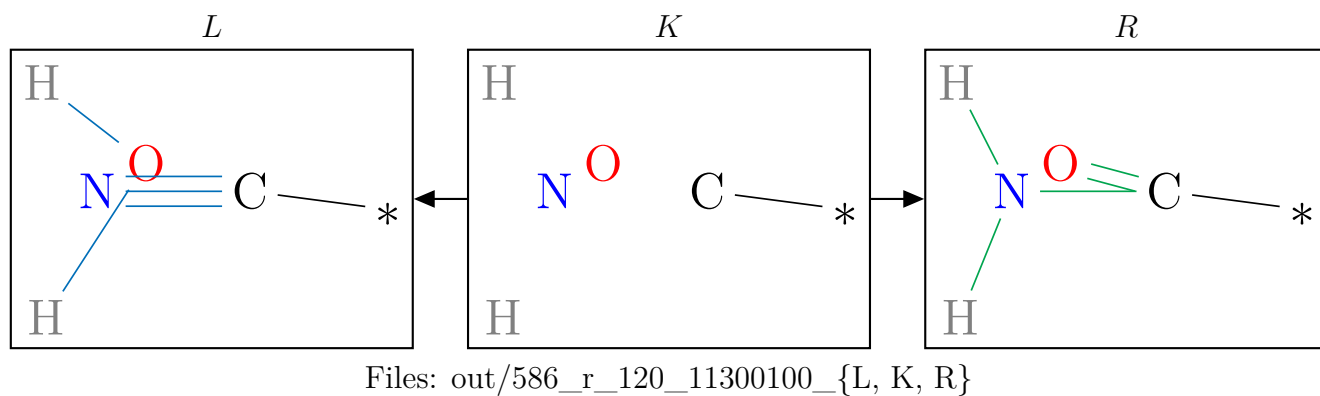
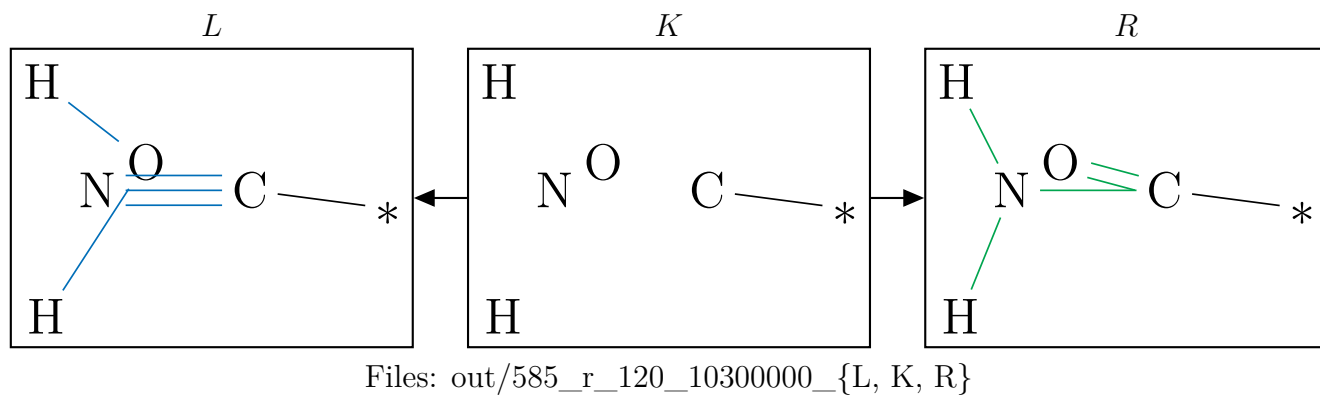
File: out/582_r_119_combined

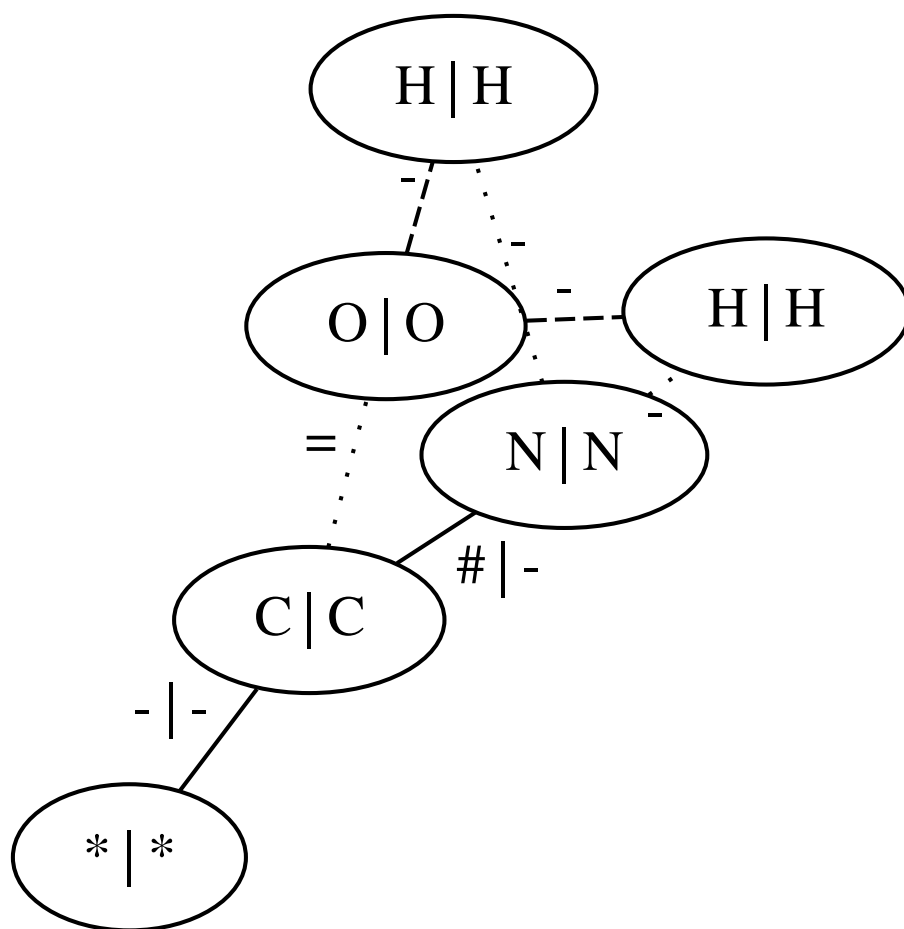
```

|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```

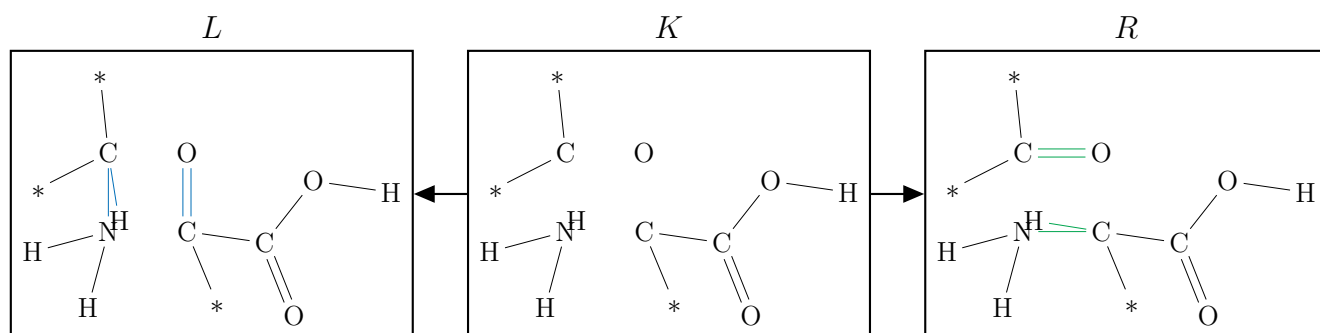
0.0.118 Nitrile Hydrolysis



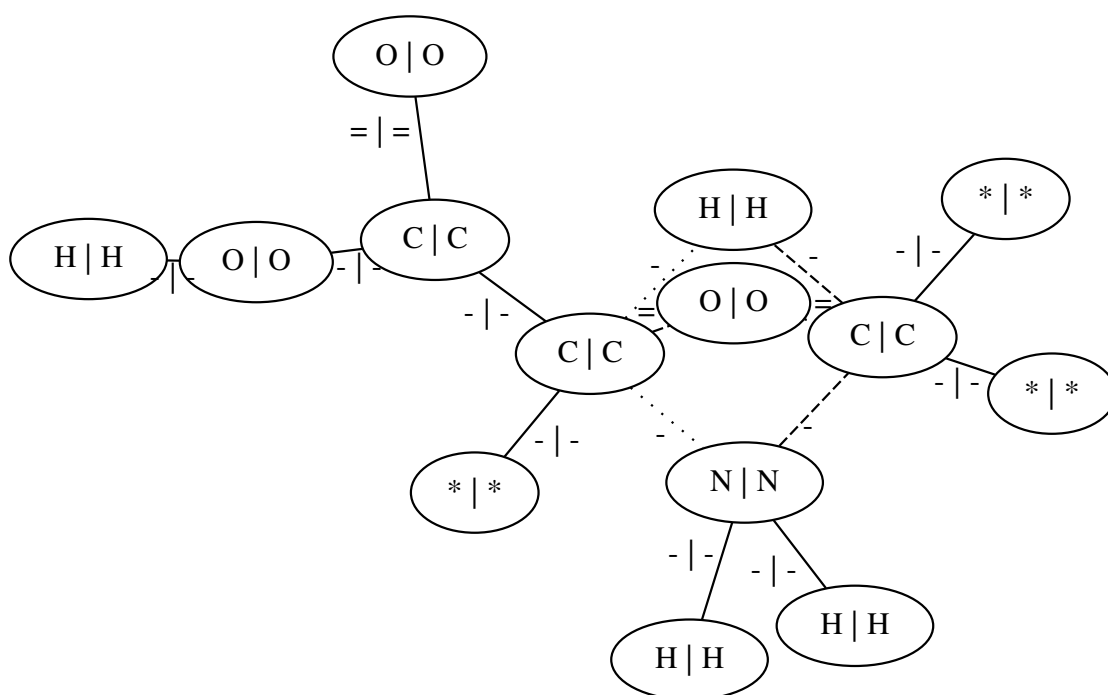
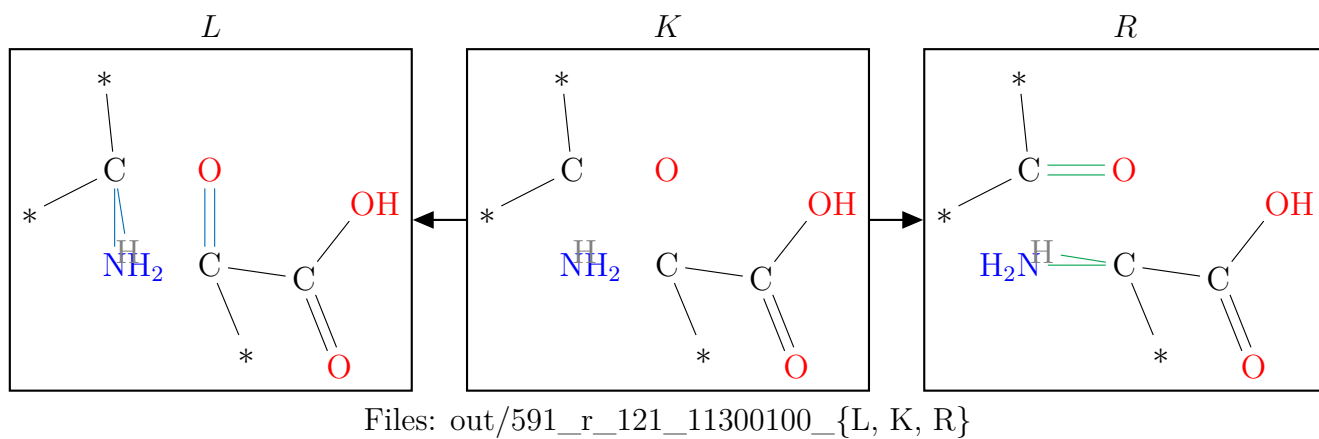


File: out/587_r_120_combined

0.0.119 Transamination



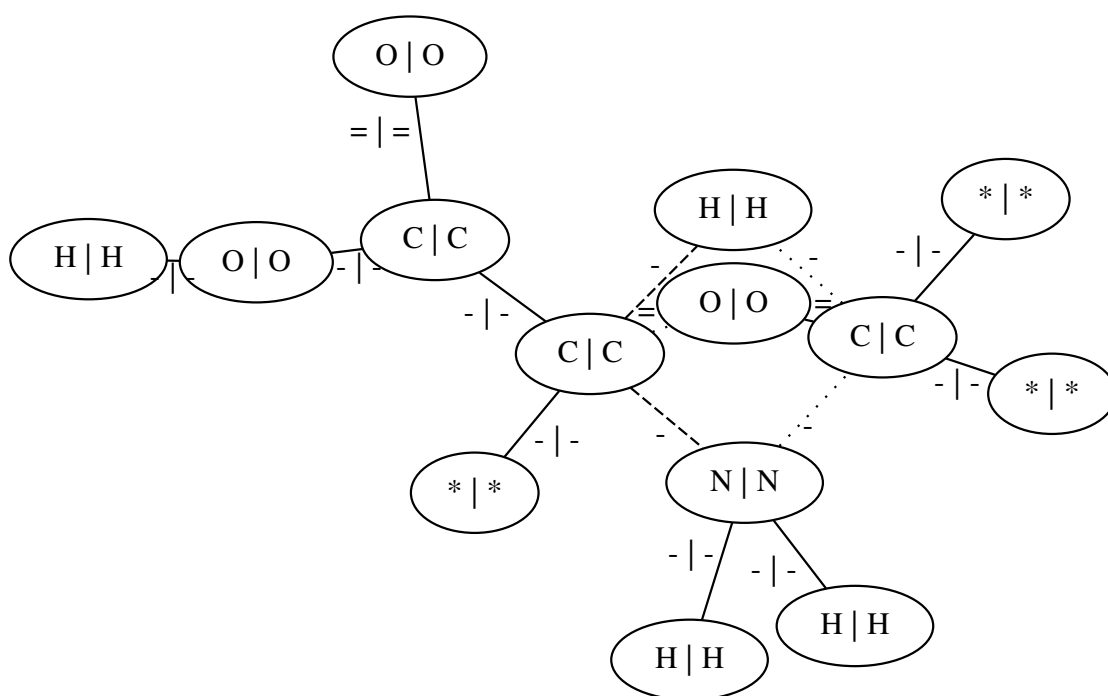
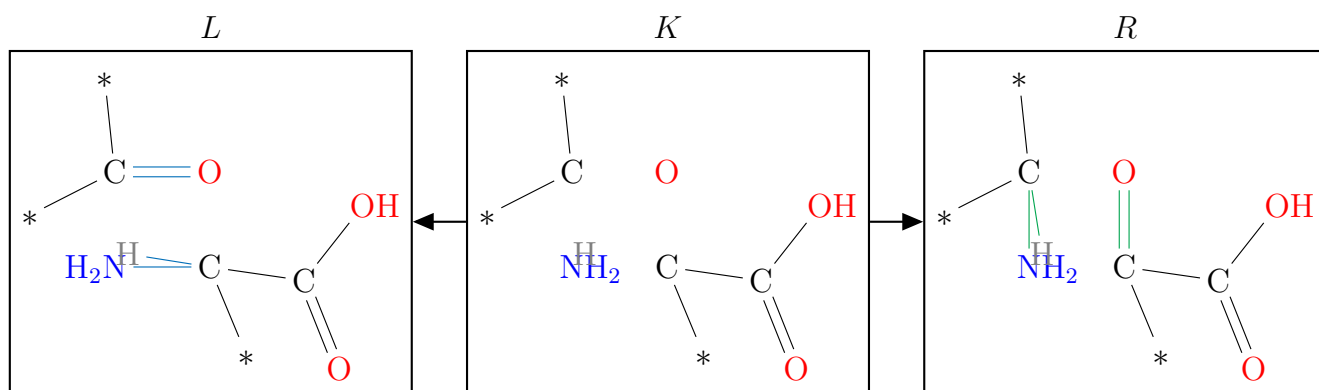
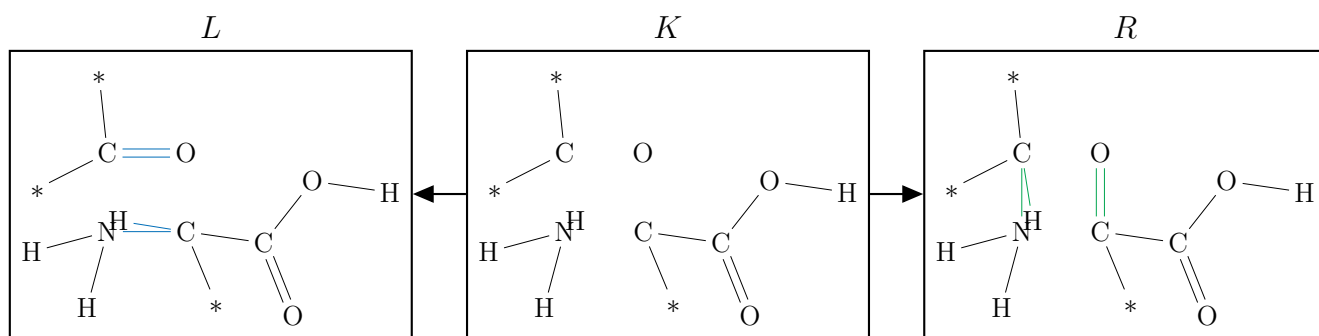
Files: out/590_r_121_10300000_{L, K, R}



File: out/592_r_121_combined

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

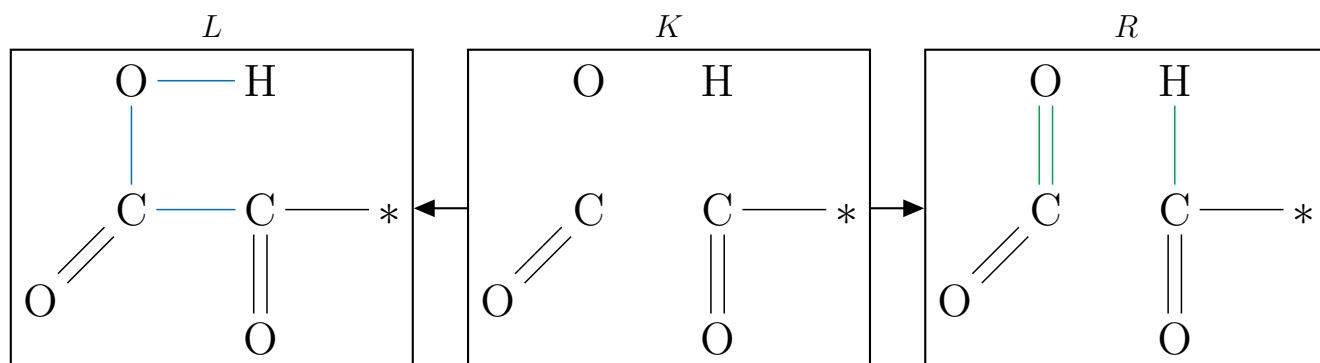
0.0.120 Transamination (inverse)



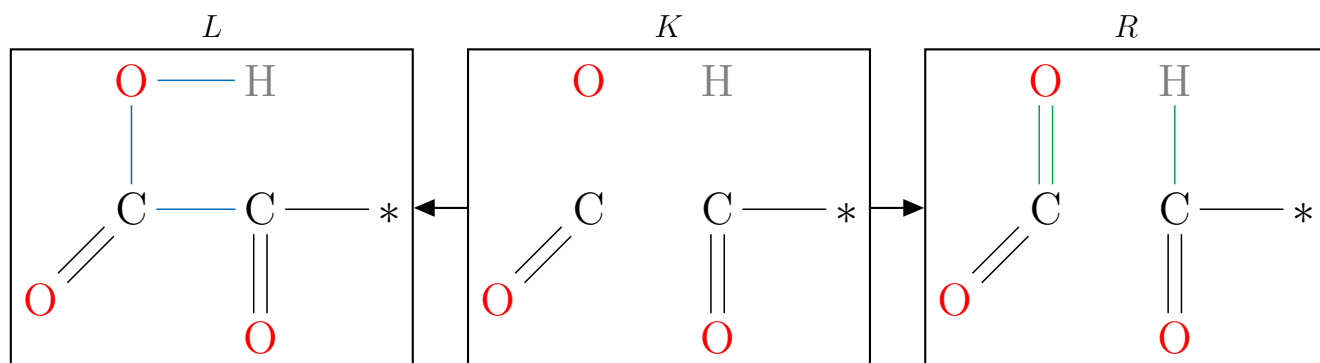
File: out/597_r_122_combined

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

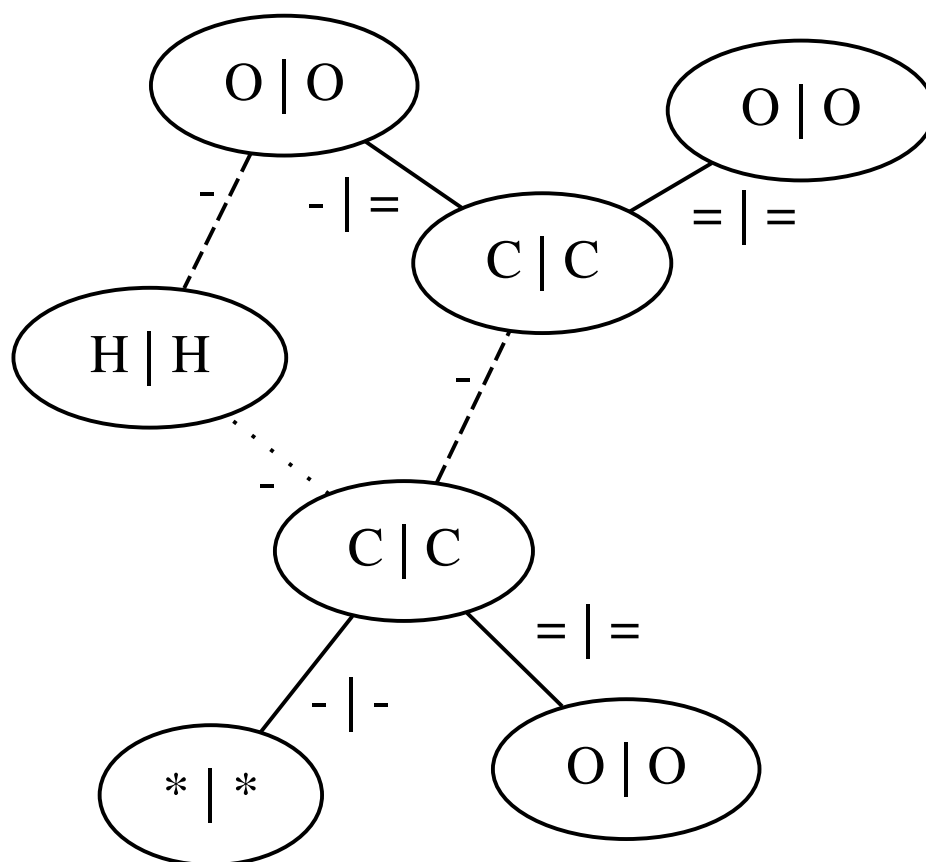
0.0.121 Alpha-Keto Acid Decarboxylation



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

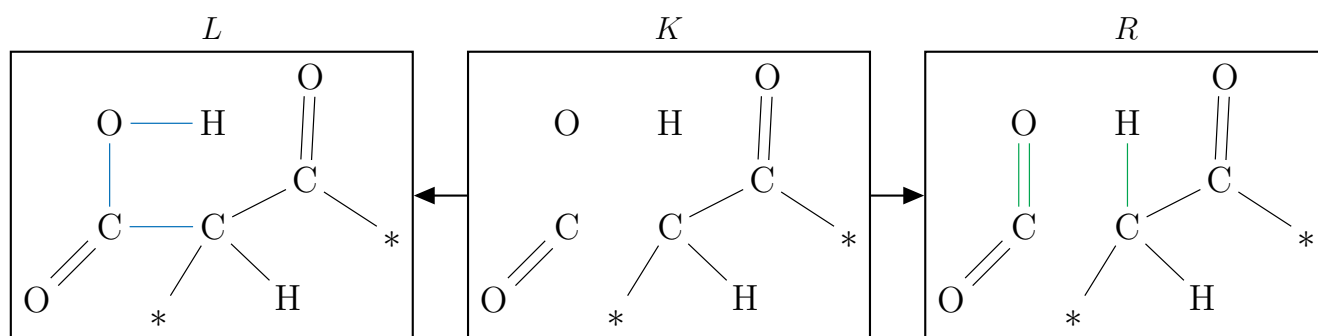


Files: out/601_r_123_11300100_{L, K, R}

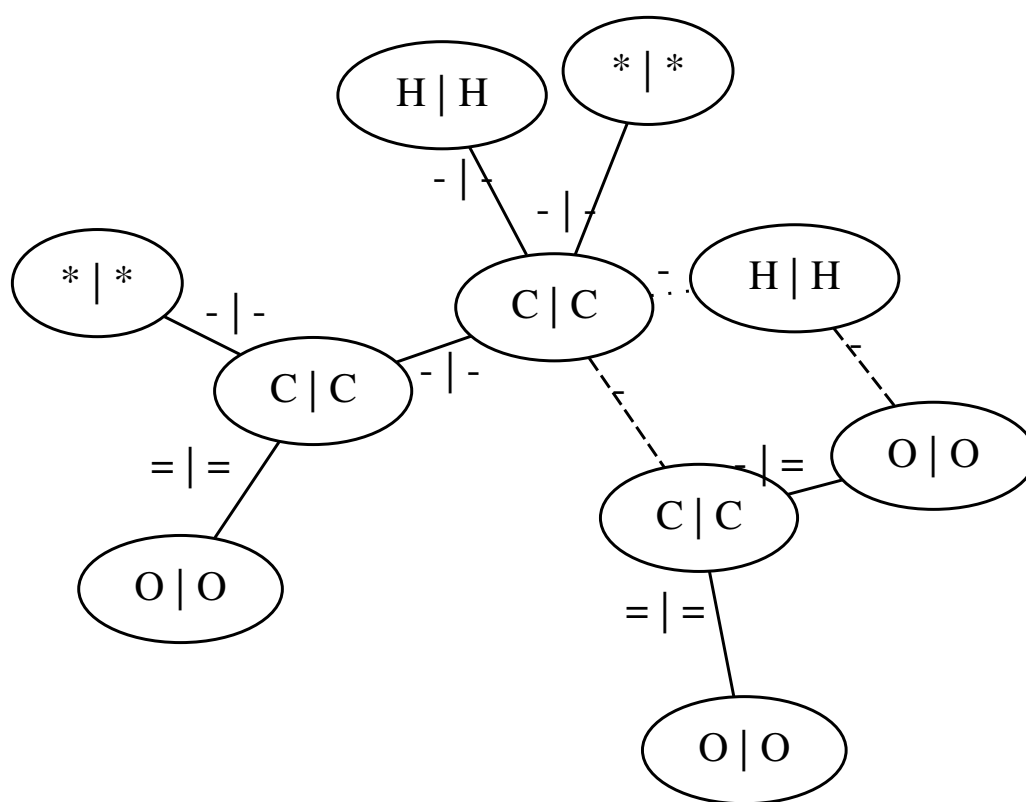
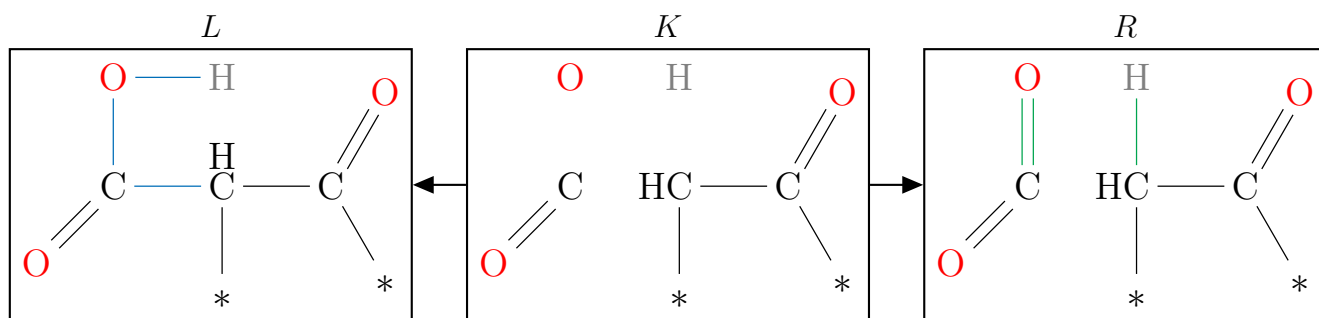


File: out/602_r_123_combined

0.0.122 Beta Decarboxylation

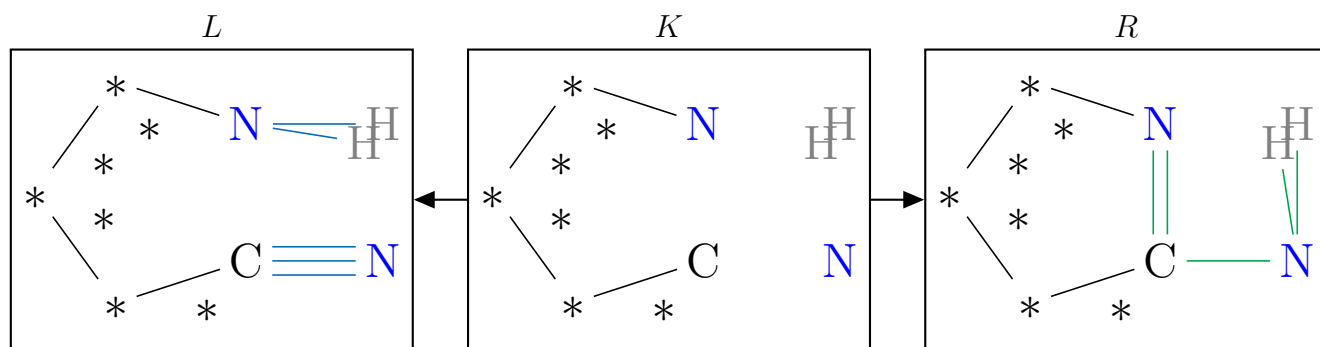
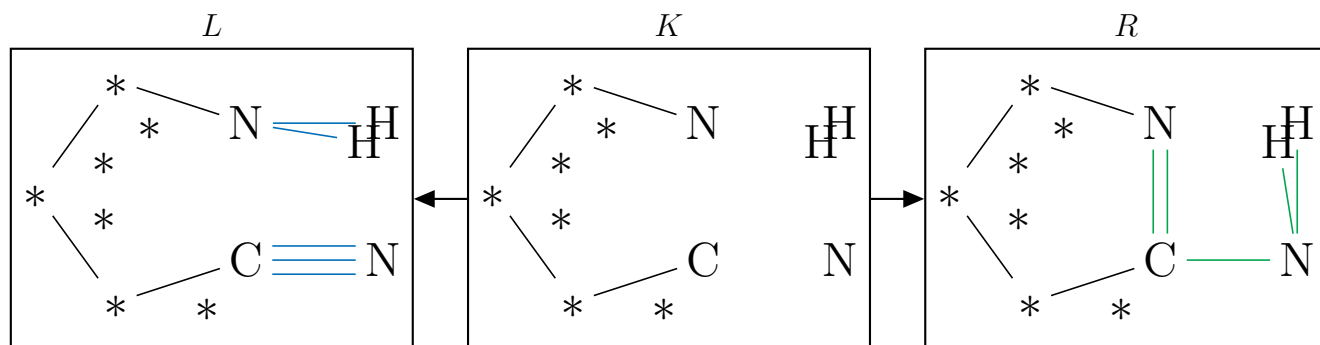


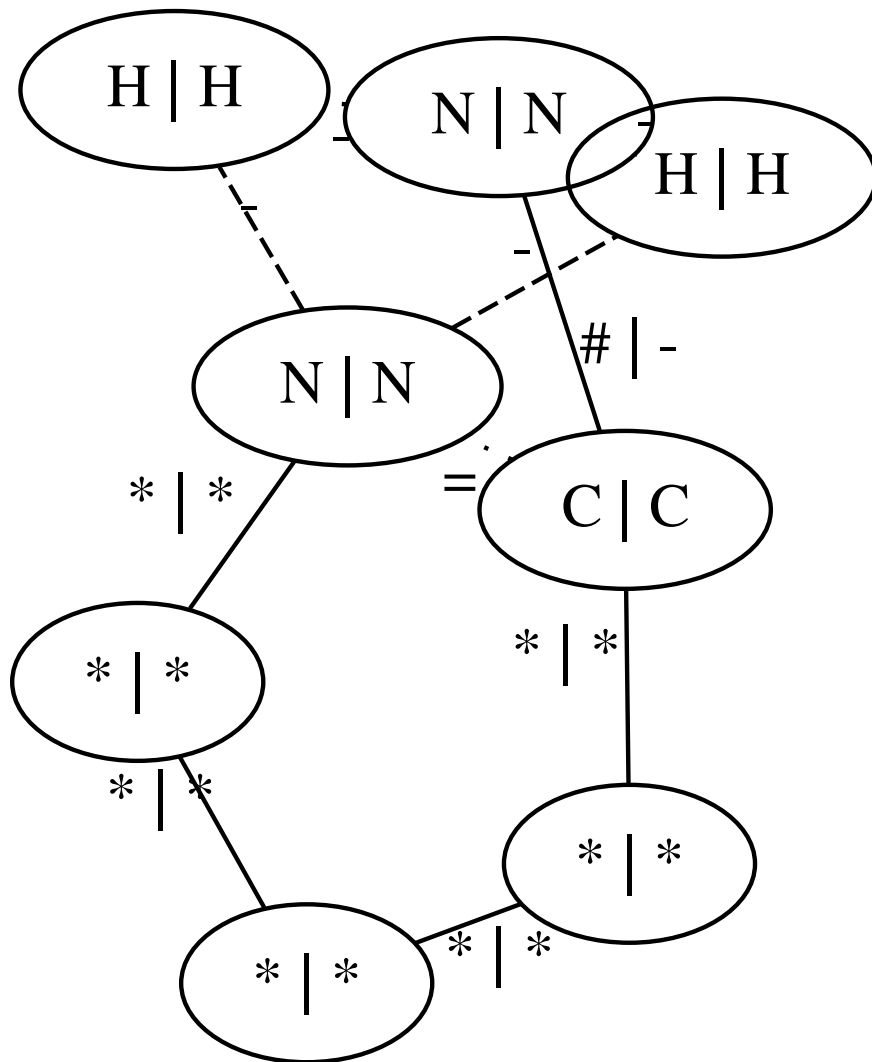
Files: out/605_r_124_10300000_{L, K, R}



File: out/607_r_124_combined

0.0.123 Nitrile Ring Closure 5





File: out/612_r_125_combined

$$|\{e \in \text{outEdges}(5) \mid$$

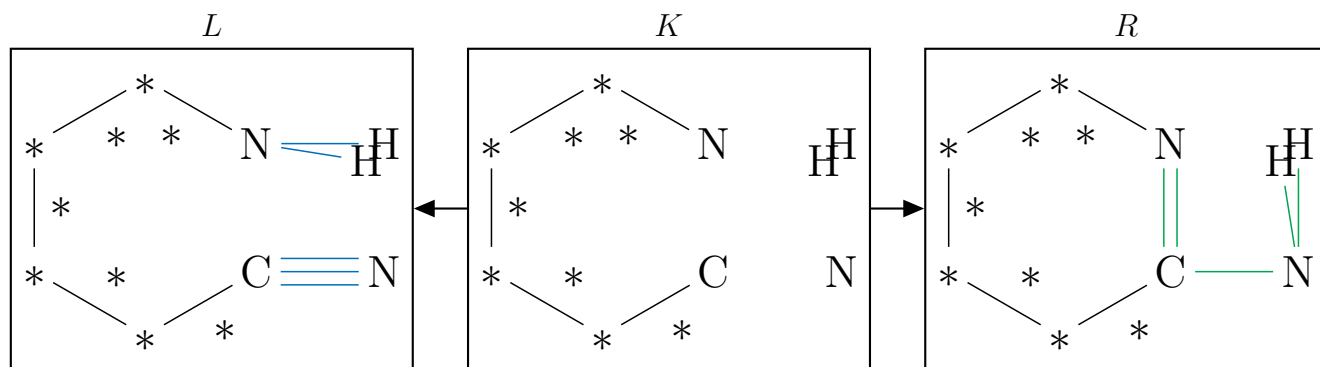
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

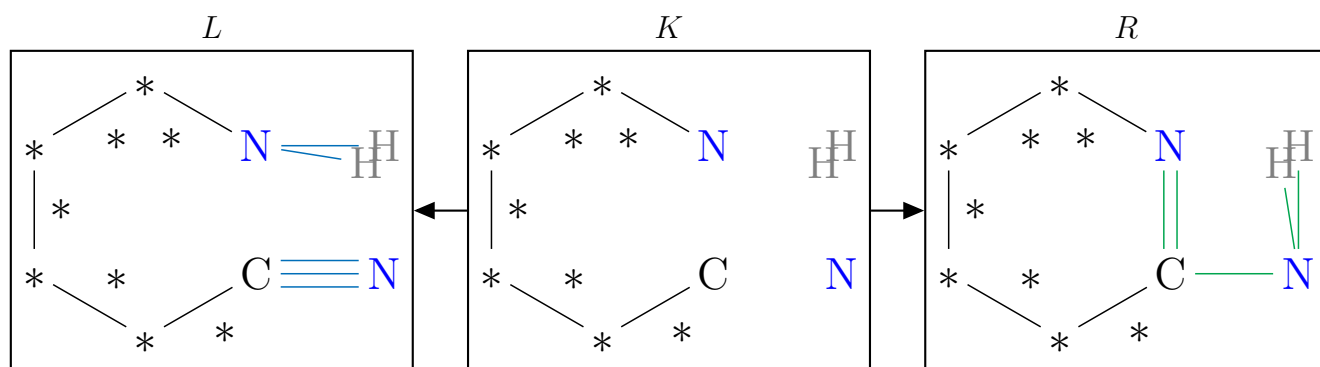
$$\text{label}(e) \in \{'=\'}\}$$

$$| = 0$$

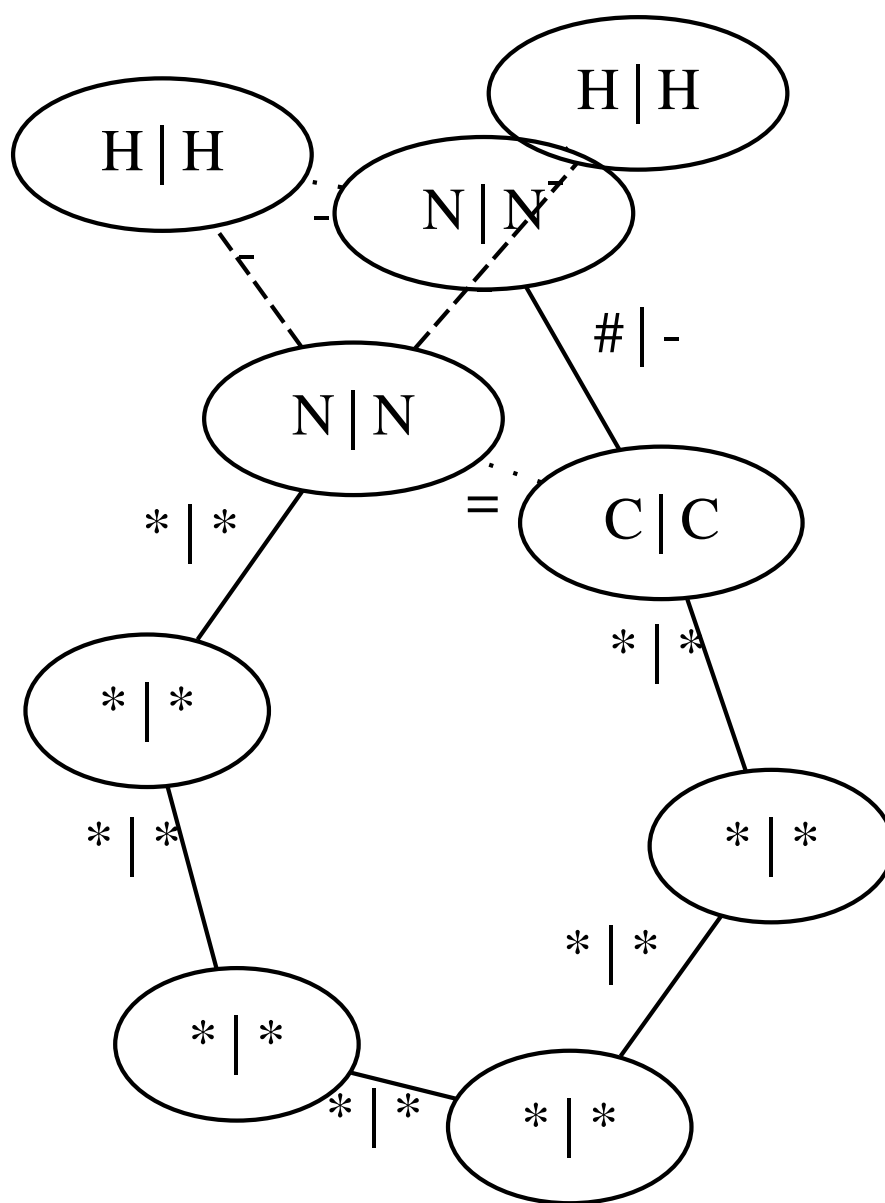
0.0.124 Nitrile Ring Closure 6



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



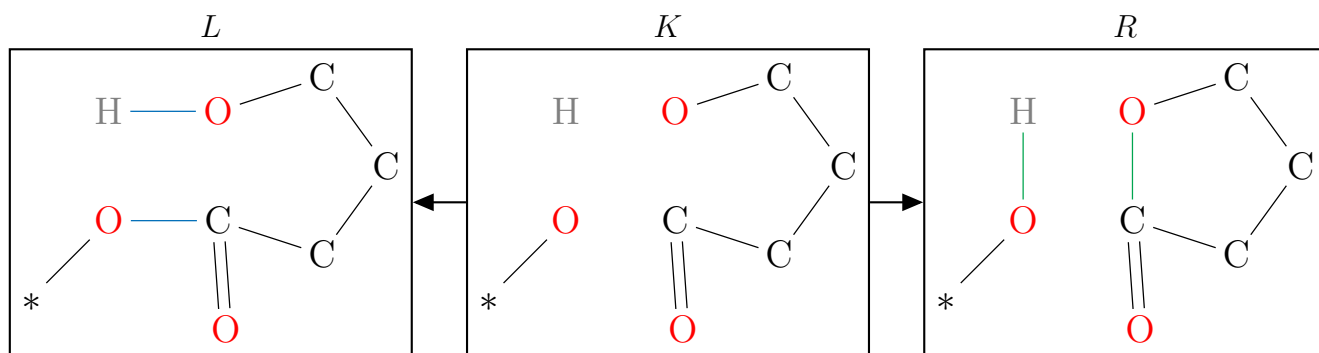
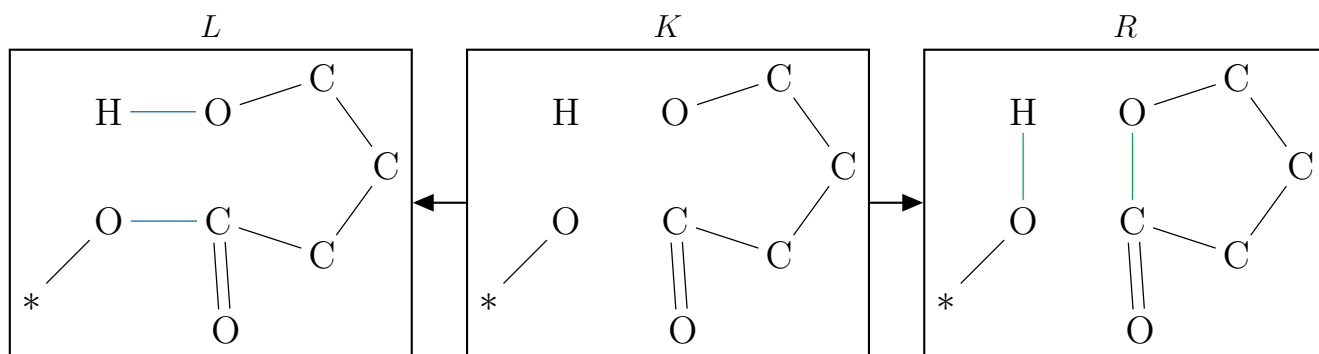
Files: out/616_r_126_11300100_{L, K, R}

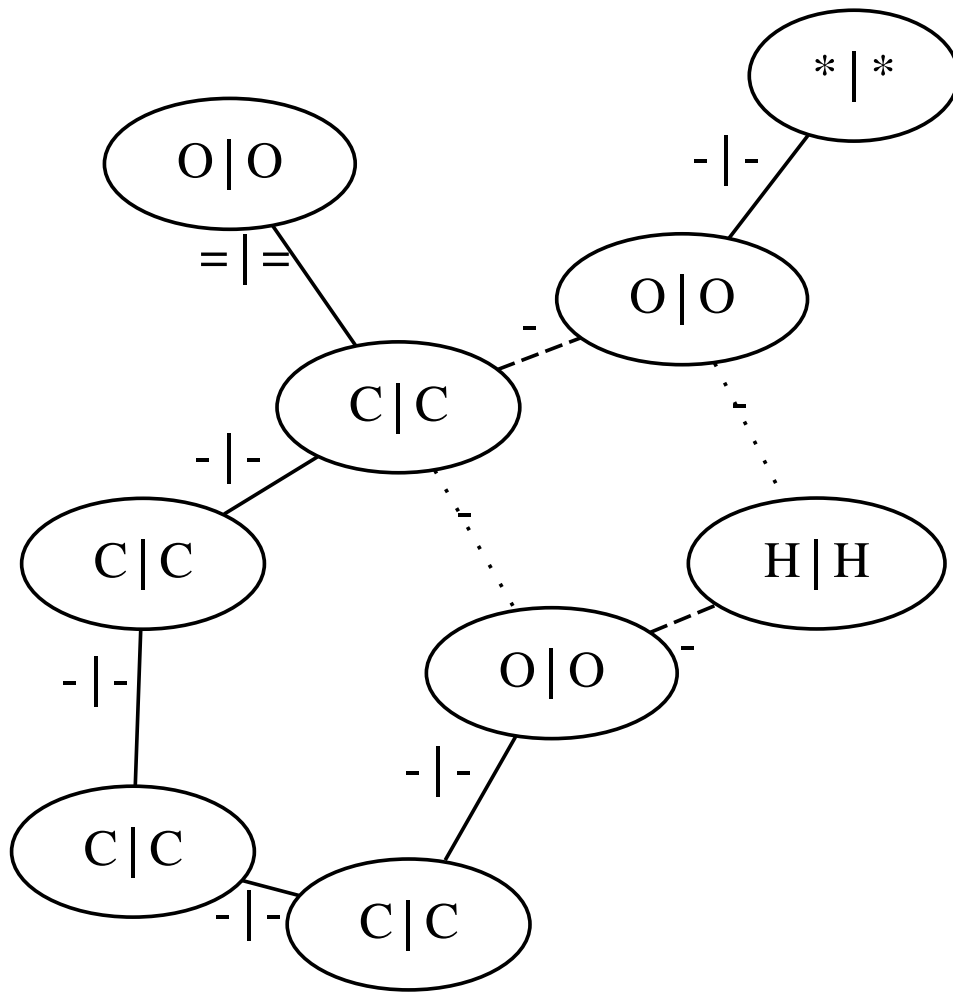


File: out/617_r_126_combined

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

0.0.125 Ring Closure 5 membered O, O





File: out/622_r_127_combined

$$|\{e \in \text{outEdges}(2) \mid$$

$$\text{label}(\text{target}(e)) \in \{ '0' \}$$

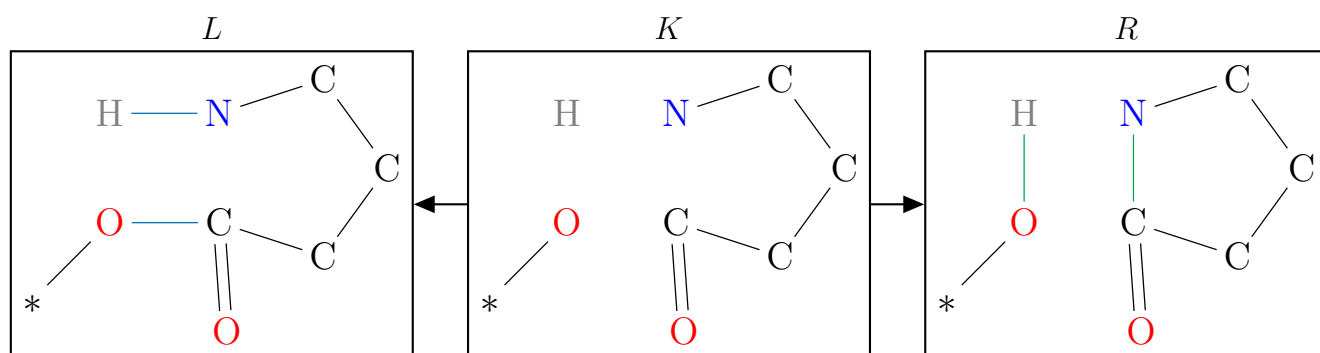
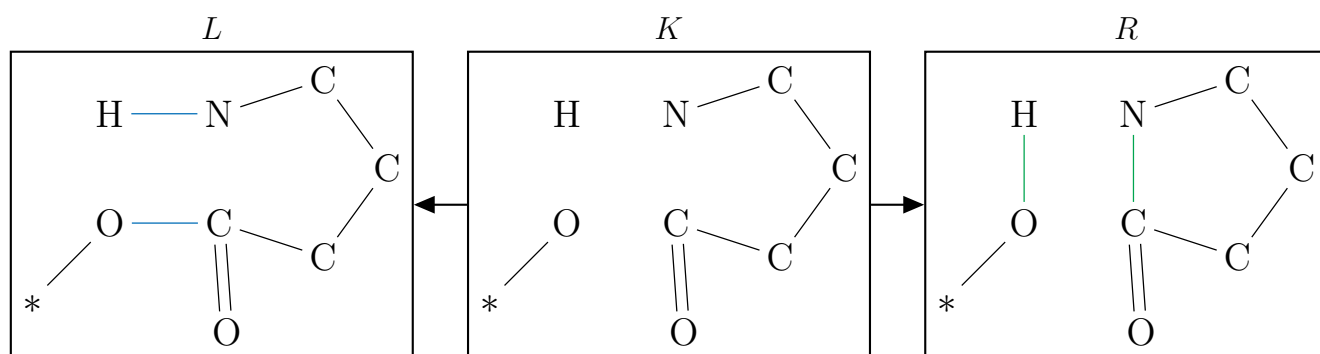
$$\wedge$$

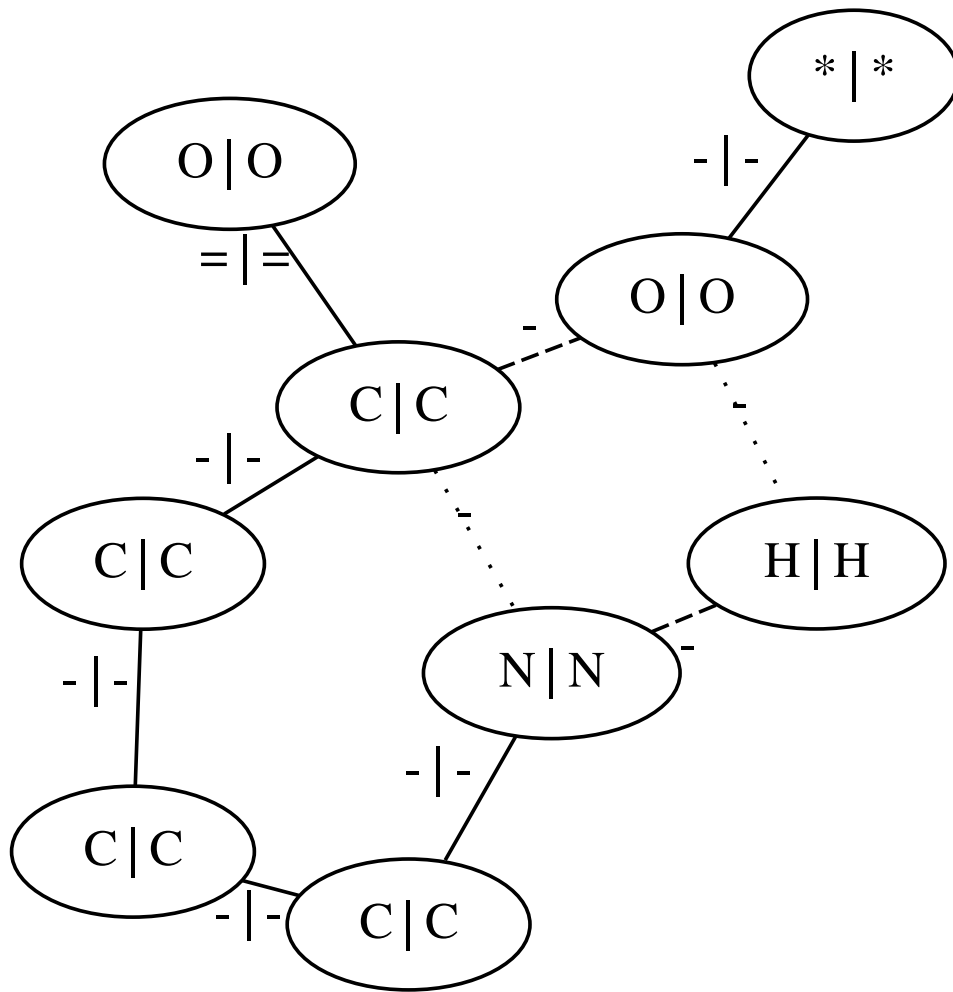
$$\text{label}(e) \in \{ '-' \}$$

$$\}| = 1$$

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

0.0.126 Ring Closure 5 membered O, N





File: out/627_r_128_combined

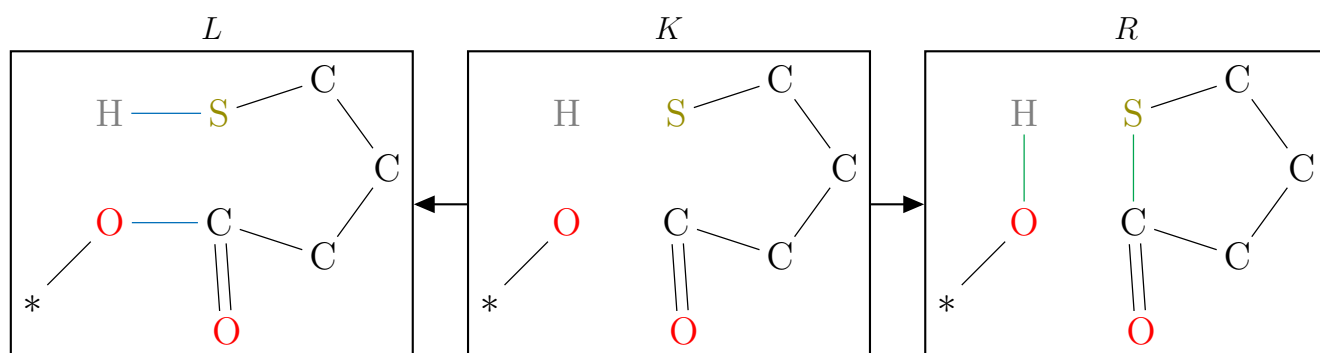
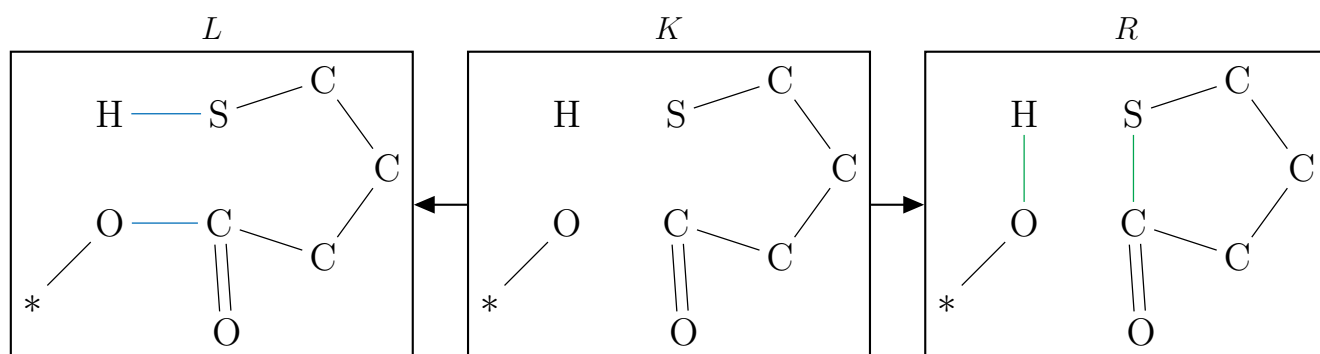
```

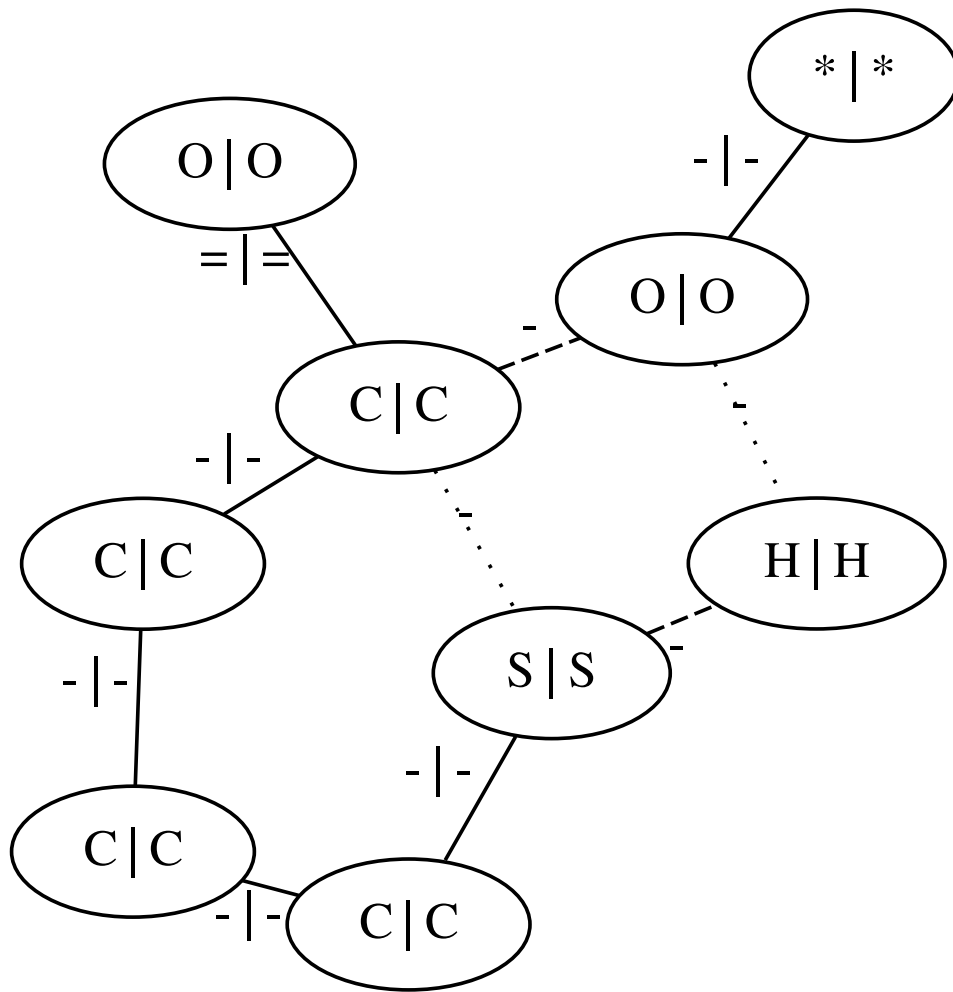
|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'0'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

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

0.0.127 Ring Closure 5 membered O, S





File: out/632_r_129_combined

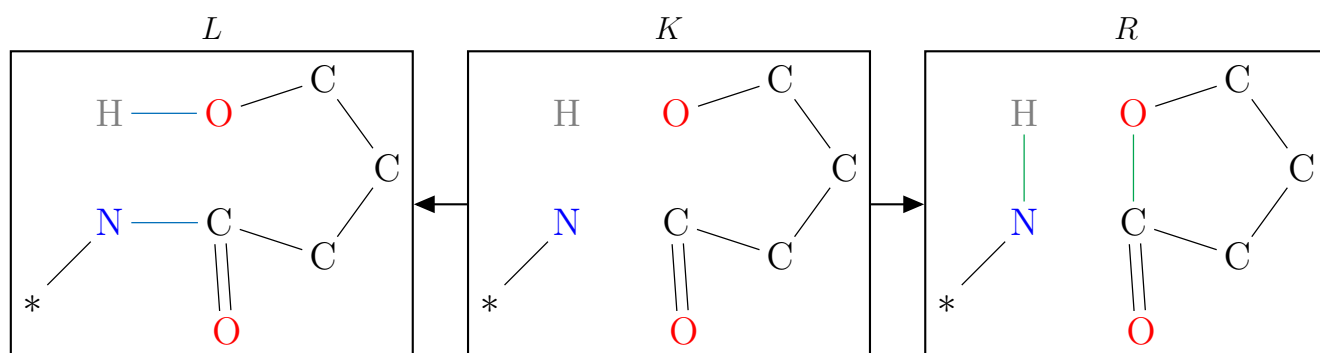
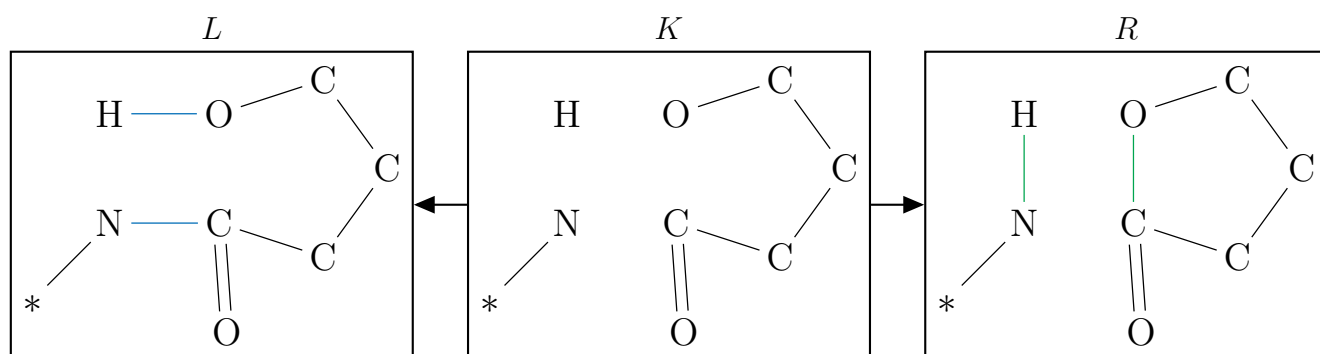
```

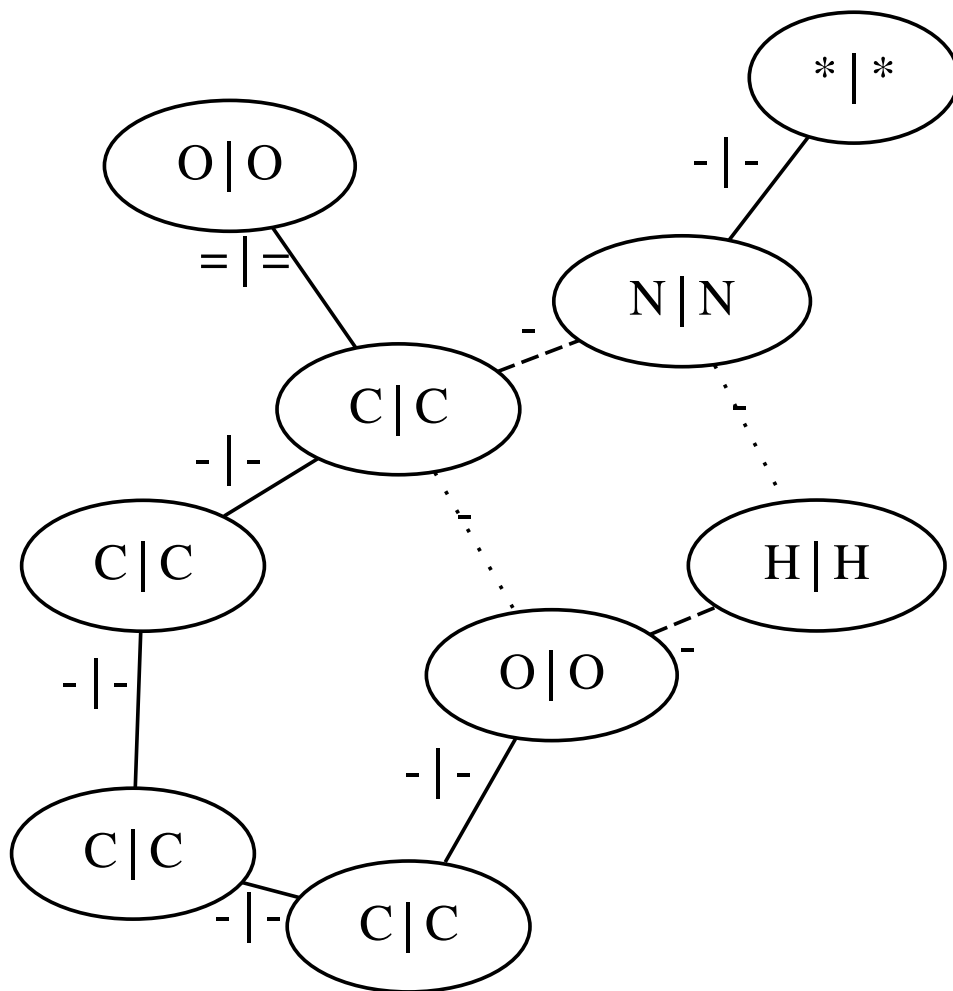
|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'0'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

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

0.0.128 Ring Closure 5 membered N, O





File: out/637_r_130_combined

$$|\{e \in \text{outEdges}(2) \mid$$

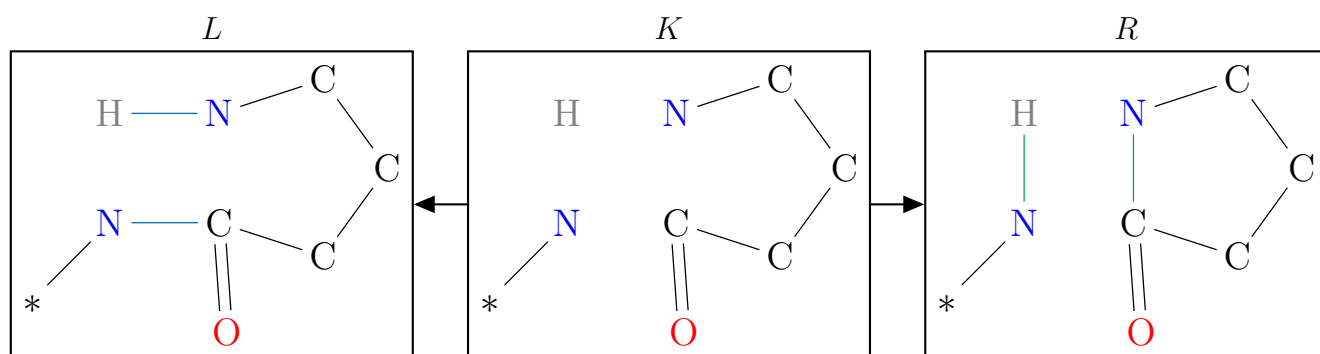
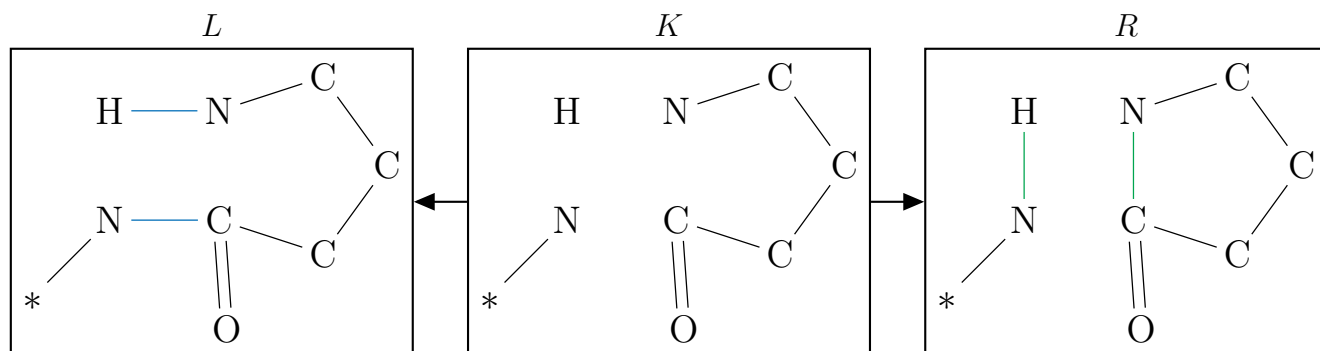
$$\text{label}(\text{target}(e)) \in \{\text{'N'}\}$$

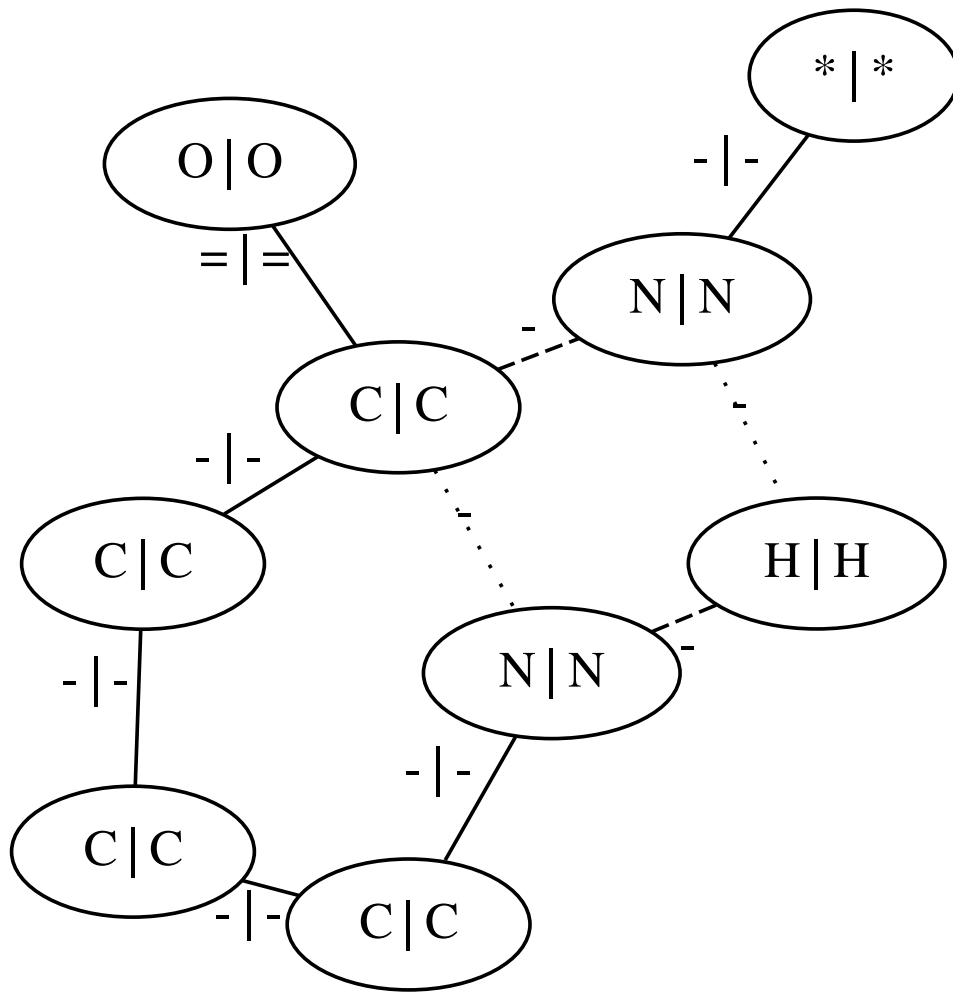
$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 1$$

0.0.129 Ring Closure 5 membered N, N





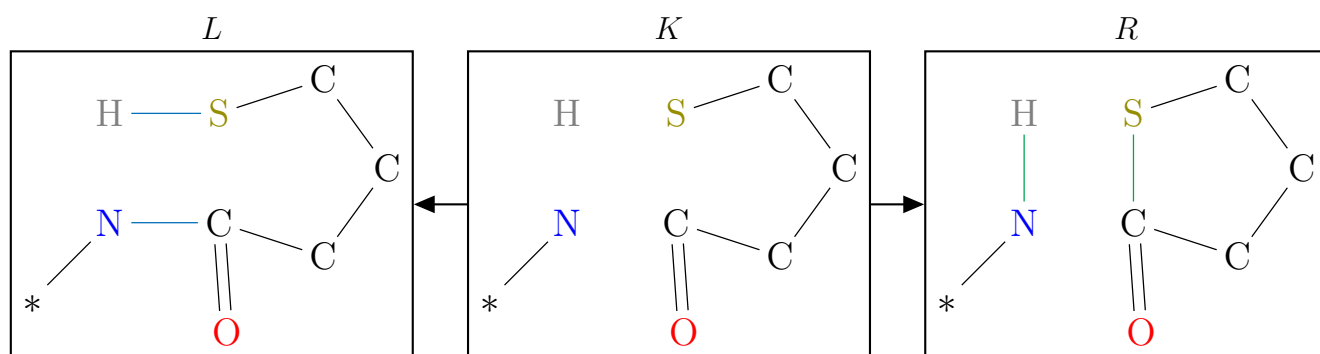
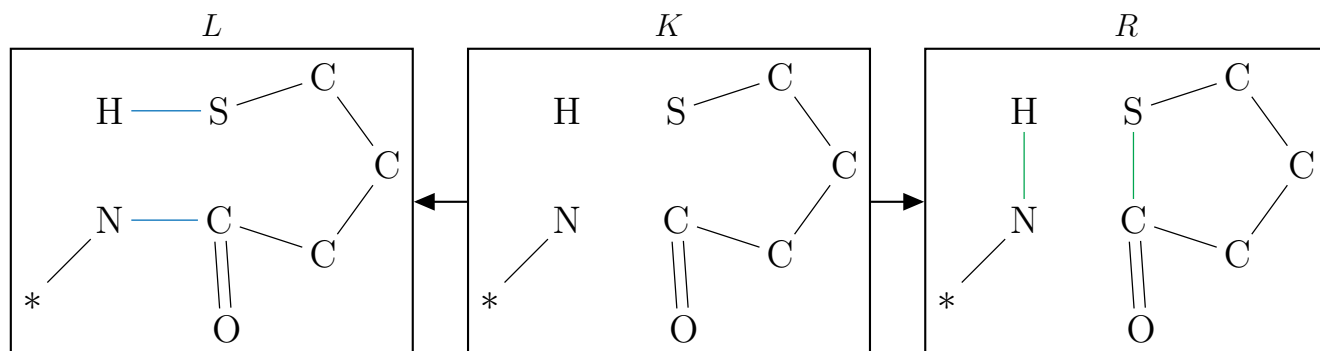
File: out/642_r_131_combined

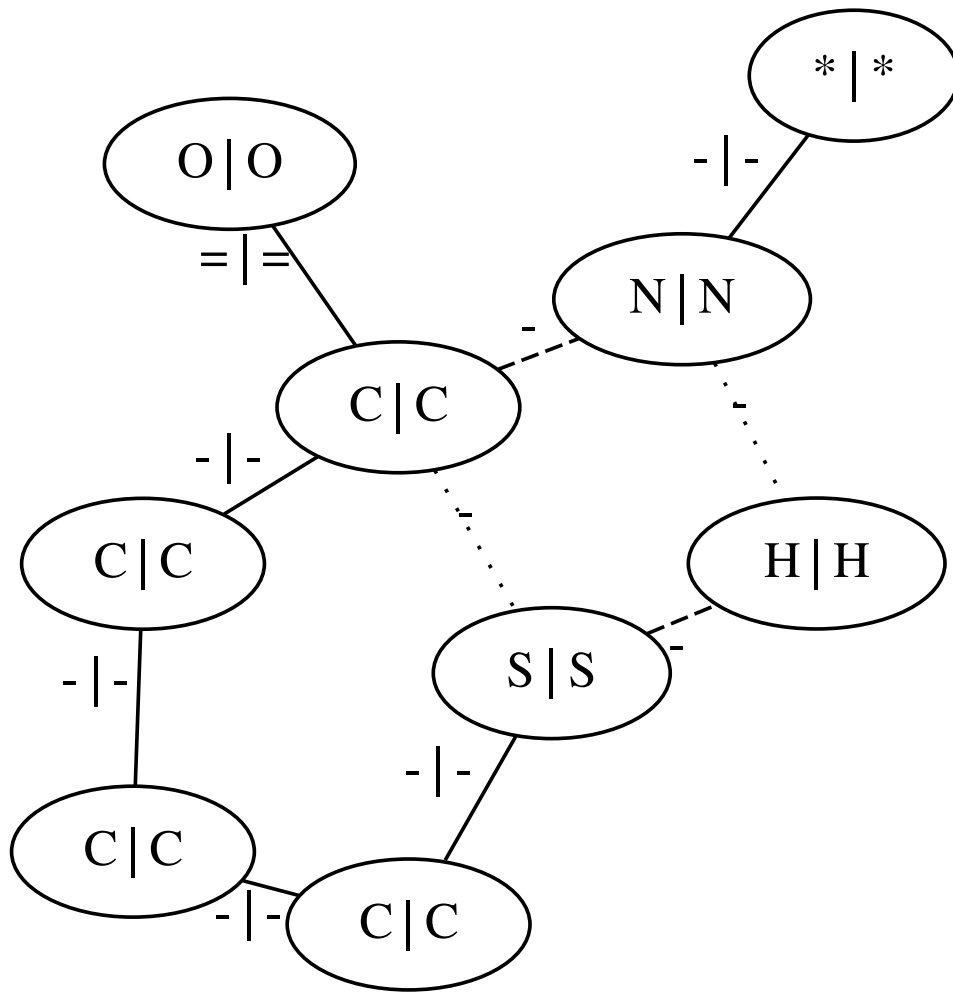
```

|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

0.0.130 Ring Closure 5 membered N, S





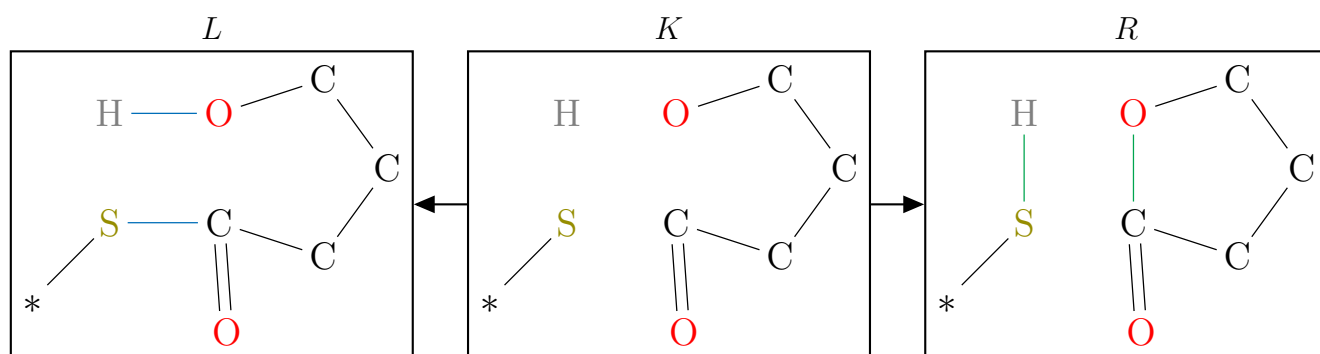
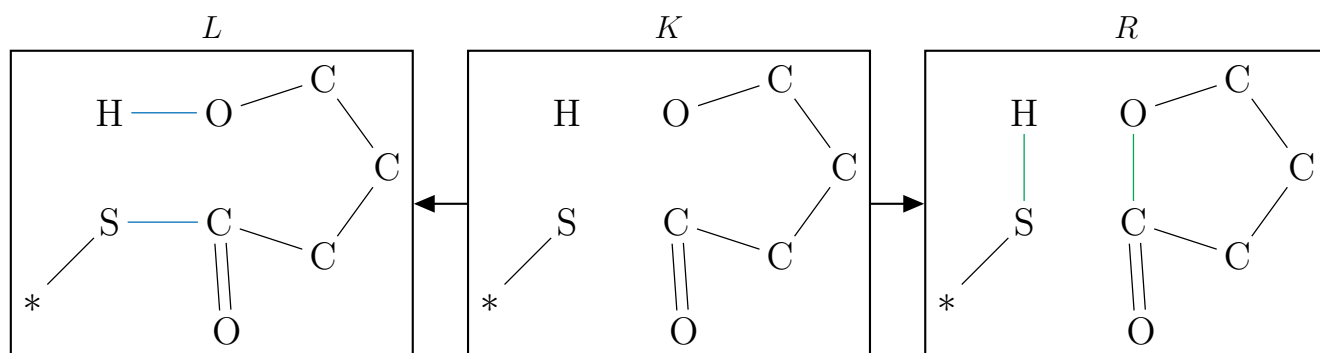
File: out/647_r_132_combined

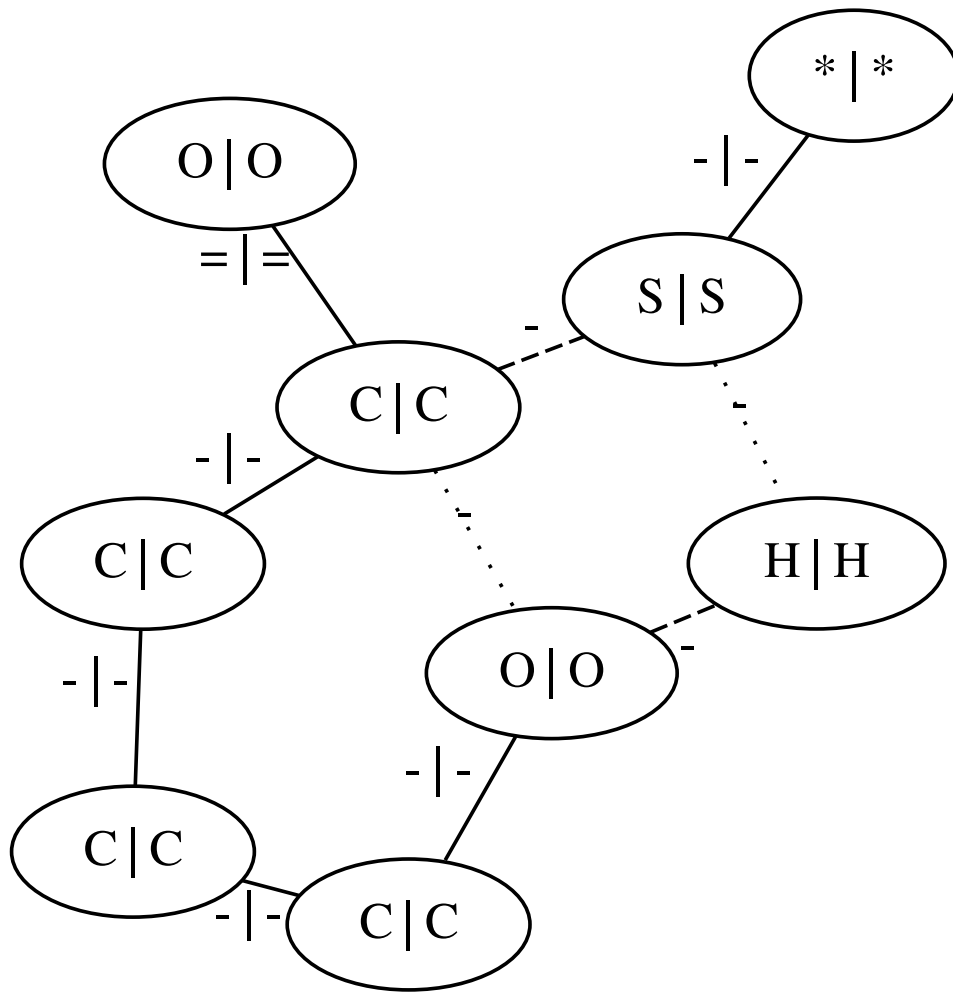
```

|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

0.0.131 Ring Closure 5 membered S, O





File: out/652_r_133_combined

$$|\{e \in \text{outEdges}(2) \mid$$

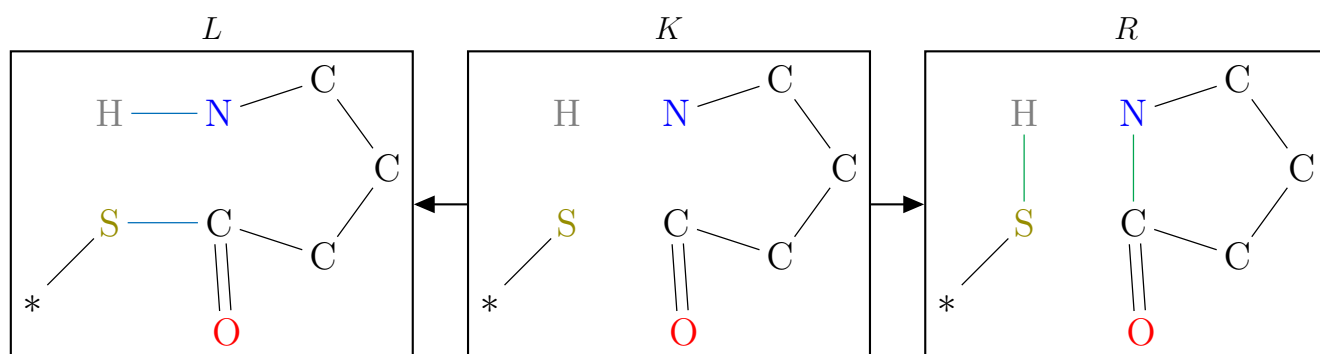
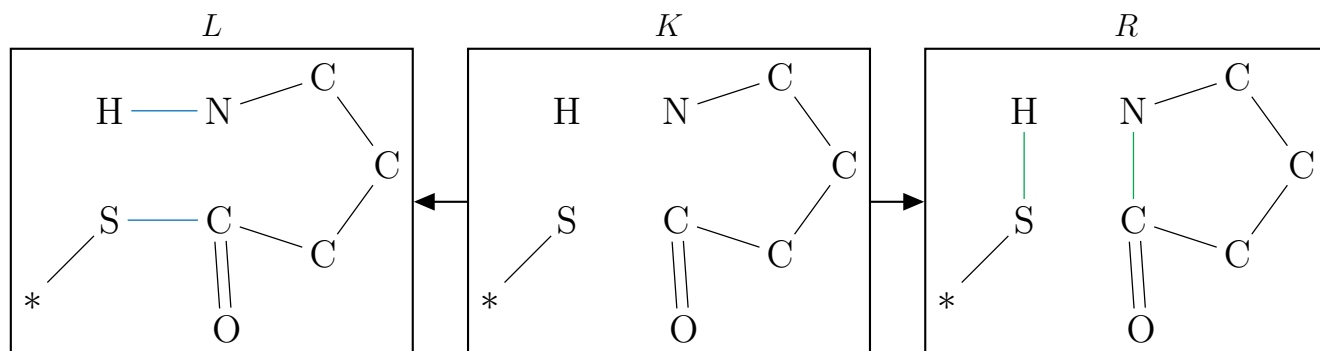
$$\text{label}(\text{target}(e)) \in \{\text{'S'}\}$$

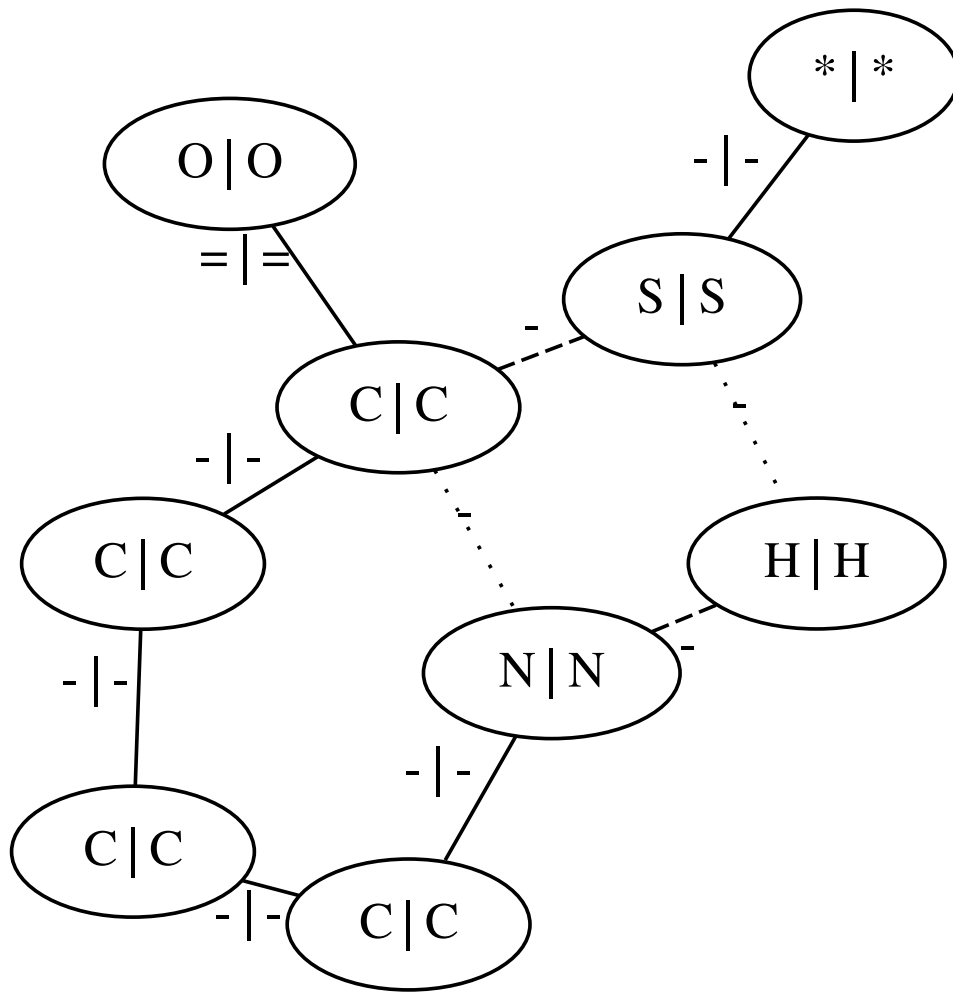
$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 1$$

0.0.132 Ring Closure 5 membered S, N

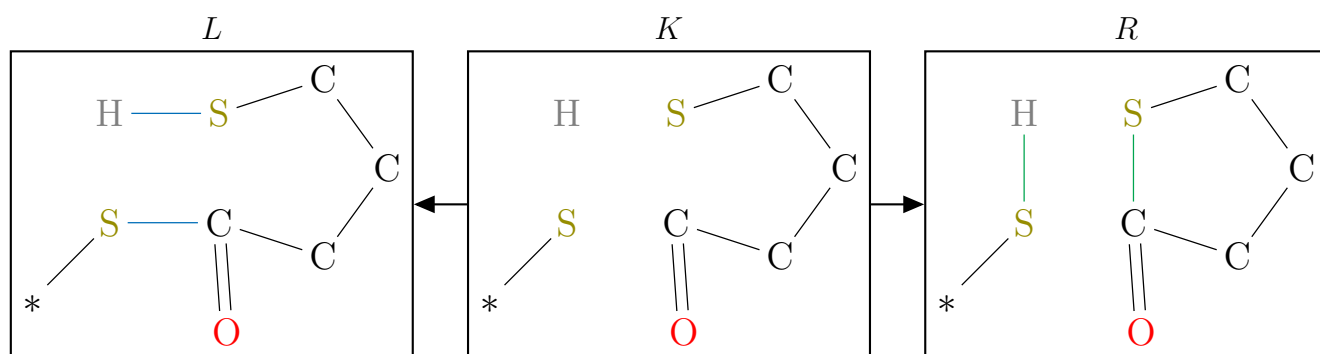
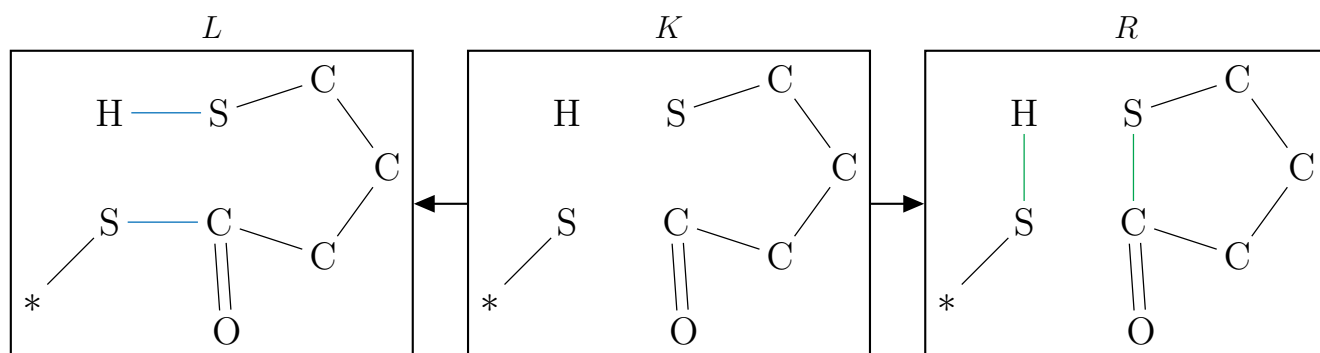


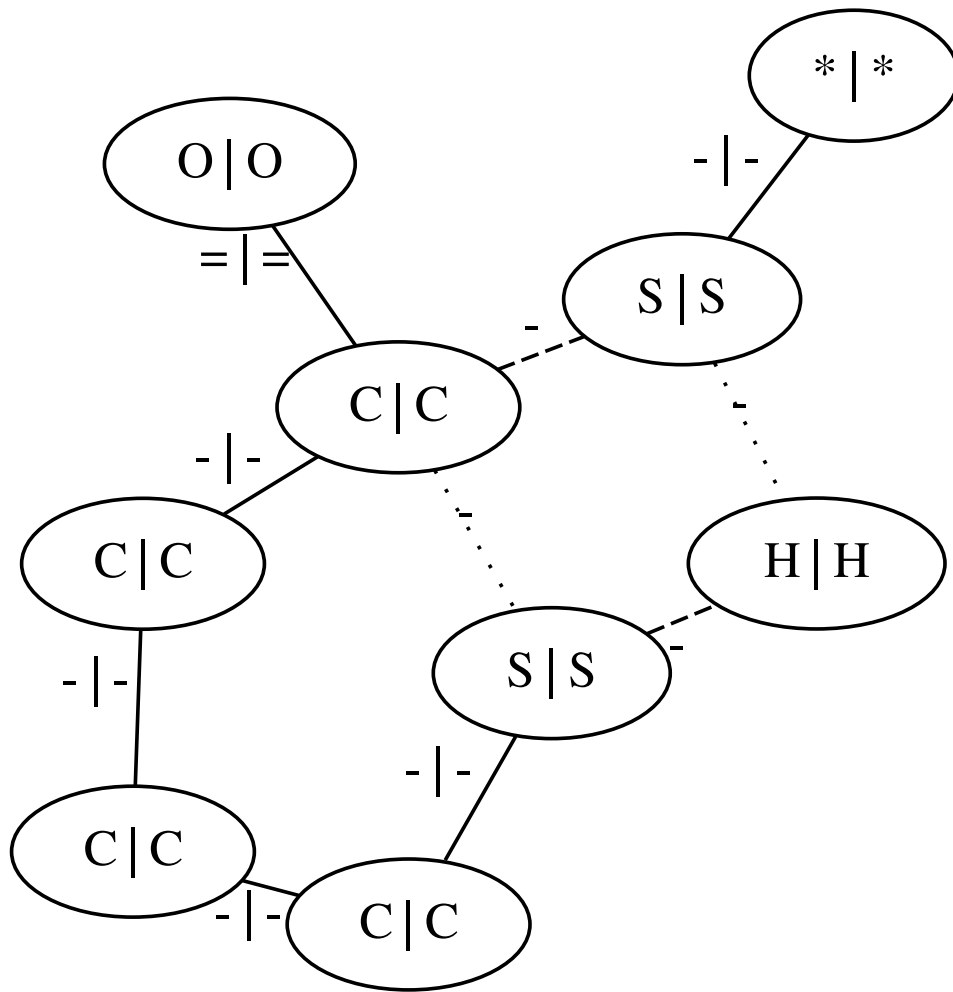


File: out/657_r_134_combined

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

0.0.133 Ring Closure 5 membered S, S





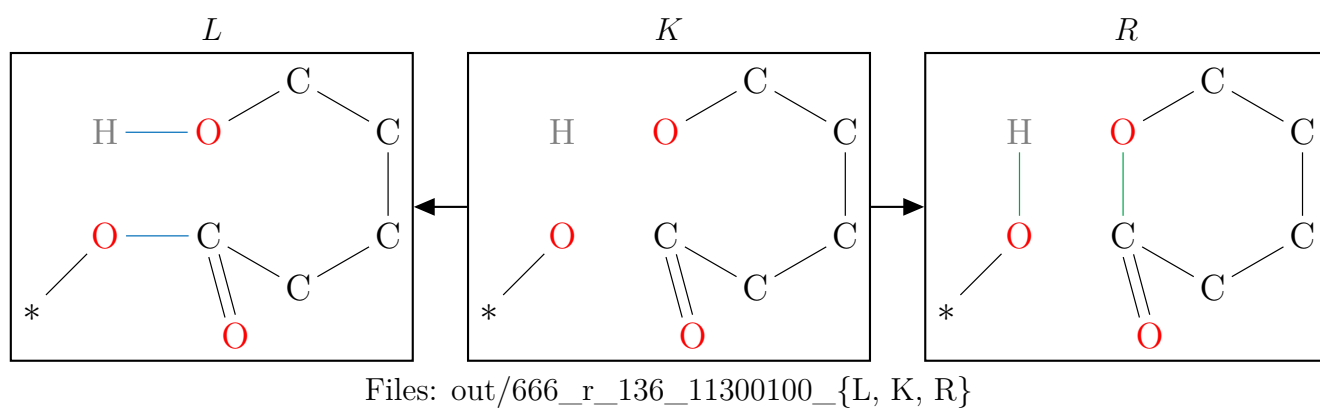
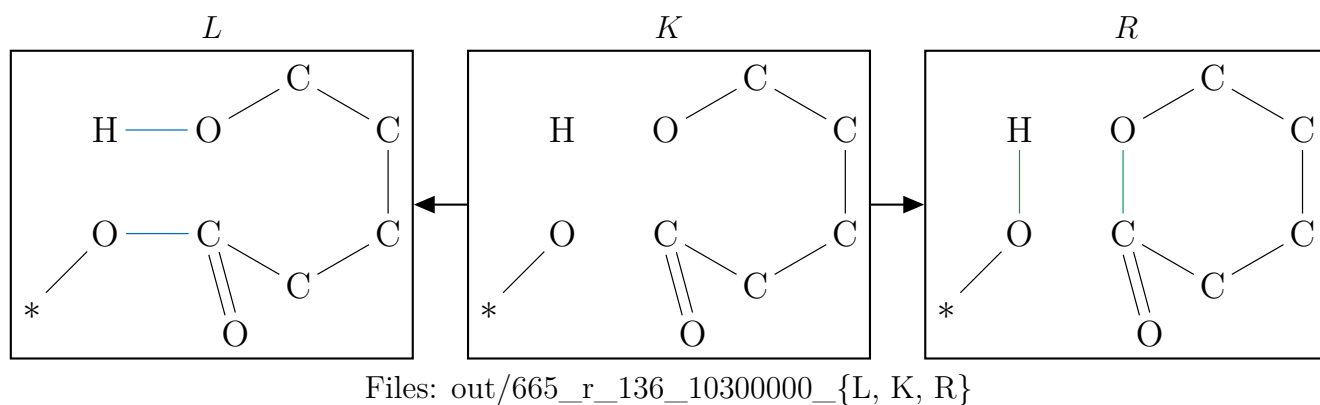
File: out/662_r_135_combined

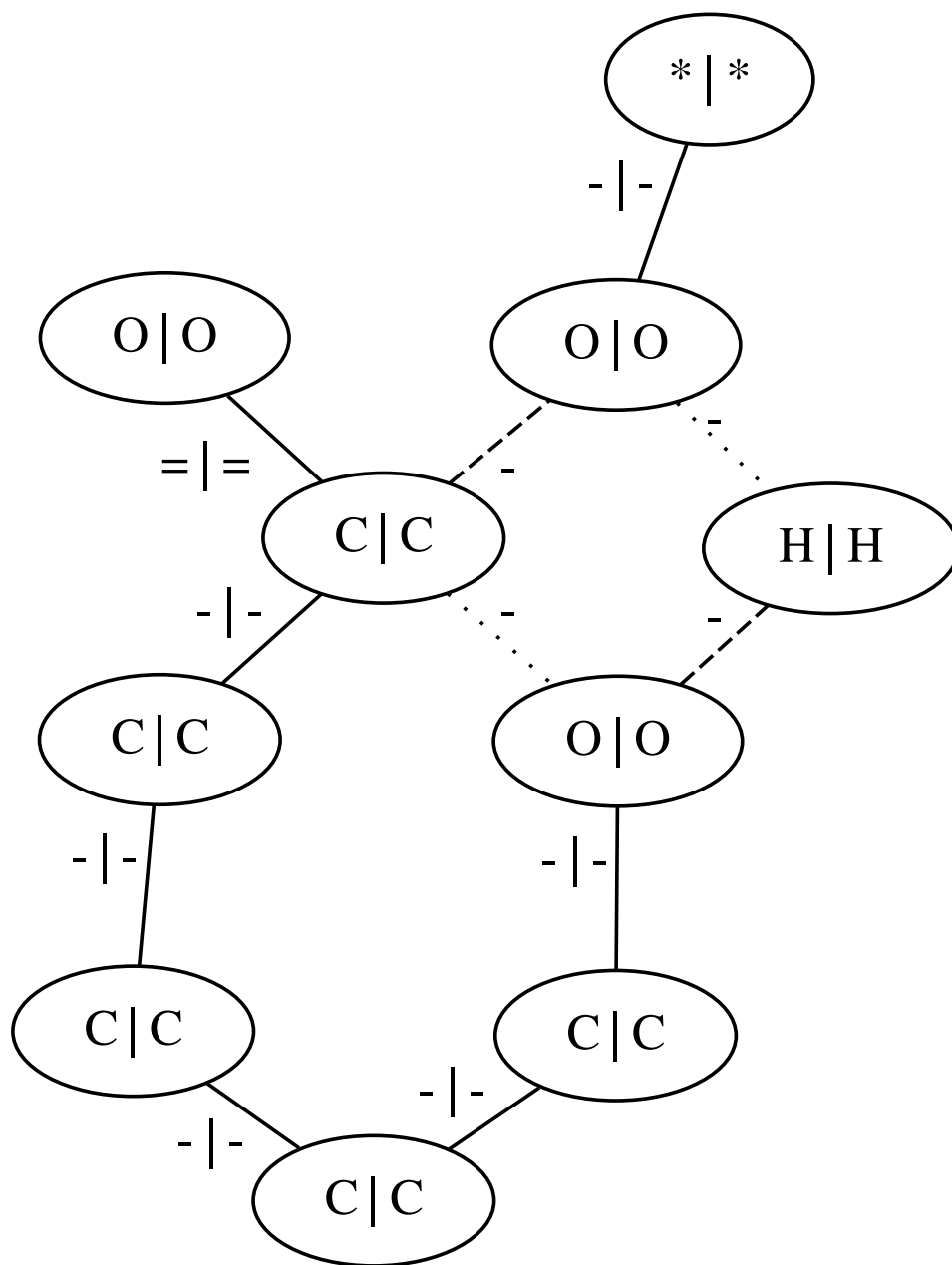
```

|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'S'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

0.0.134 Ring Closure 6 membered O, O





File: out/667_r_136_combined

$$|\{e \in \text{outEdges}(2) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 1$$

$$|\{e \in \text{outEdges}(2) \mid$$

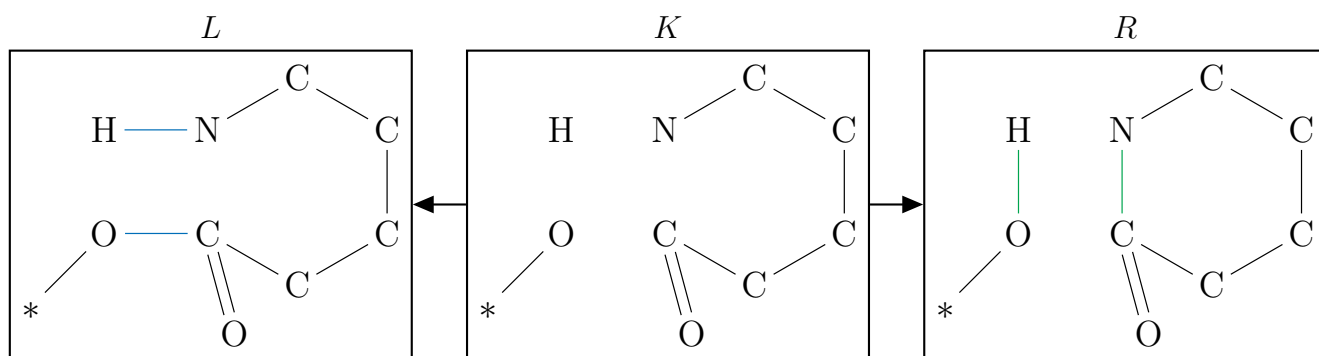
$$\text{label}(\text{target}(e)) \in \{\text{'C'}\}$$

$$\wedge$$

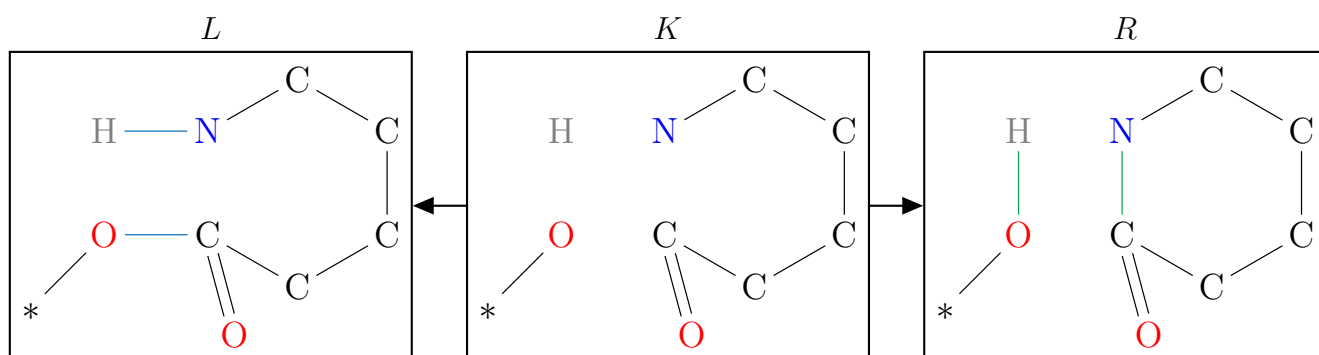
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

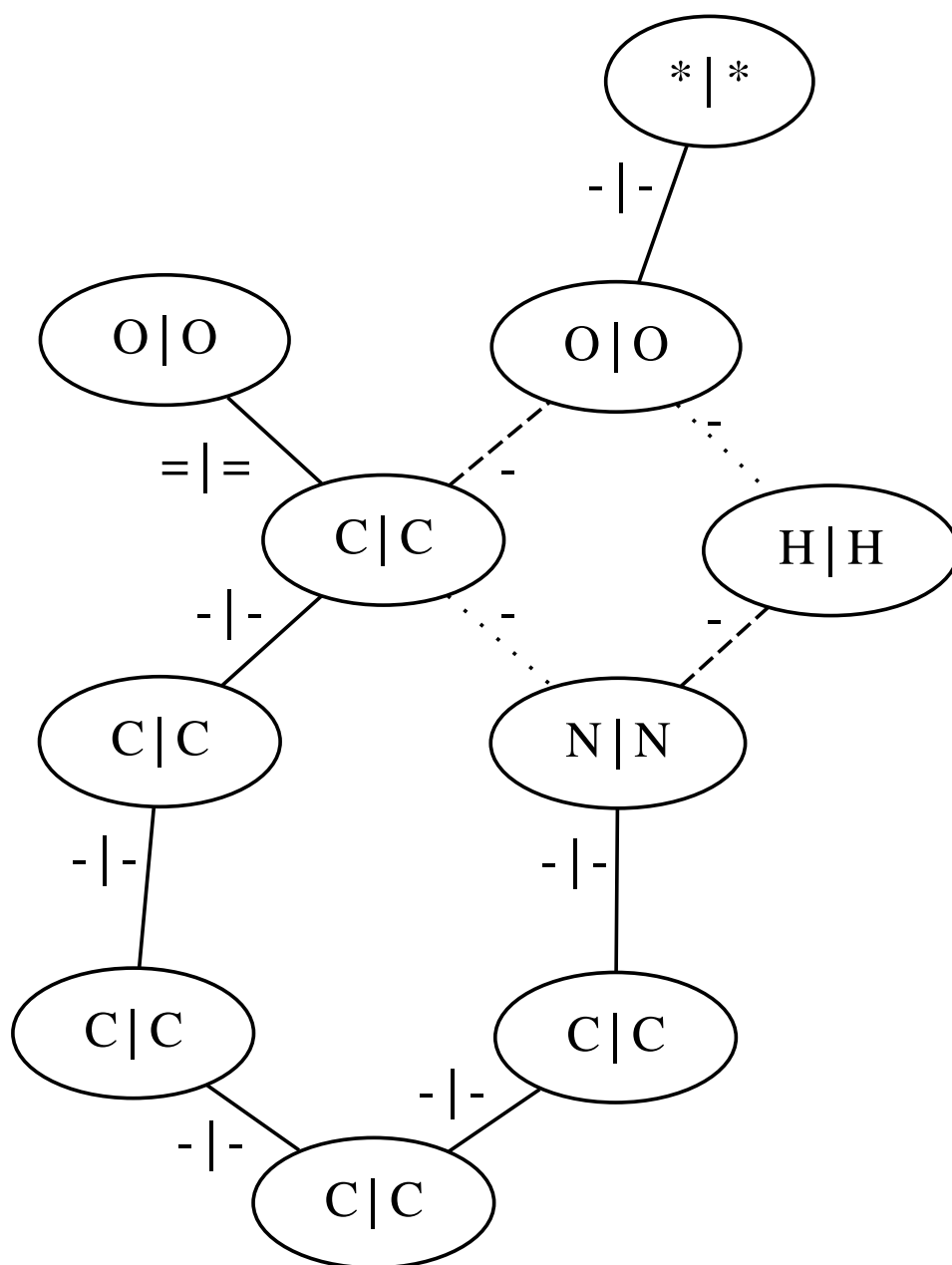
0.0.135 Ring Closure 6 membered O, N



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



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

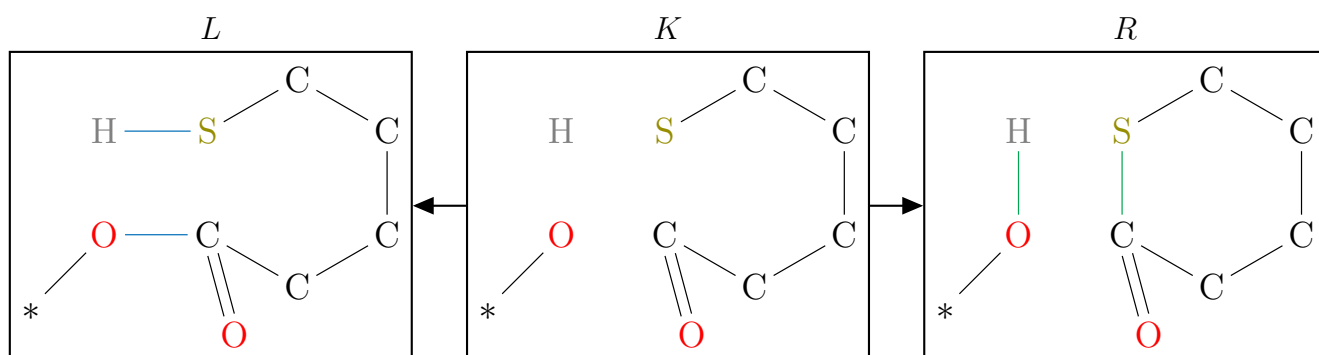
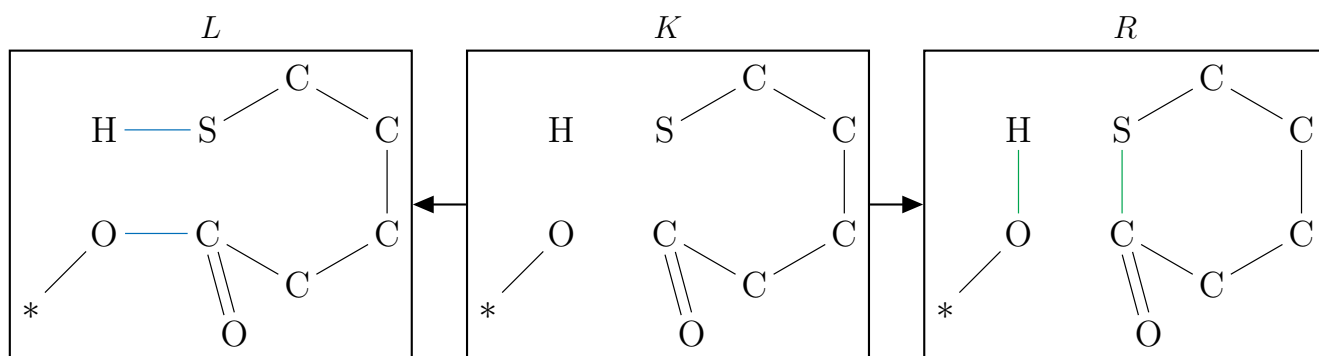


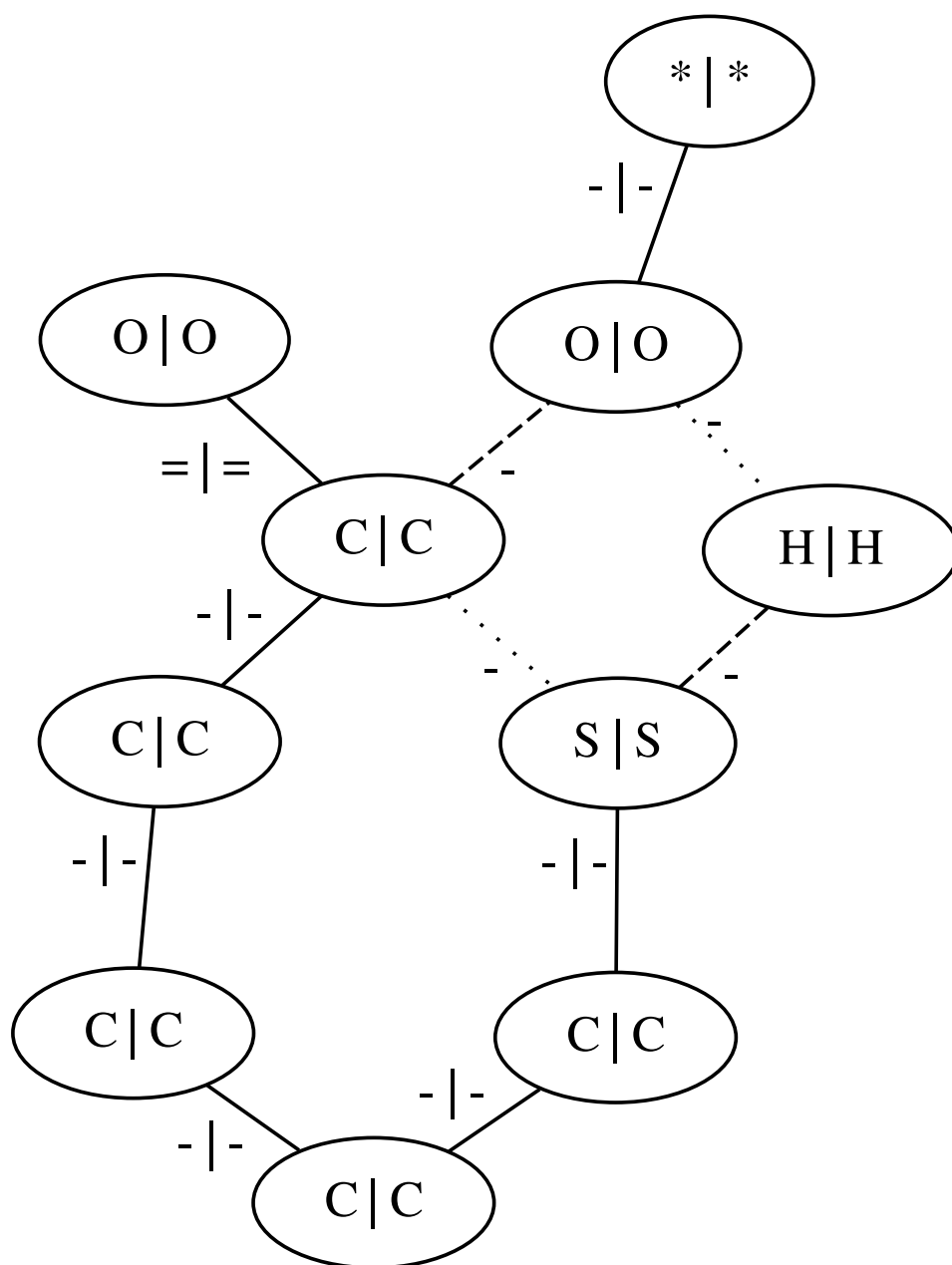
File: out/672_r_137_combined

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

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

0.0.136 Ring Closure 6 membered O, S



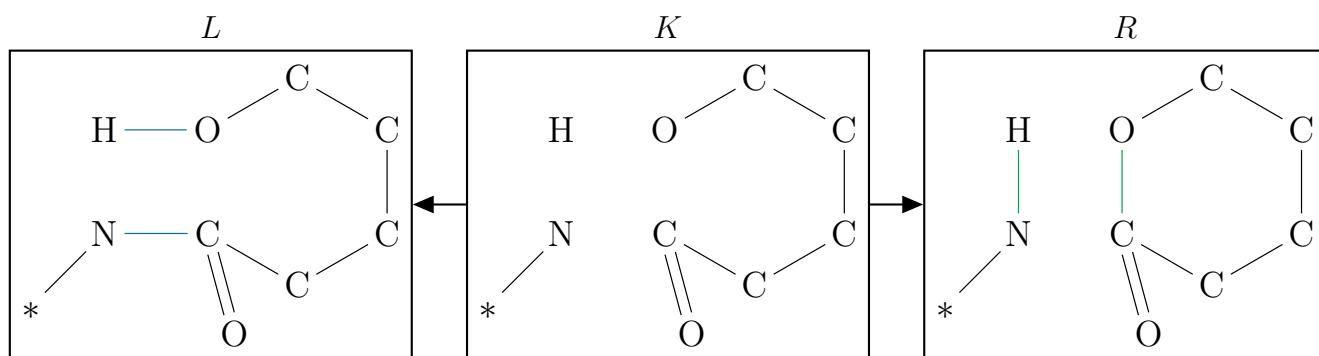


File: out/677_r_138_combined

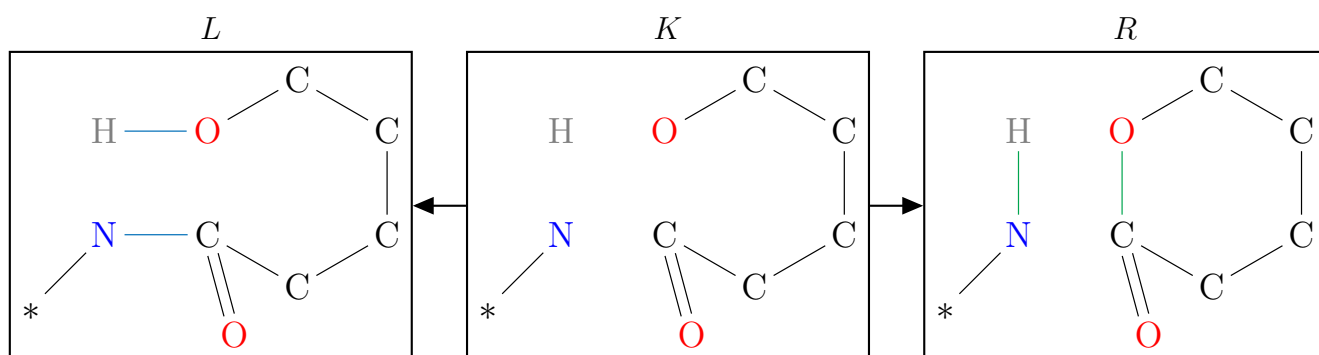
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid = 1
\end{aligned}$$

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

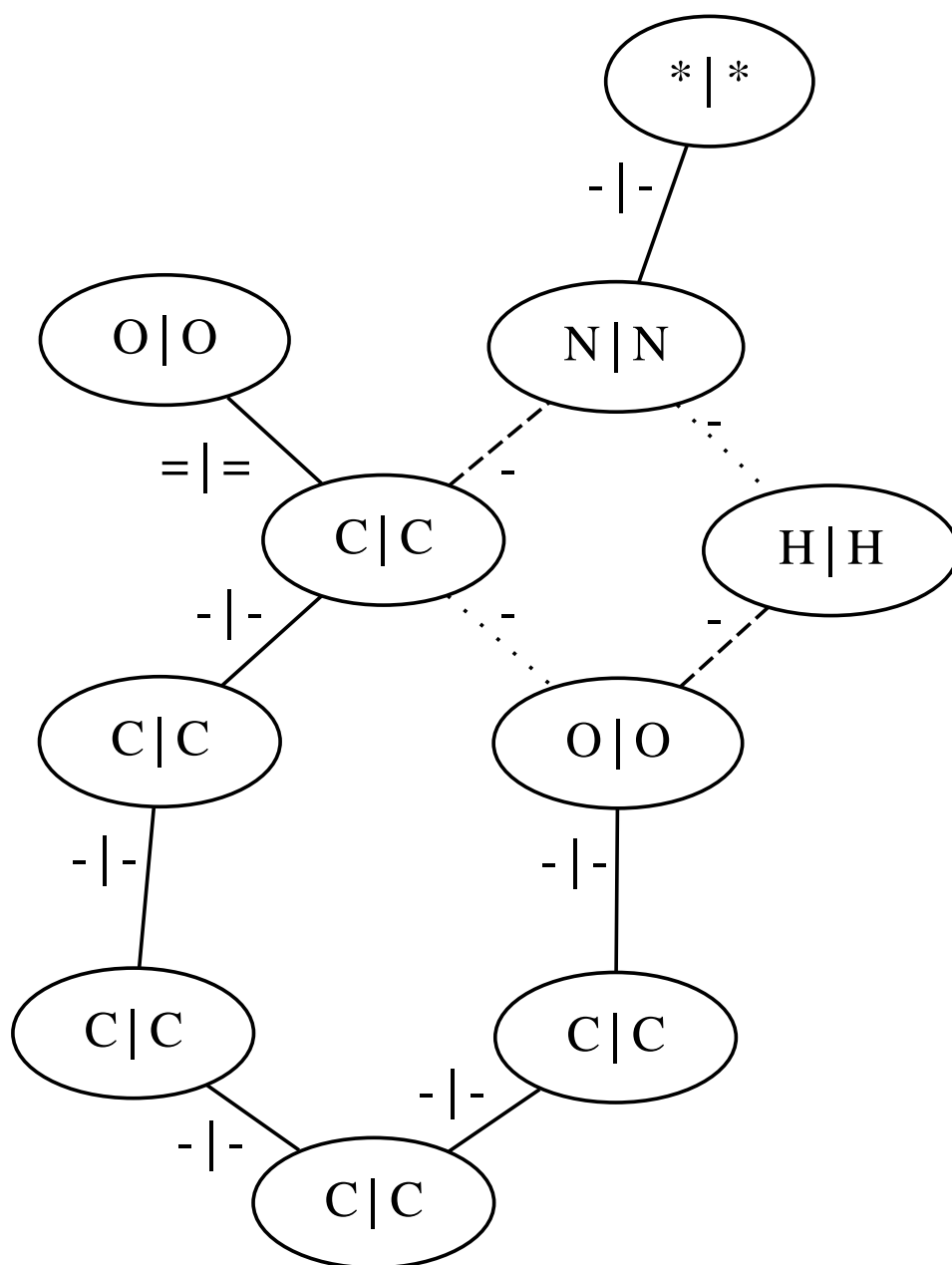
0.0.137 Ring Closure 6 membered N, O



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



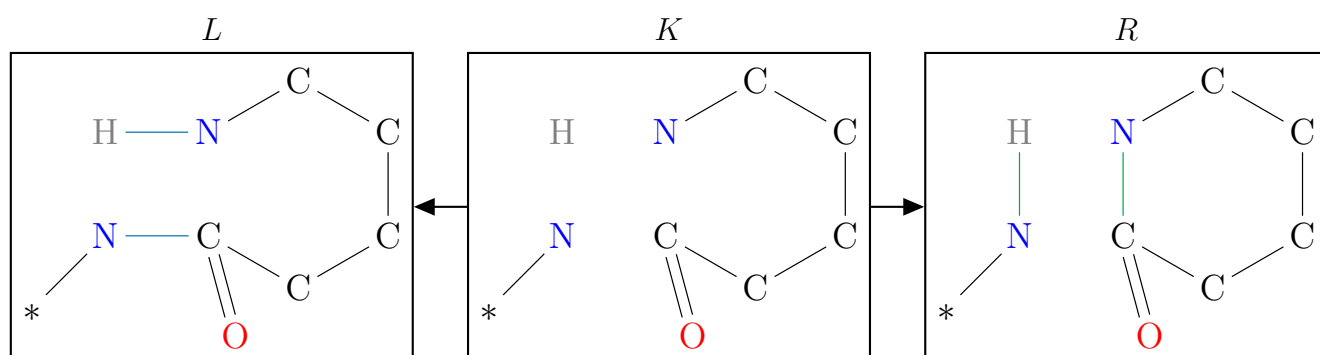
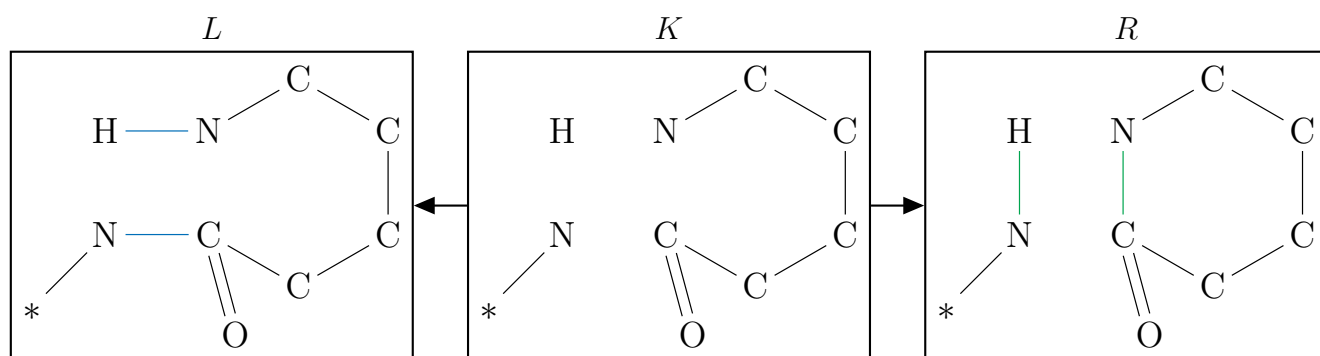
Files: out/681_r_139_11300100_{L, K, R}

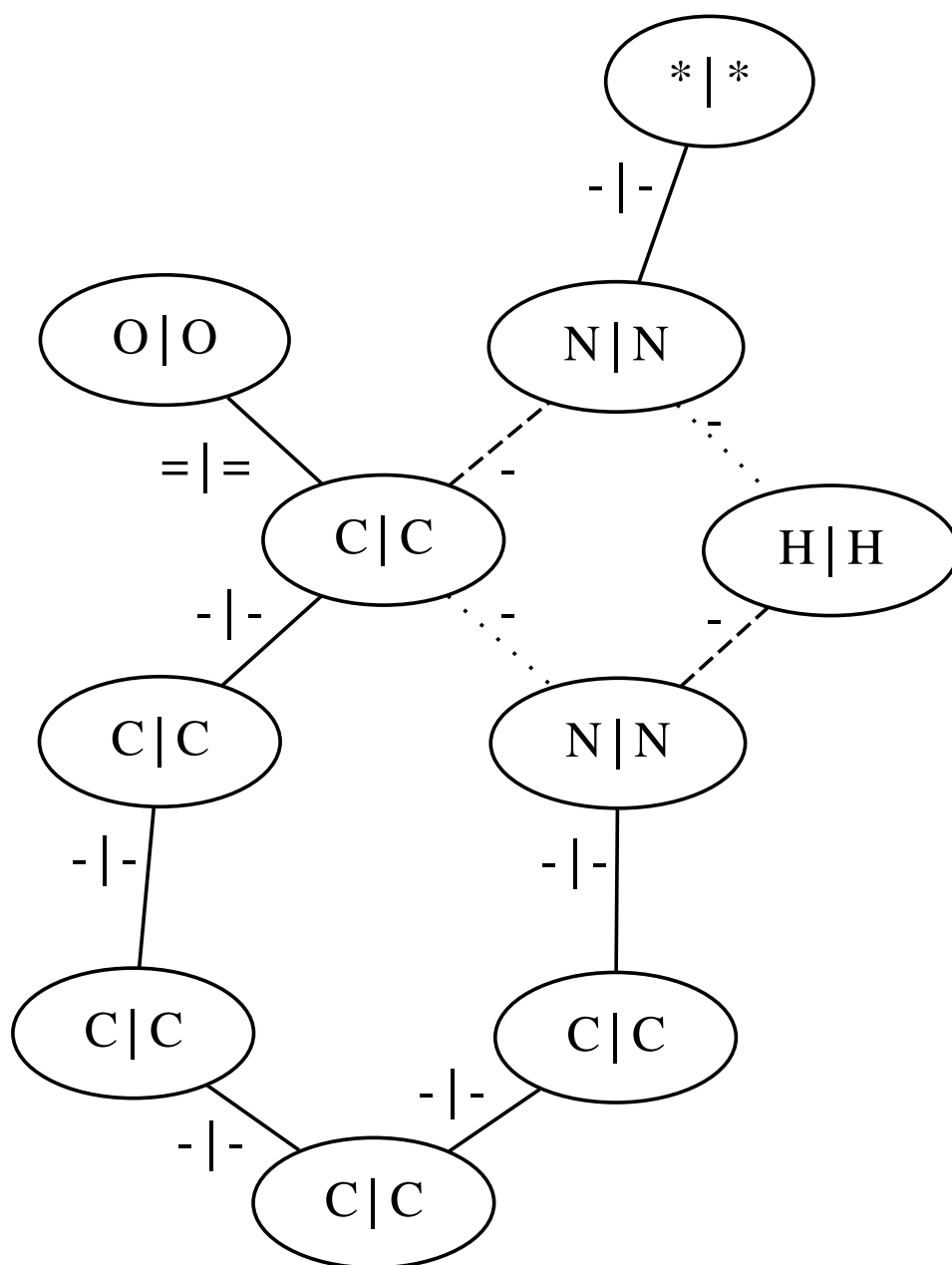


File: out/682_r_139_combined

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

0.0.138 Ring Closure 6 membered N, N

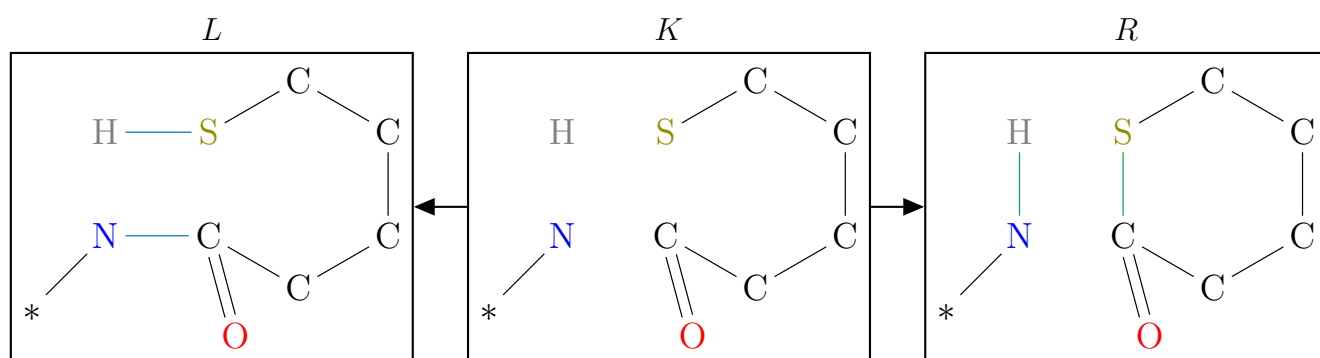
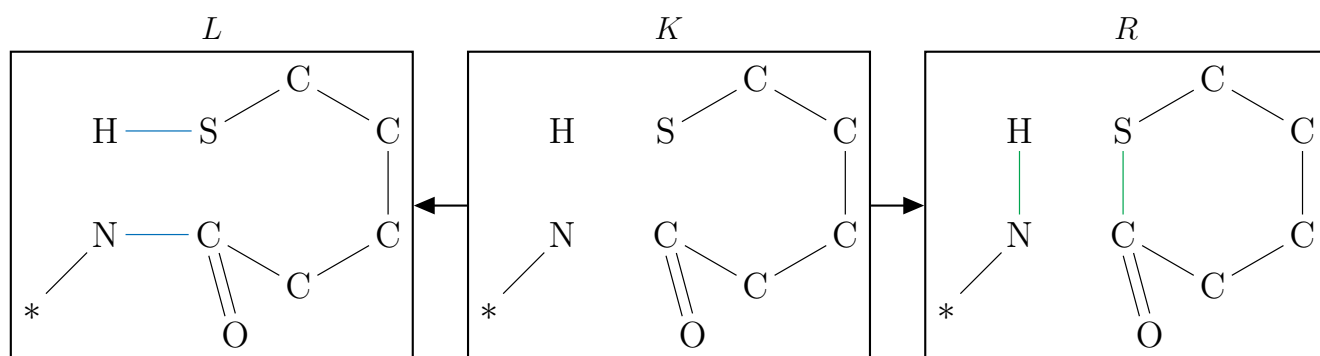


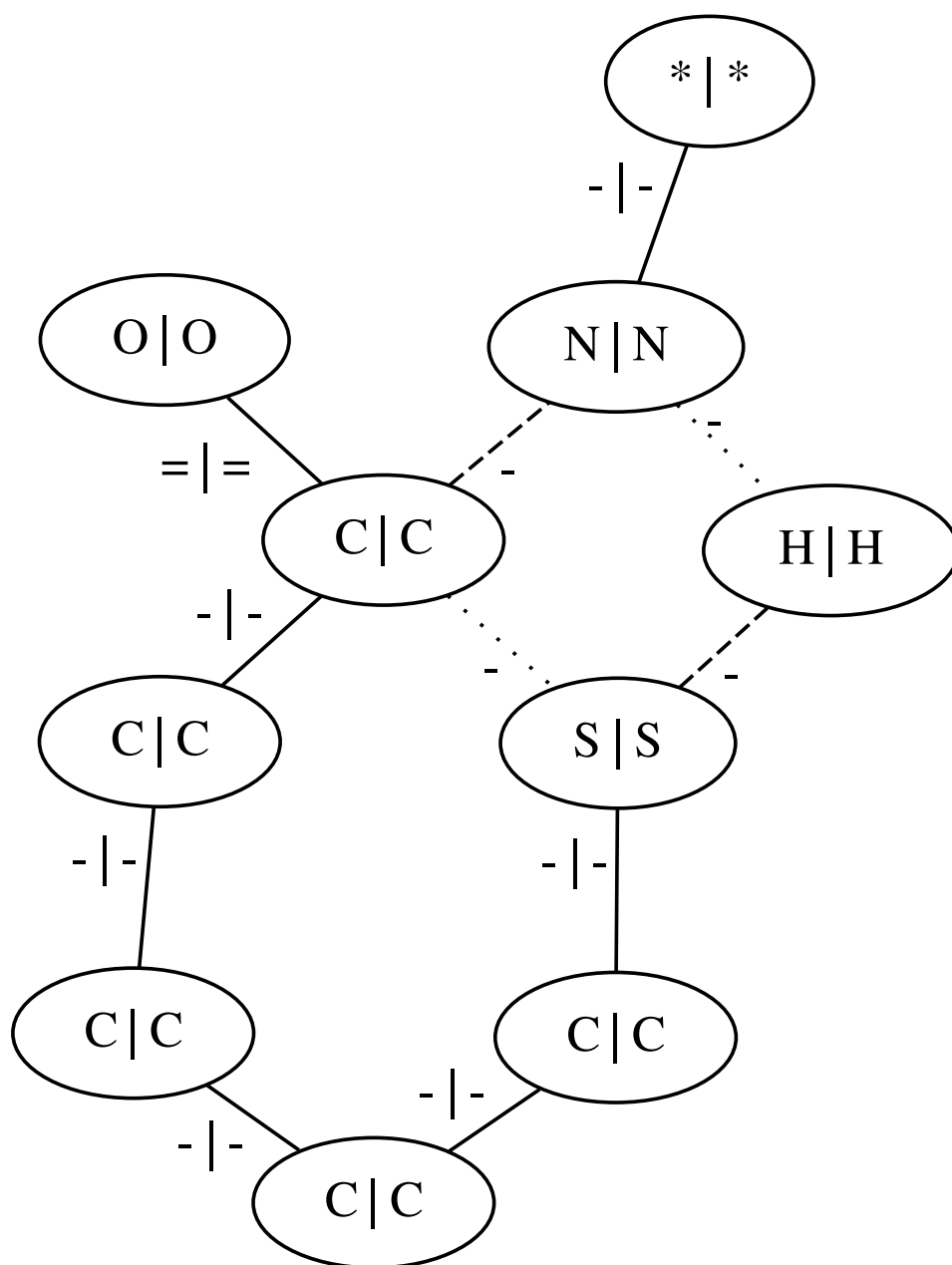


File: out/687_r_140_combined

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

0.0.139 Ring Closure 6 membered N, S

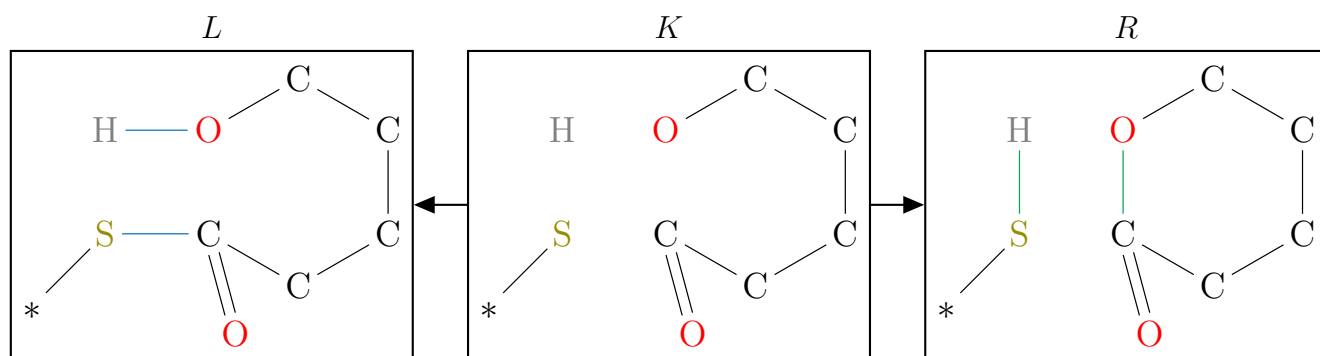
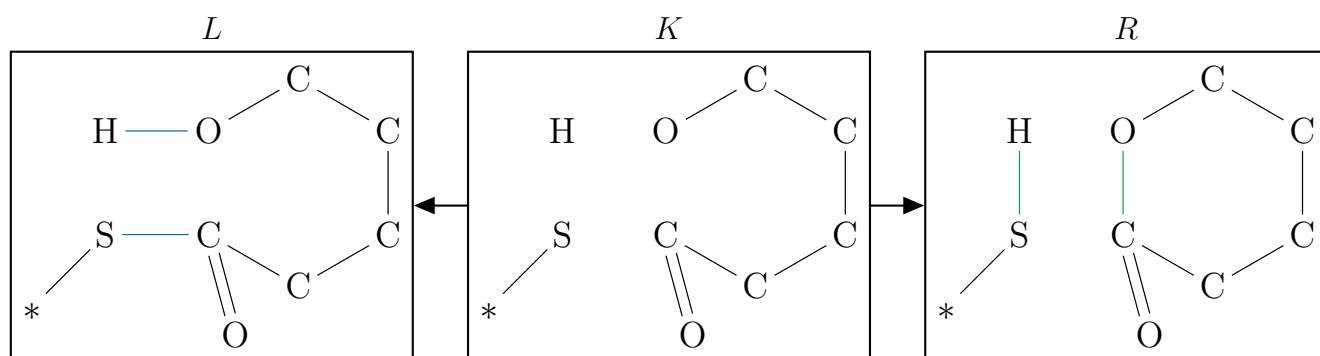


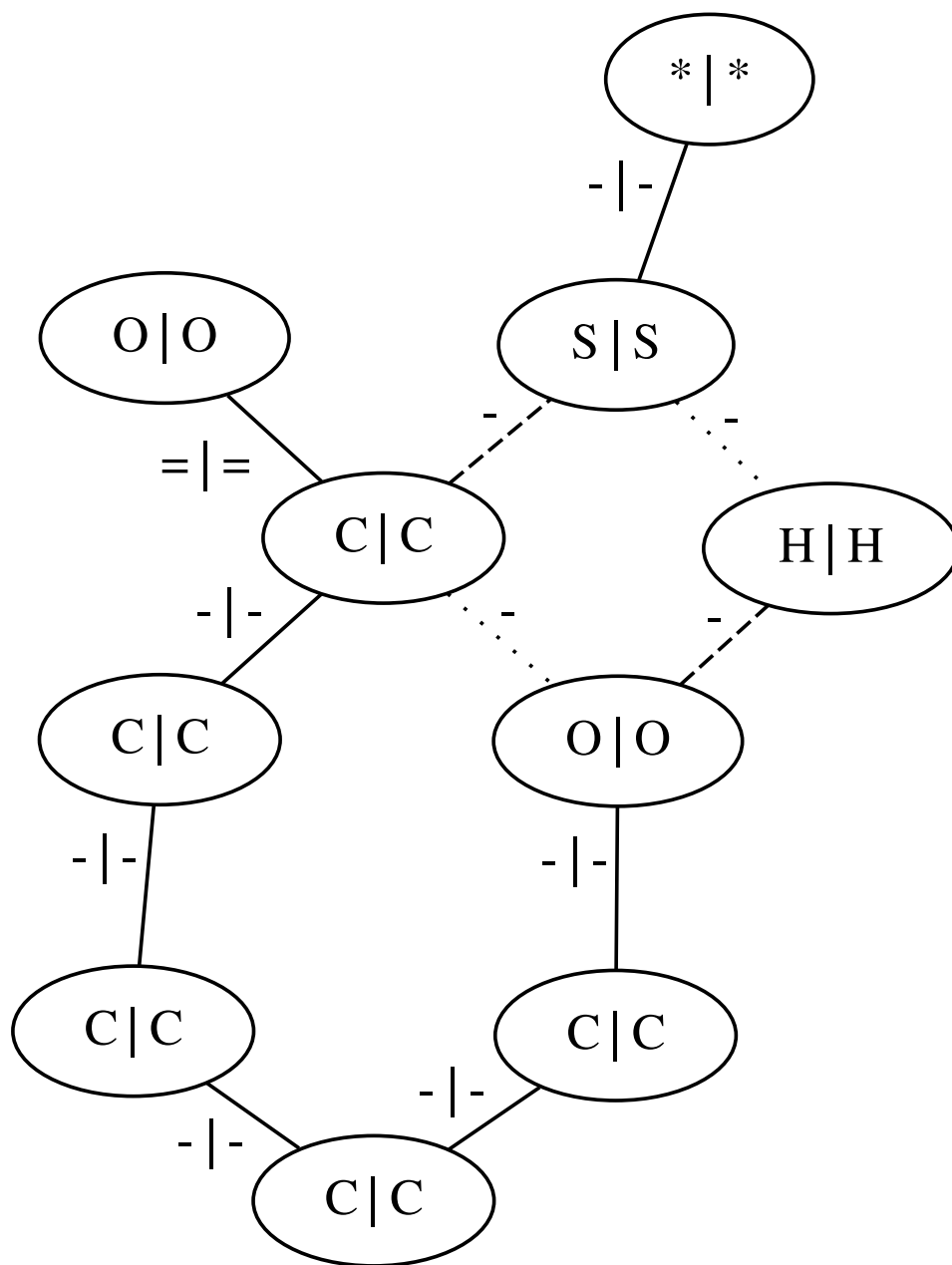


File: out/692_r_141_combined

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

0.0.140 Ring Closure 6 membered S, O

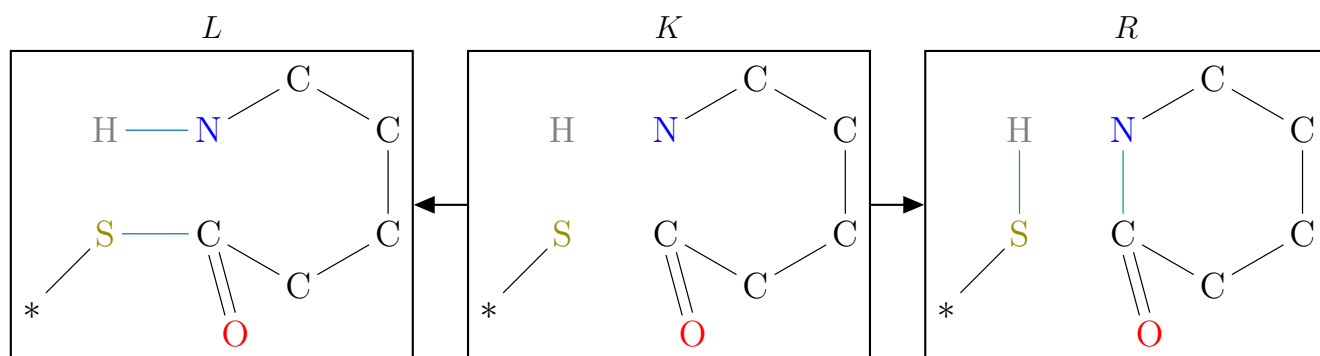
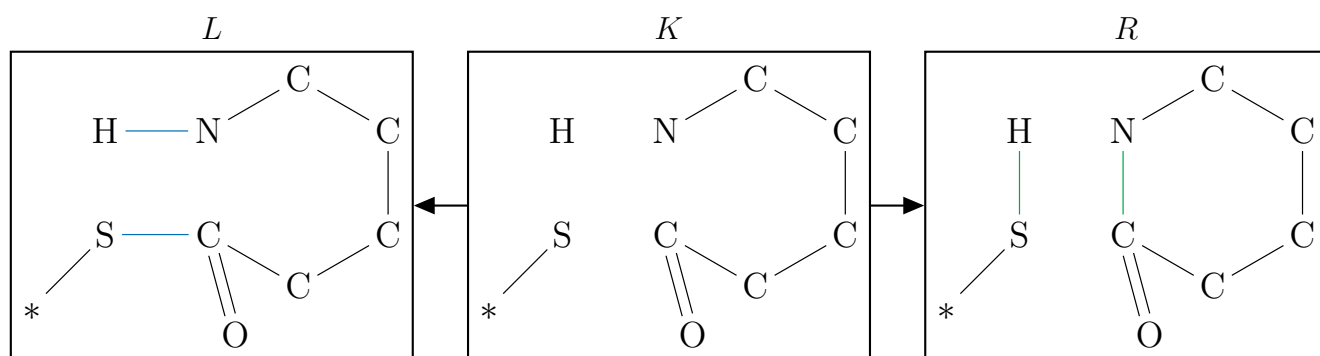


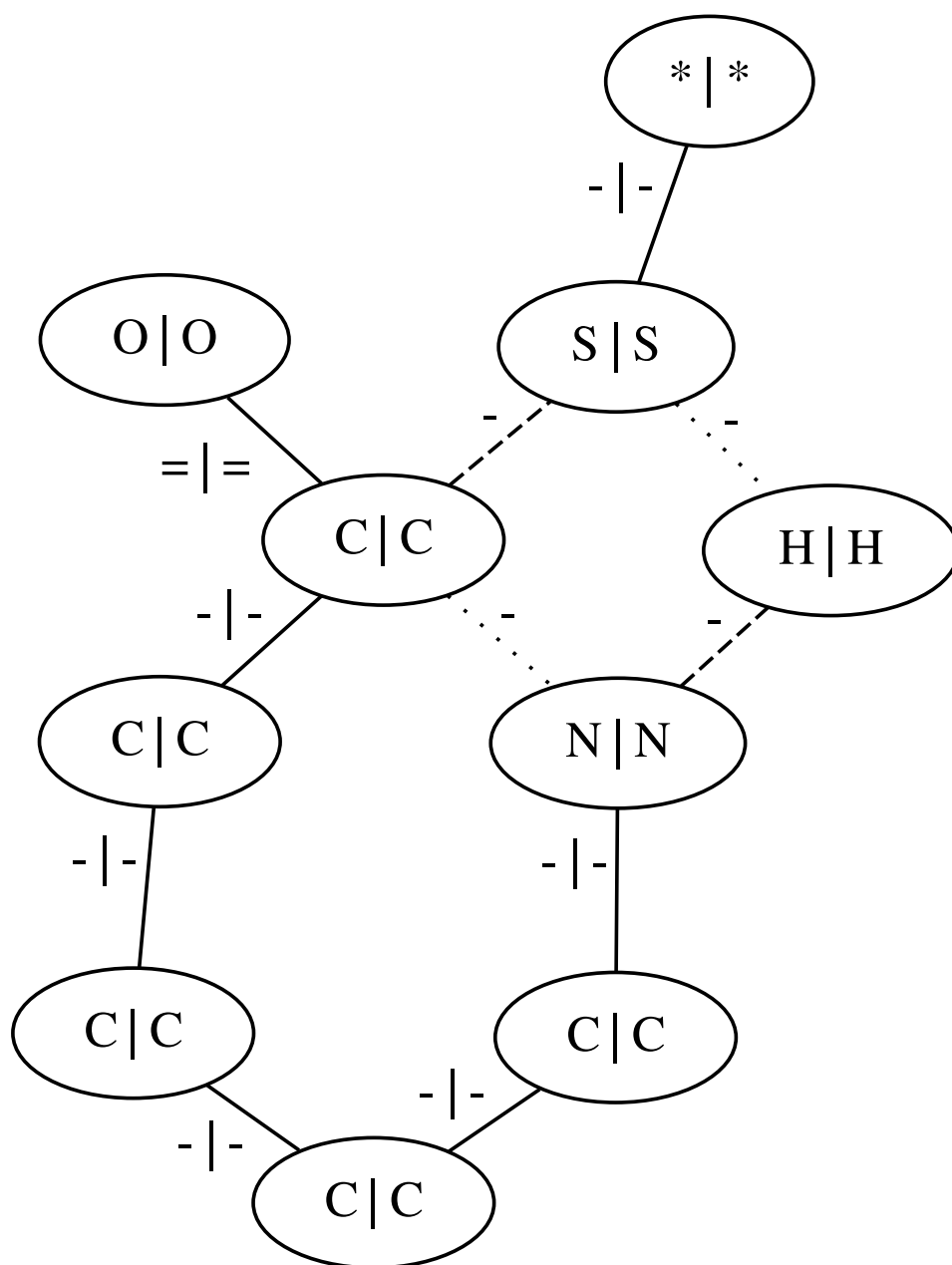


File: out/697_r_142_combined

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

0.0.141 Ring Closure 6 membered S, N

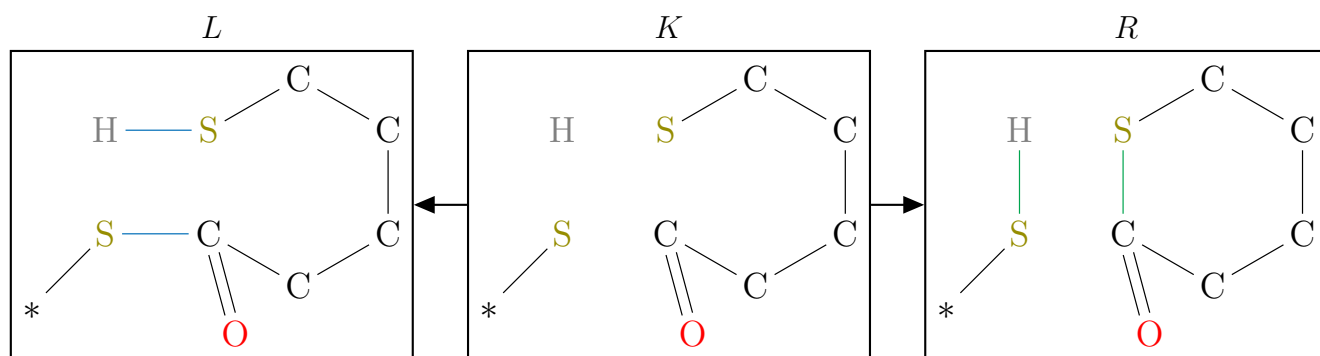
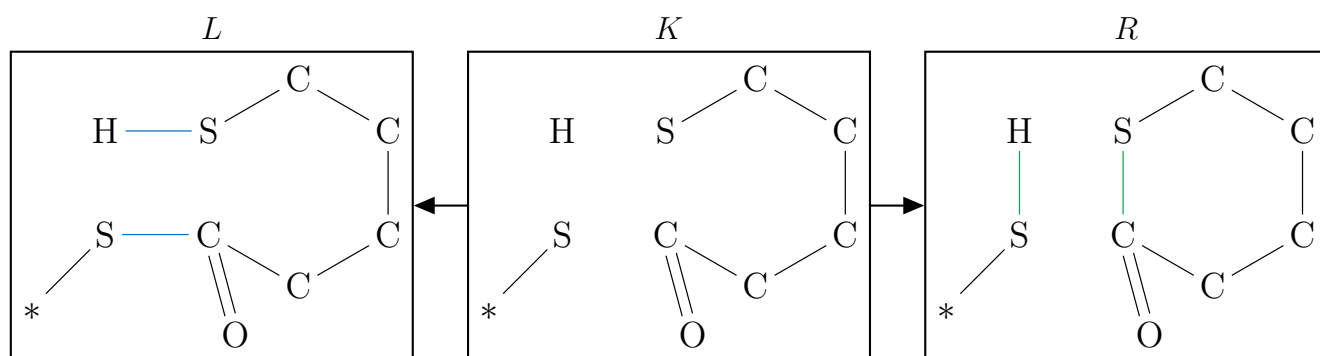


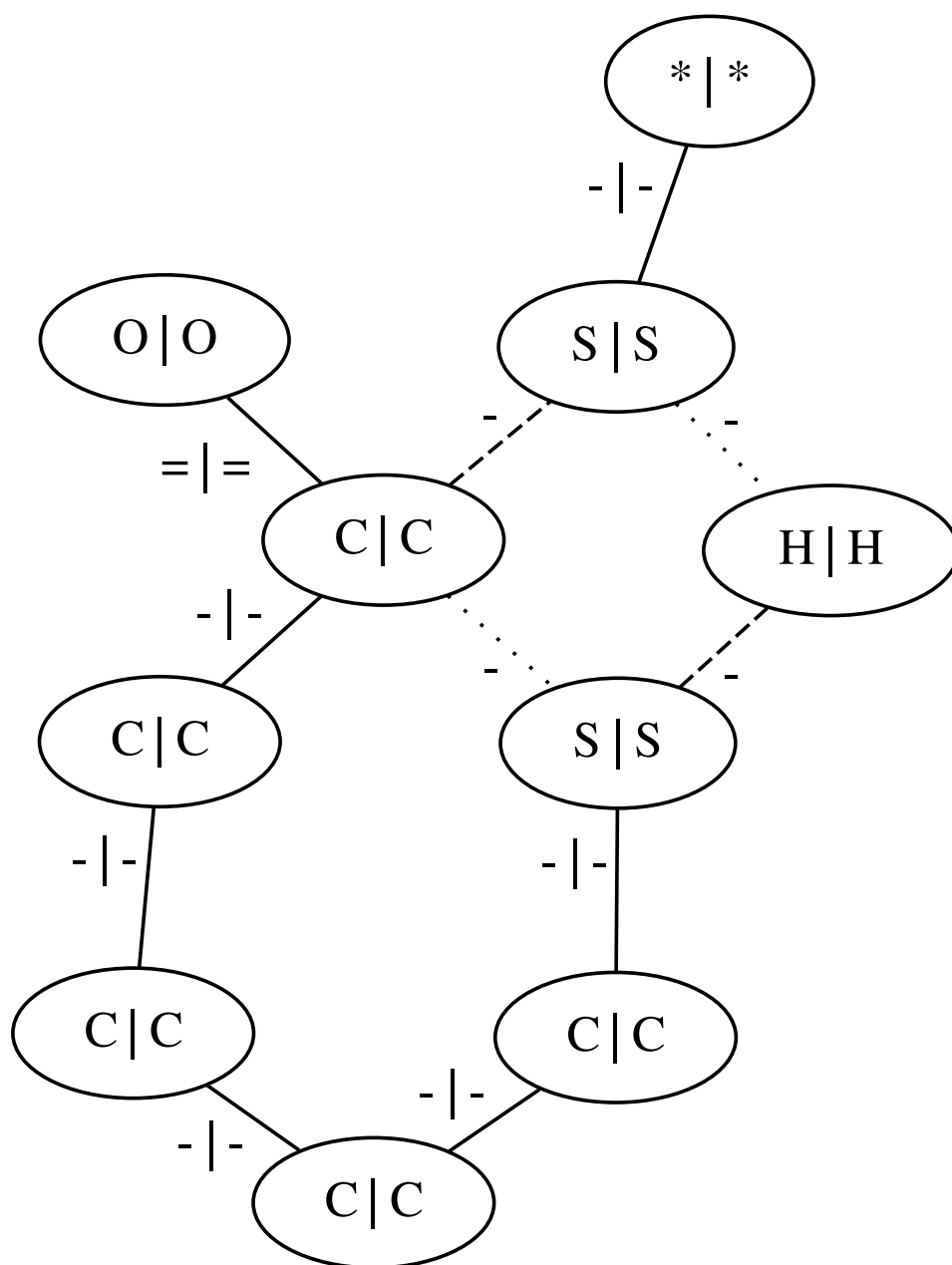


File: out/702_r_143_combined

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

0.0.142 Ring Closure 6 membered S, S

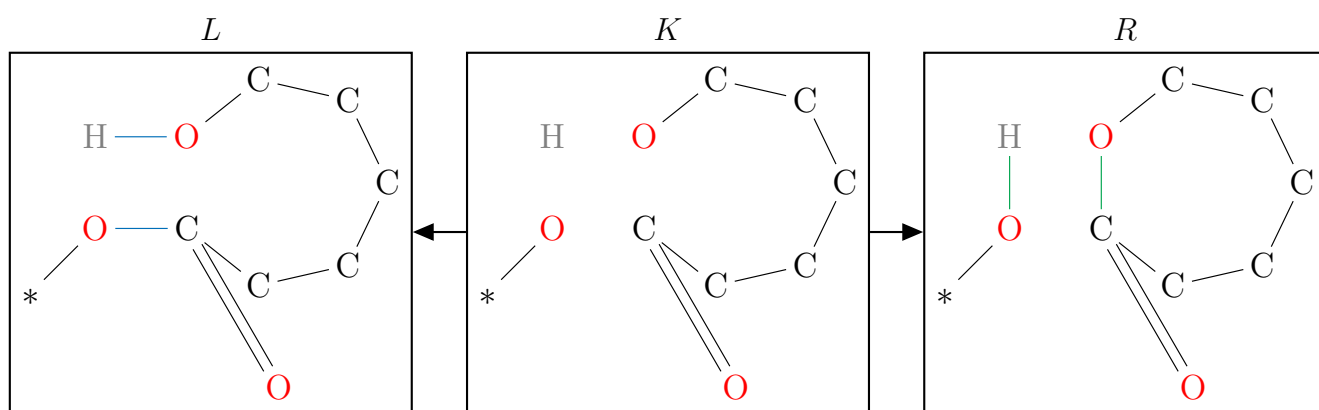
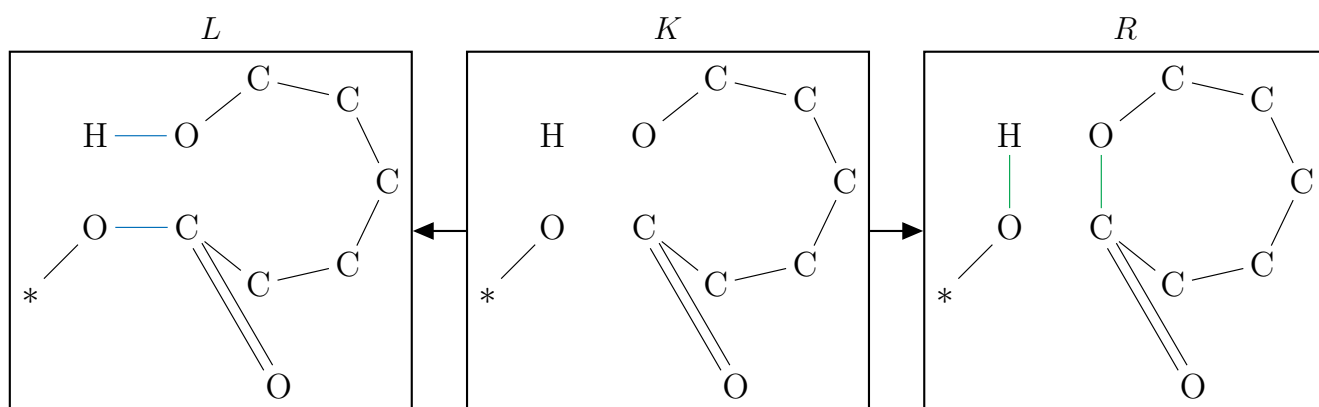


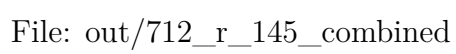


File: out/707_r_144_combined

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

0.0.143 Ring Closure 7 membered O, O

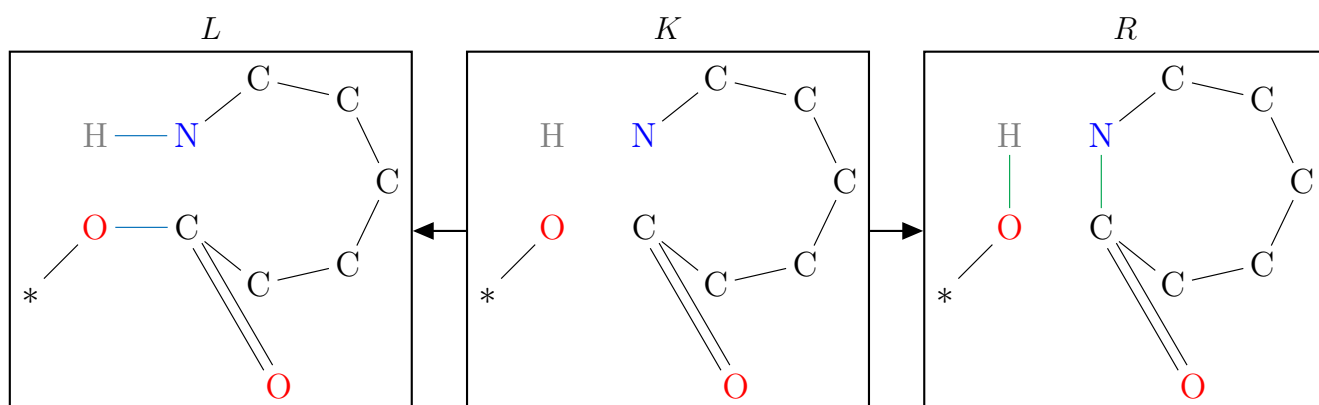
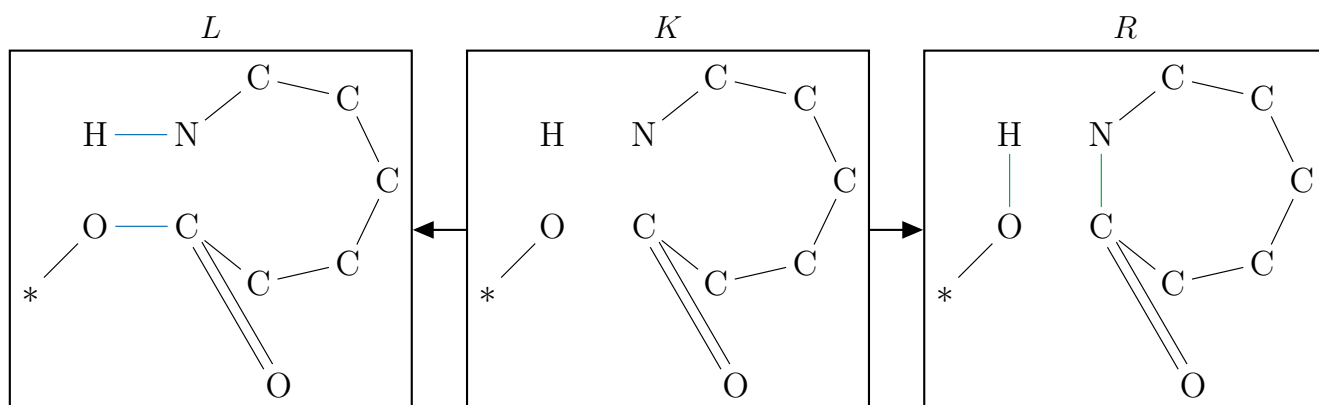


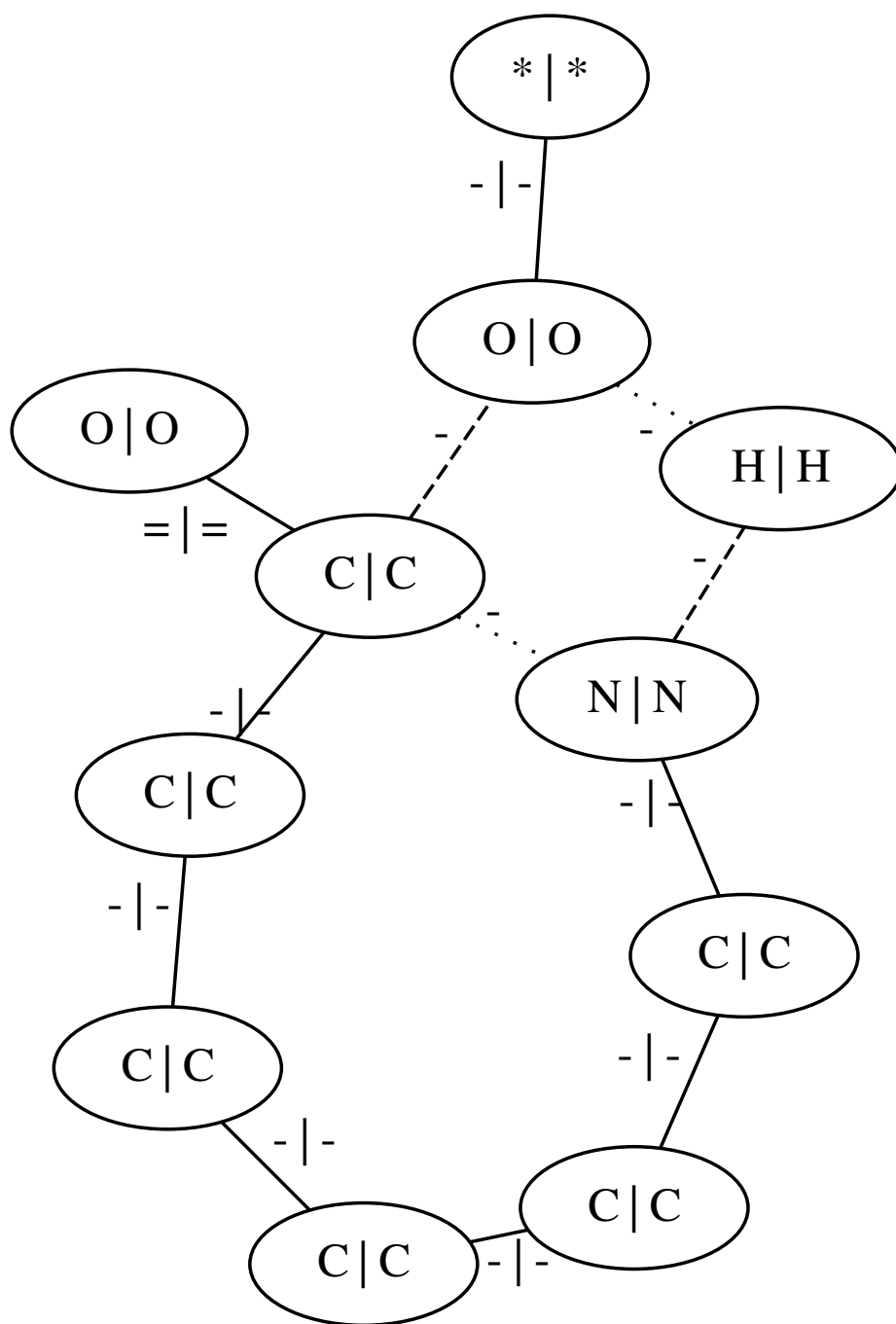


$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 1
\end{aligned}$$

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

0.0.144 Ring Closure 7 membered O, N



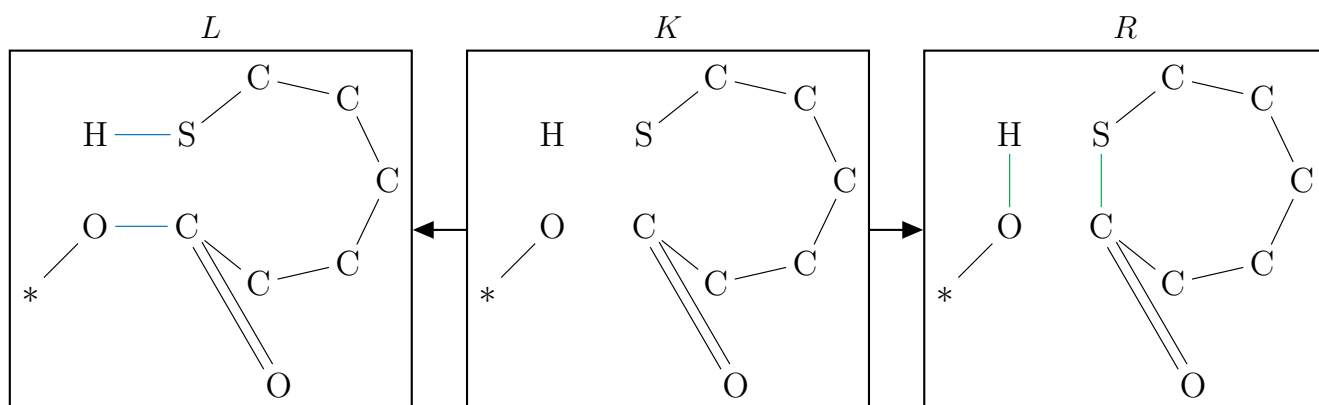


File: out/717_r_146_combined

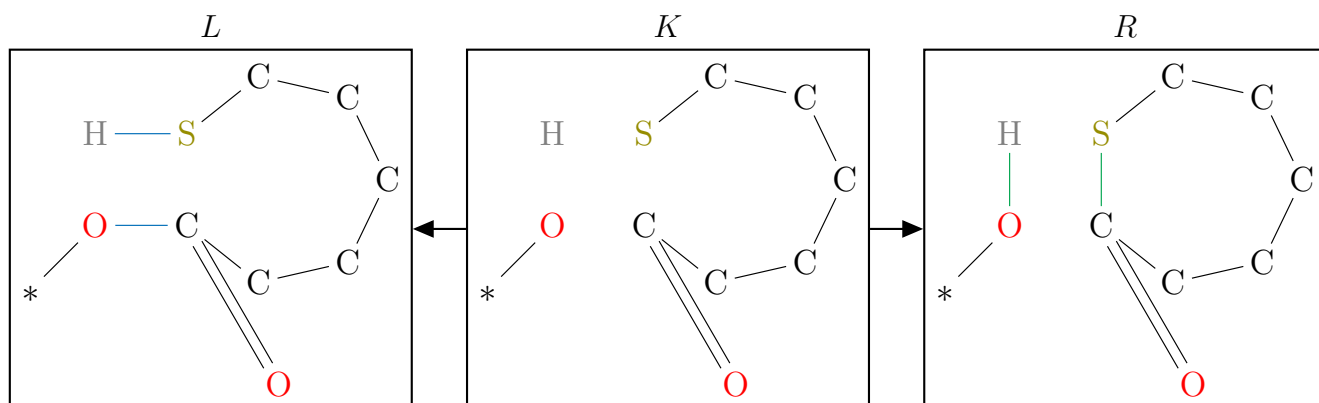
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 1
\end{aligned}$$

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

0.0.145 Ring Closure 7 membered O, S



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

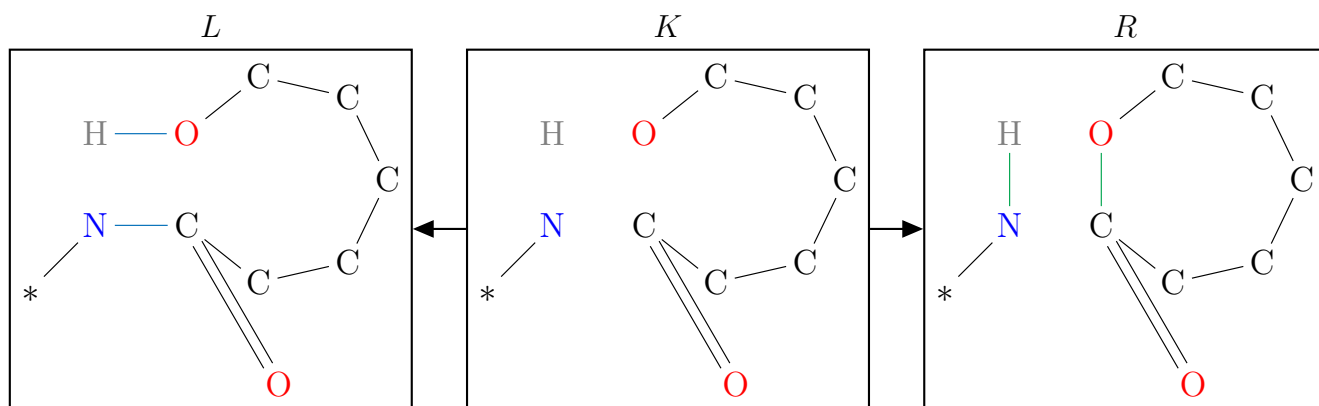
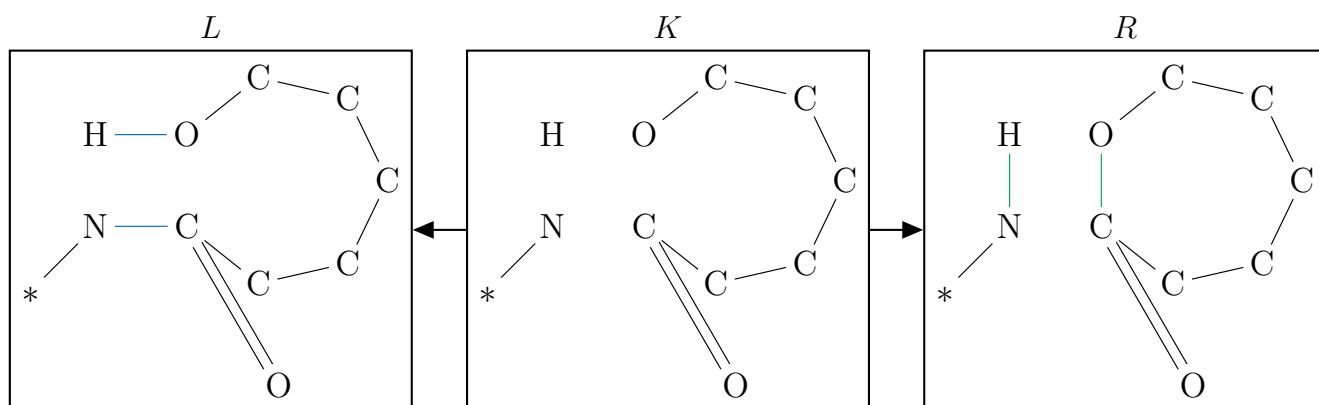


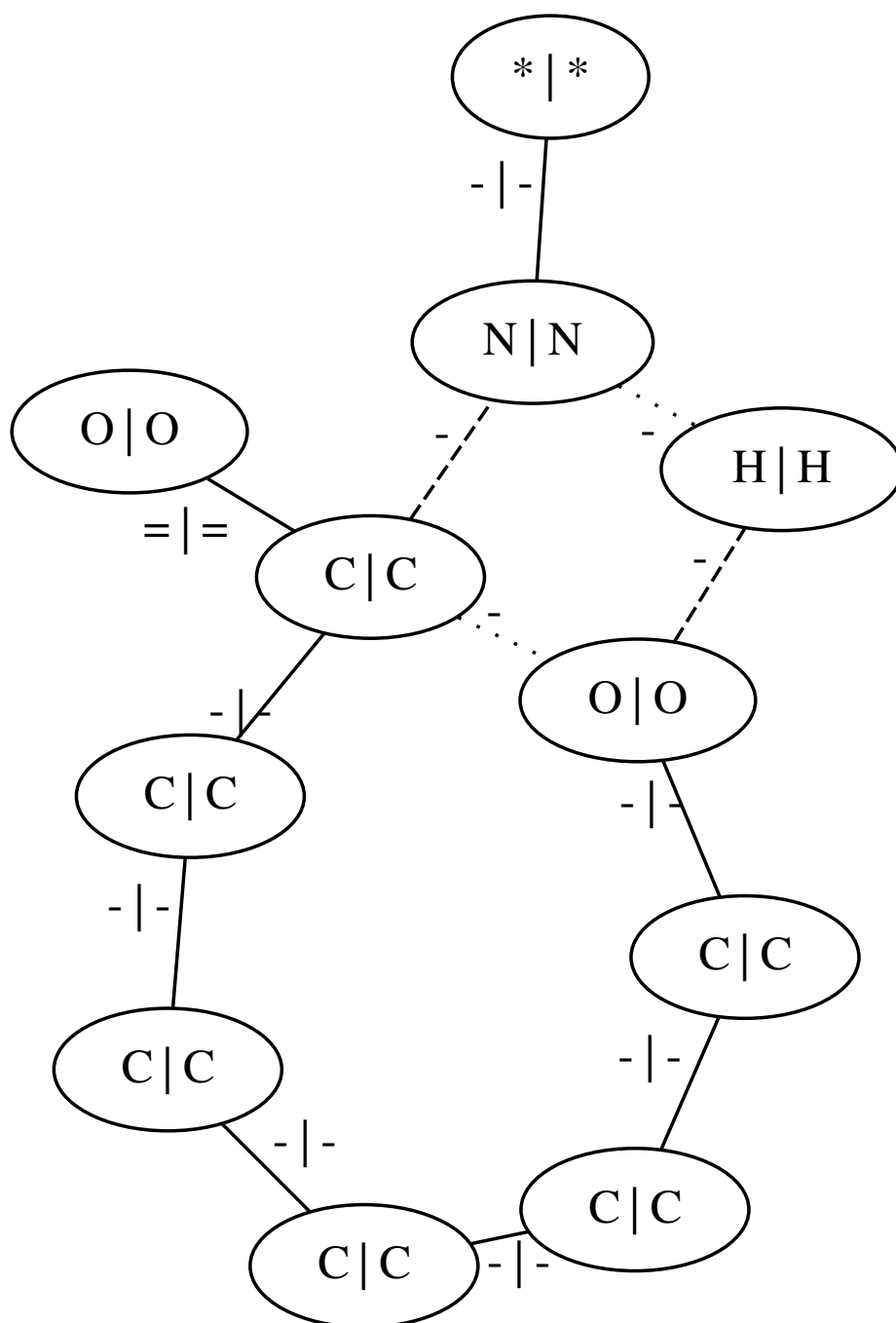
Files: out/721_r_147_11300100_{L, K, R}

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

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

0.0.146 Ring Closure 7 membered N, O

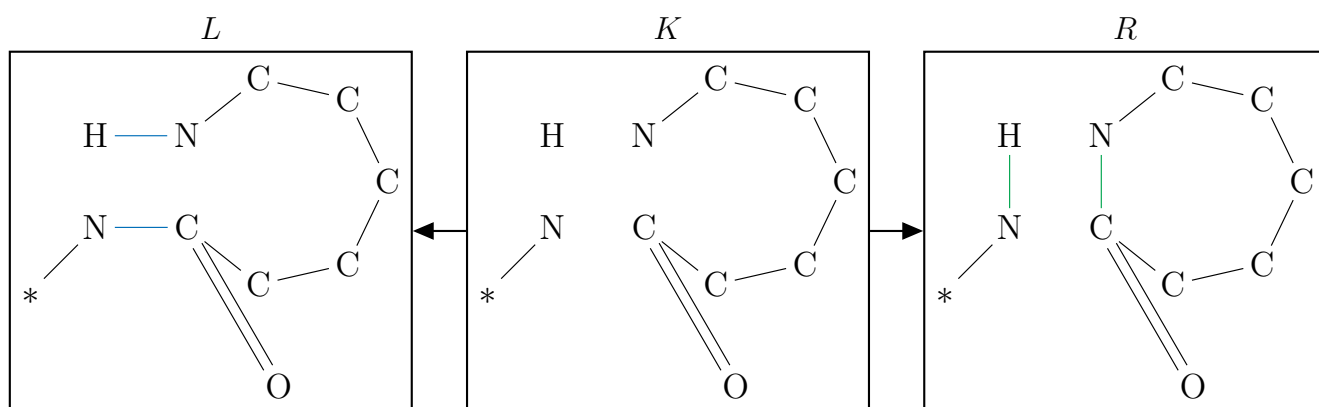




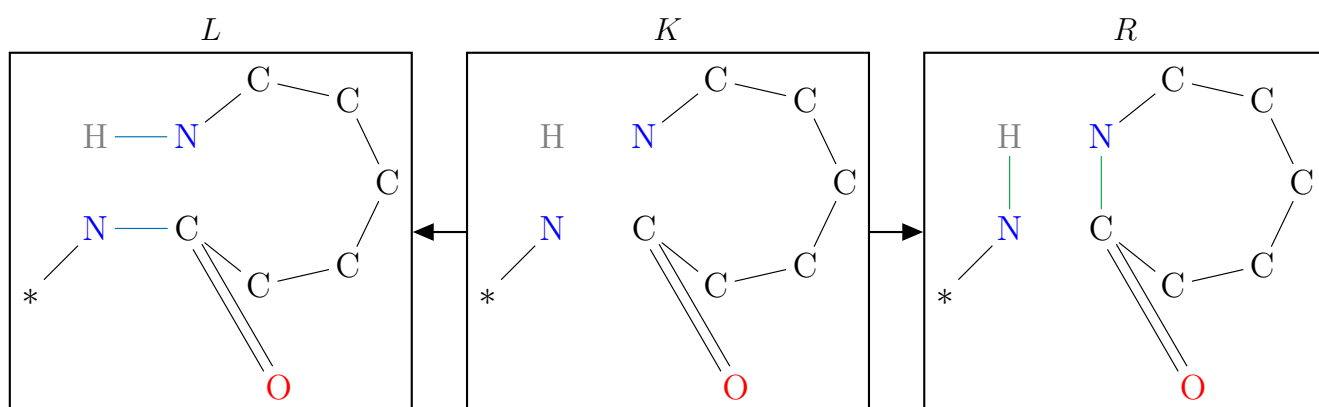
File: out/727_r_148_combined

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

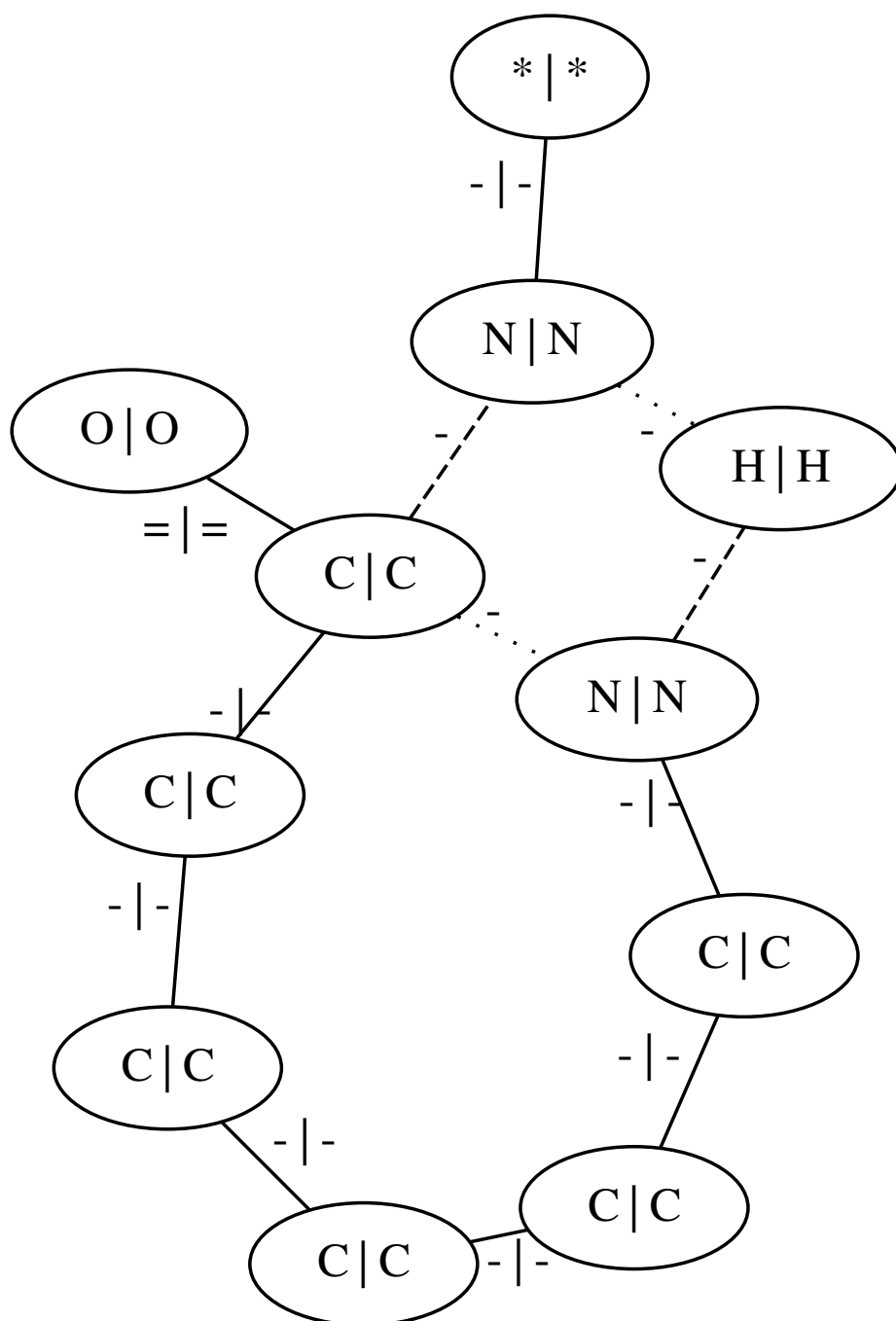
0.0.147 Ring Closure 7 membered N, N



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



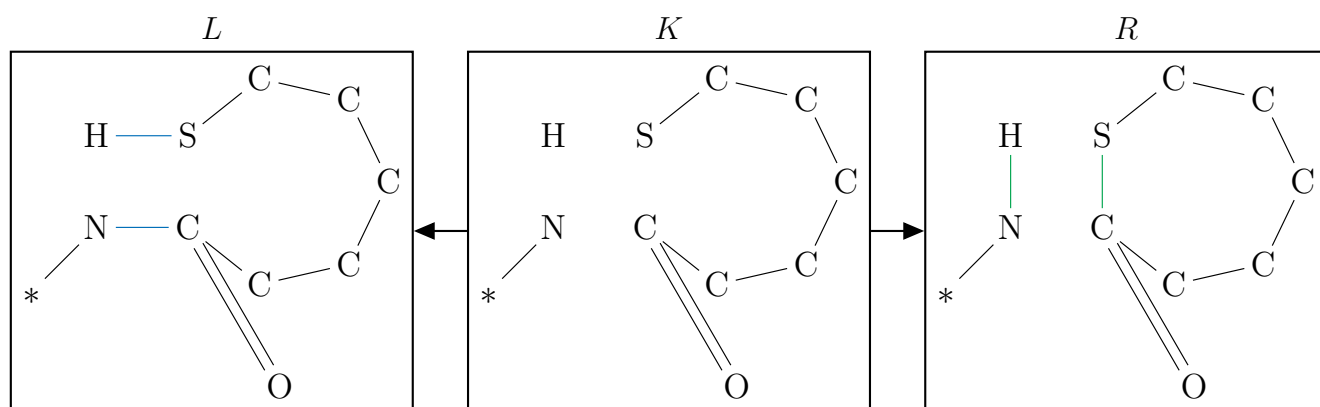
Files: out/731_r_149_11300100_{L, K, R}



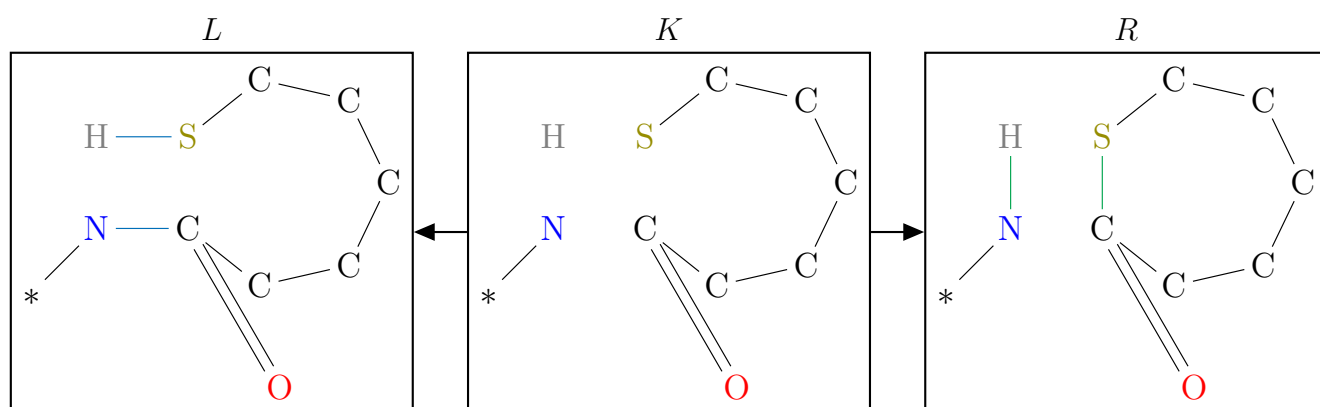
File: out/732_r_149_combined

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

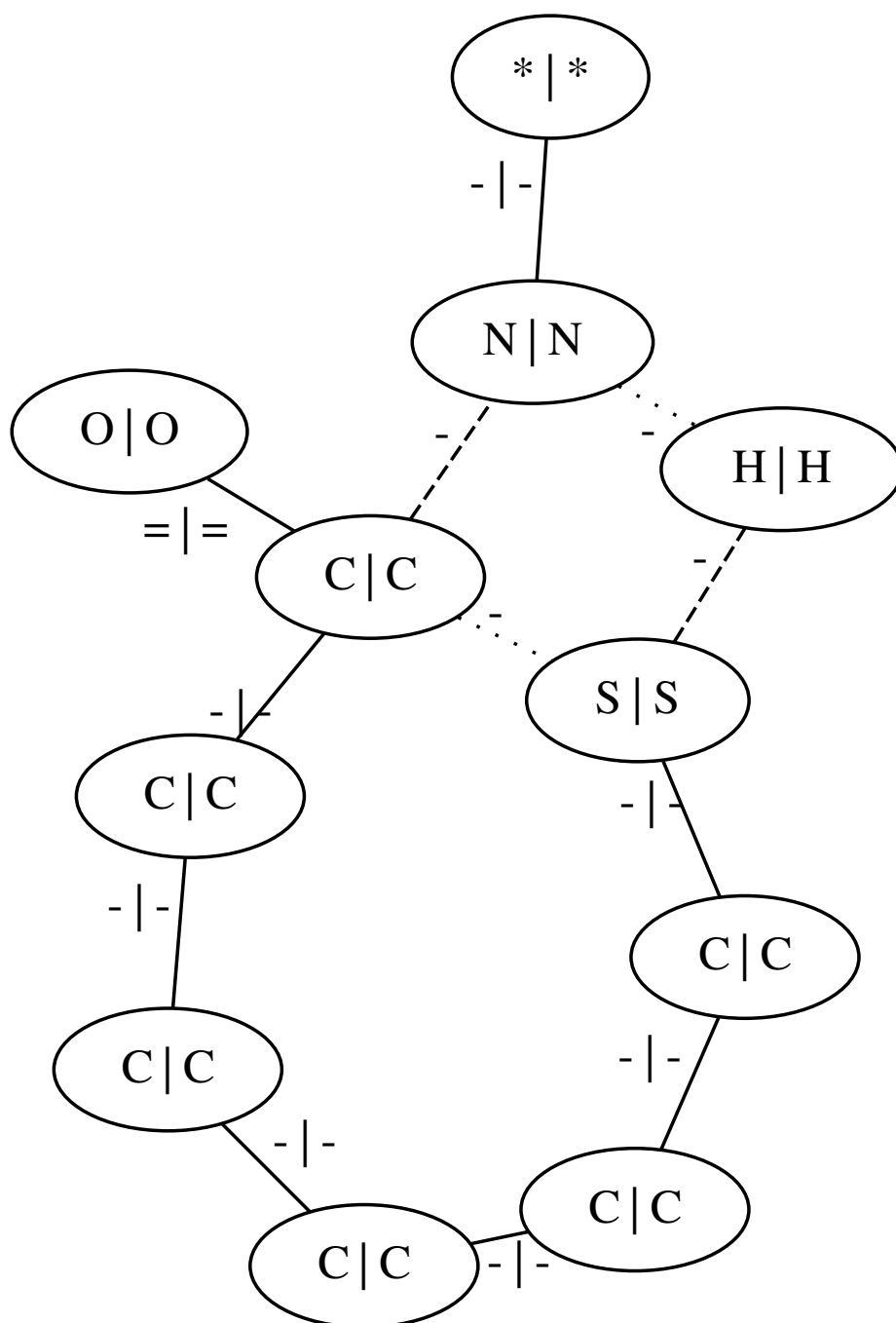
0.0.148 Ring Closure 7 membered N, S



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



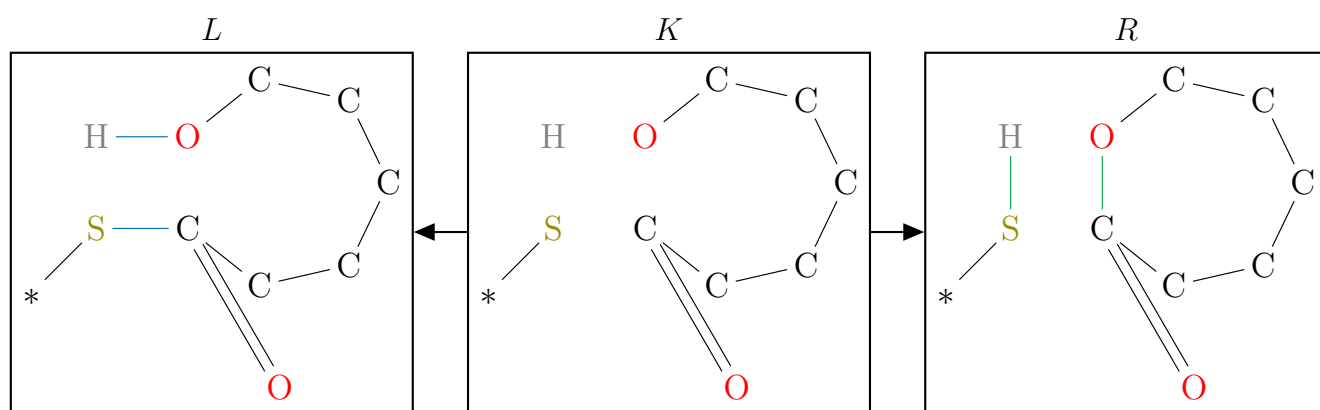
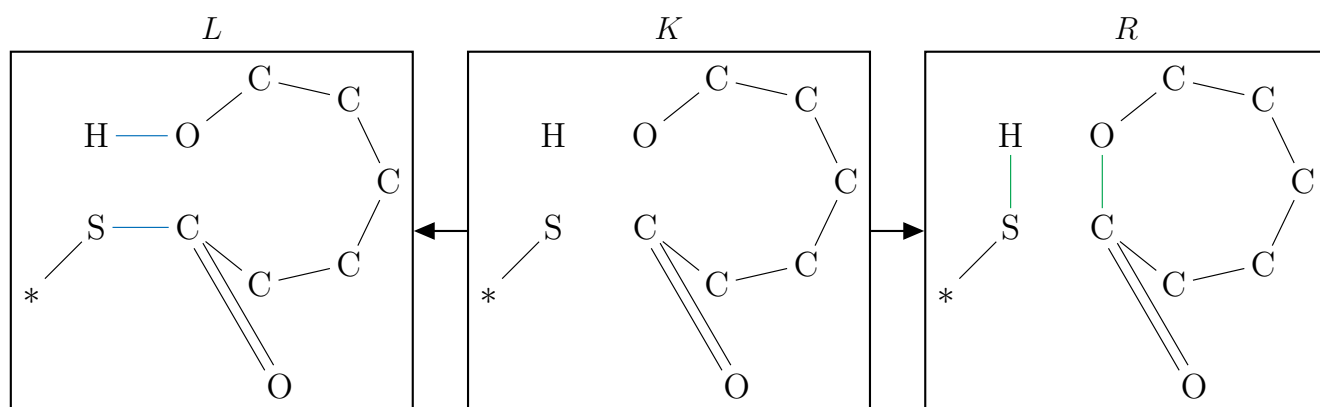
Files: out/736_r_150_11300100_{L, K, R}

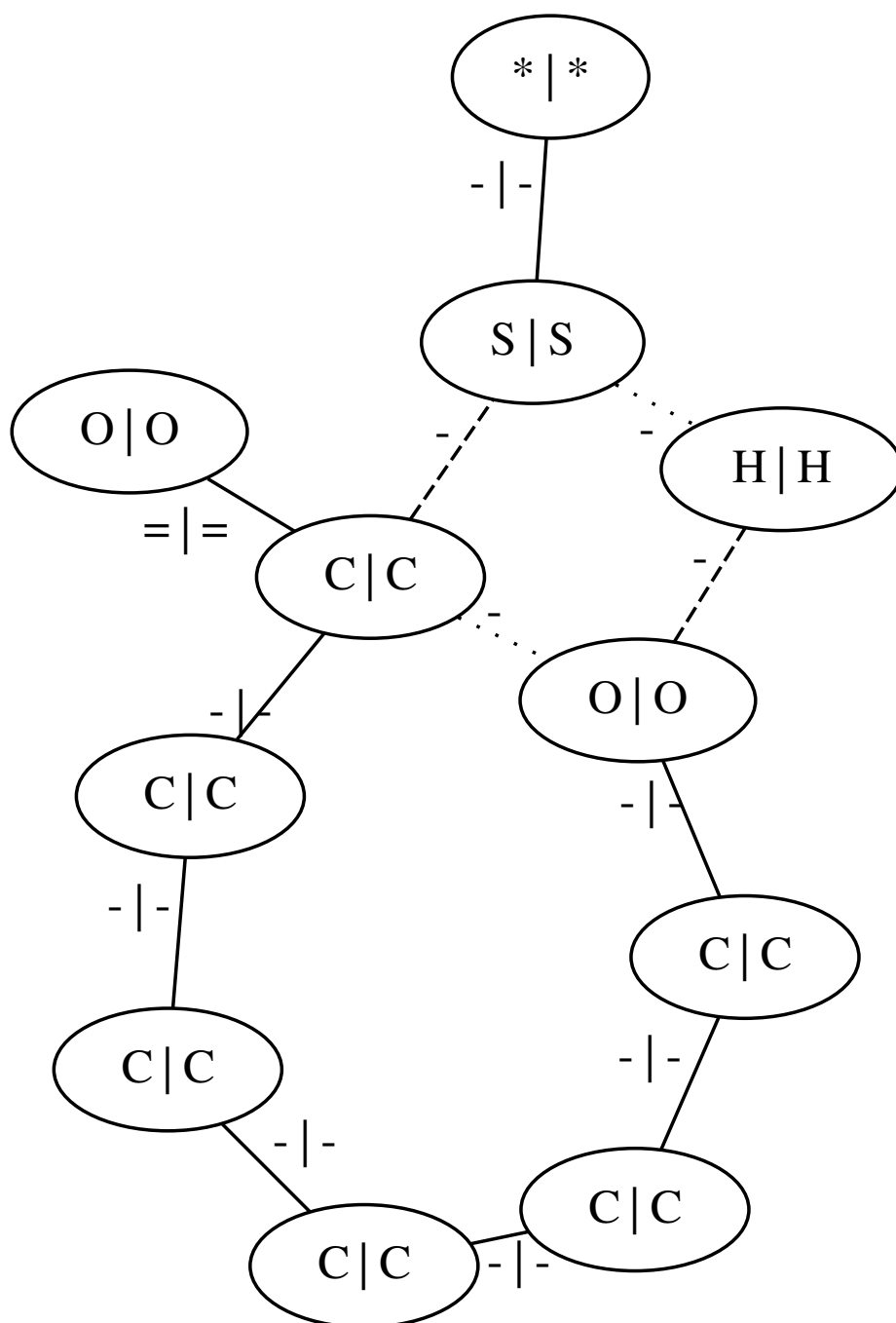


File: out/737_r_150_combined

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

0.0.149 Ring Closure 7 membered S, O

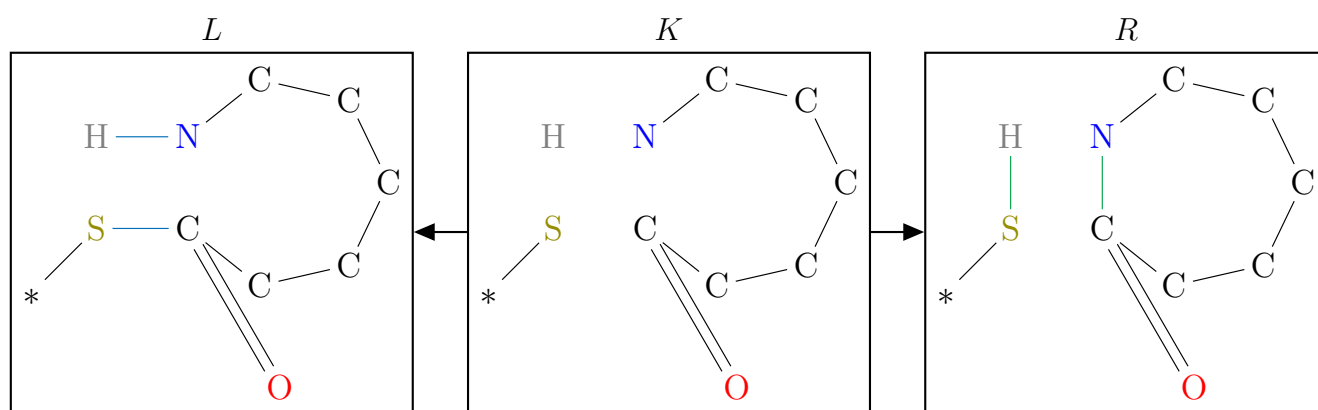
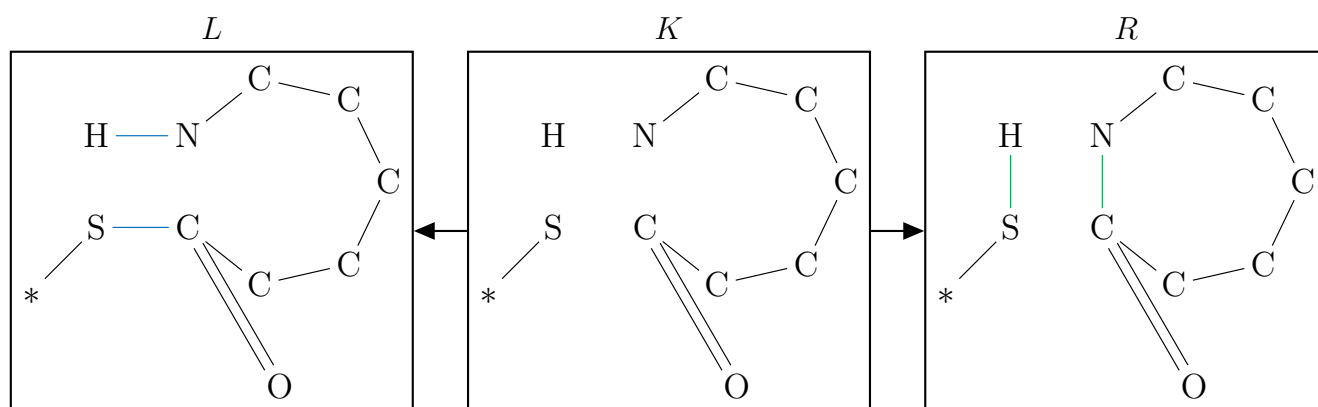


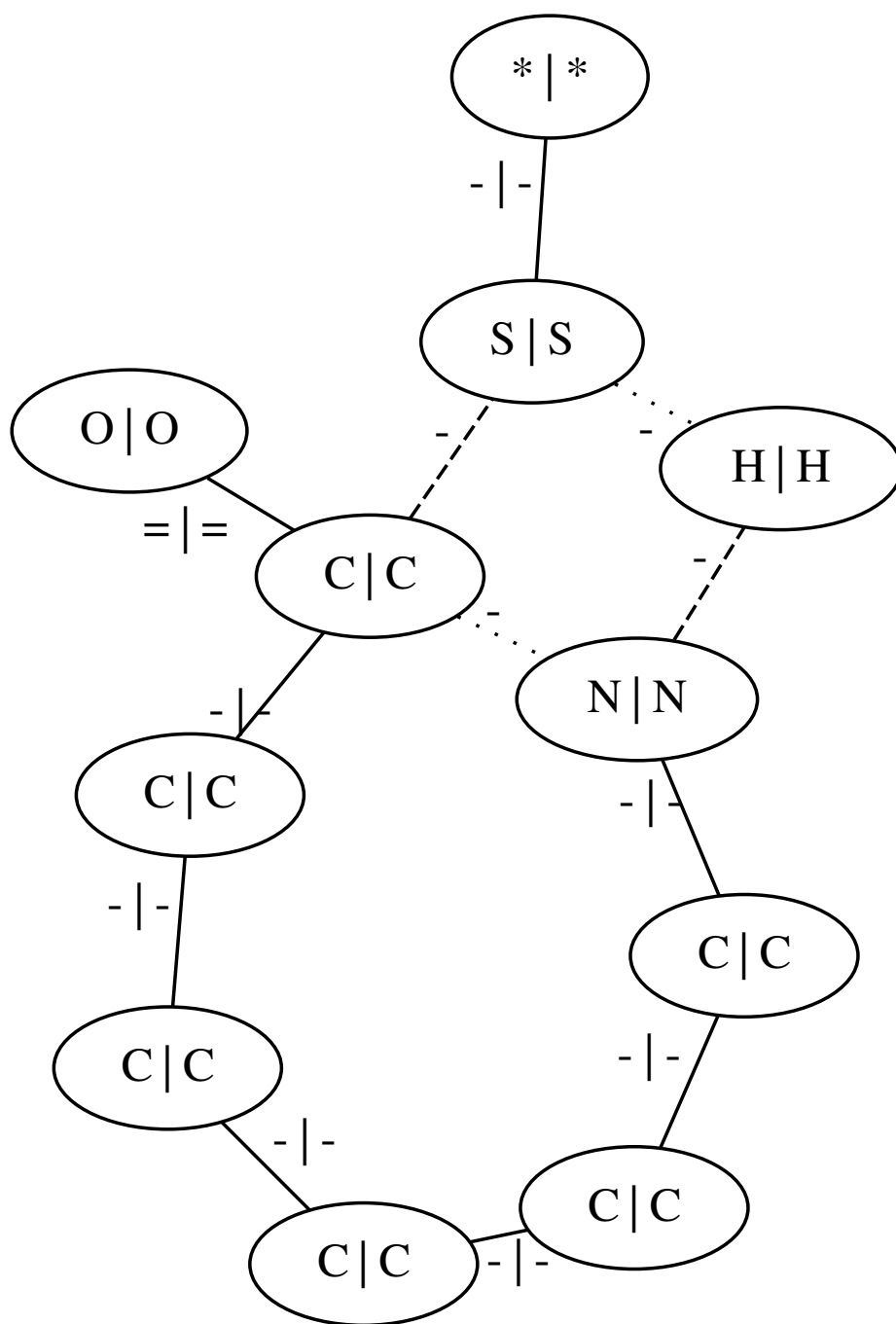


File: out/742_r_151_combined

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

0.0.150 Ring Closure 7 membered S, N

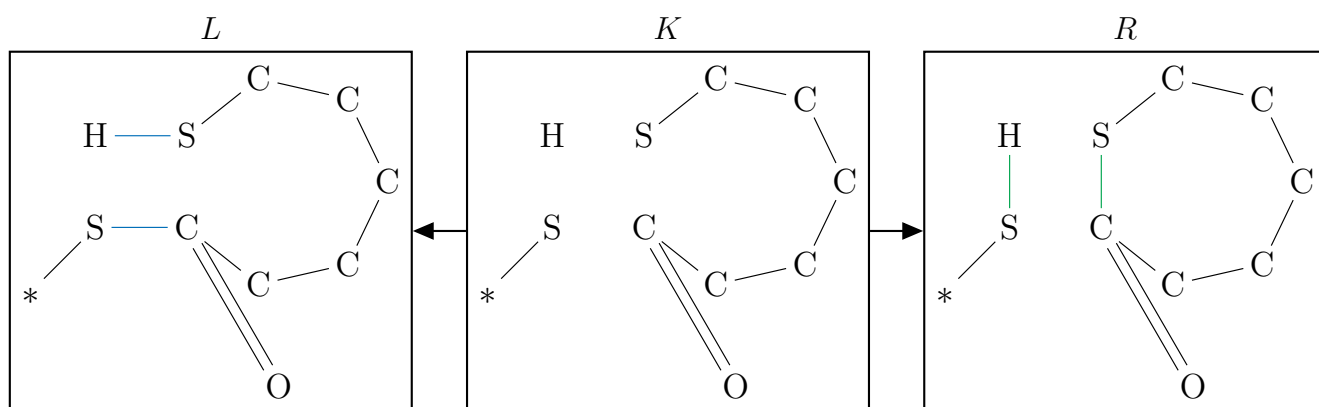




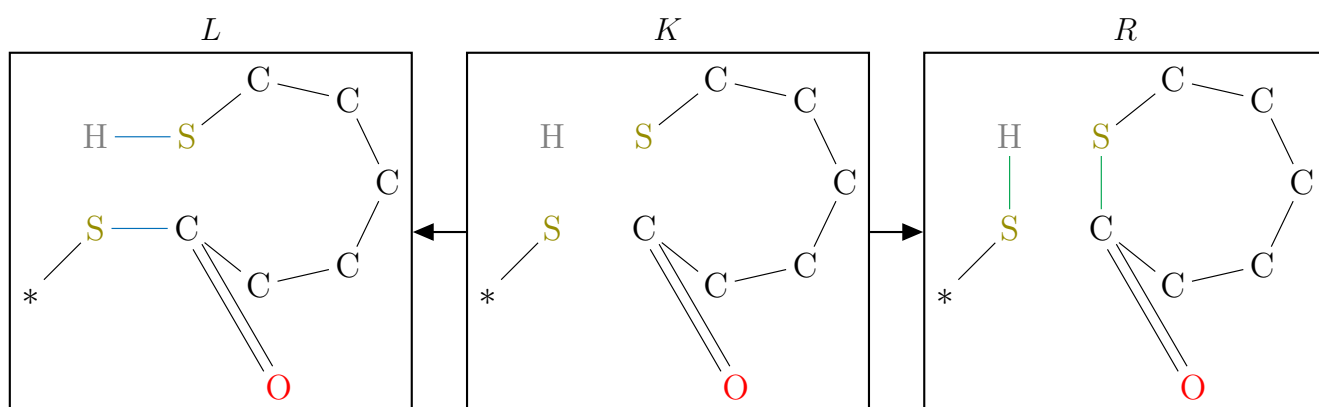
File: out/747_r_152_combined

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

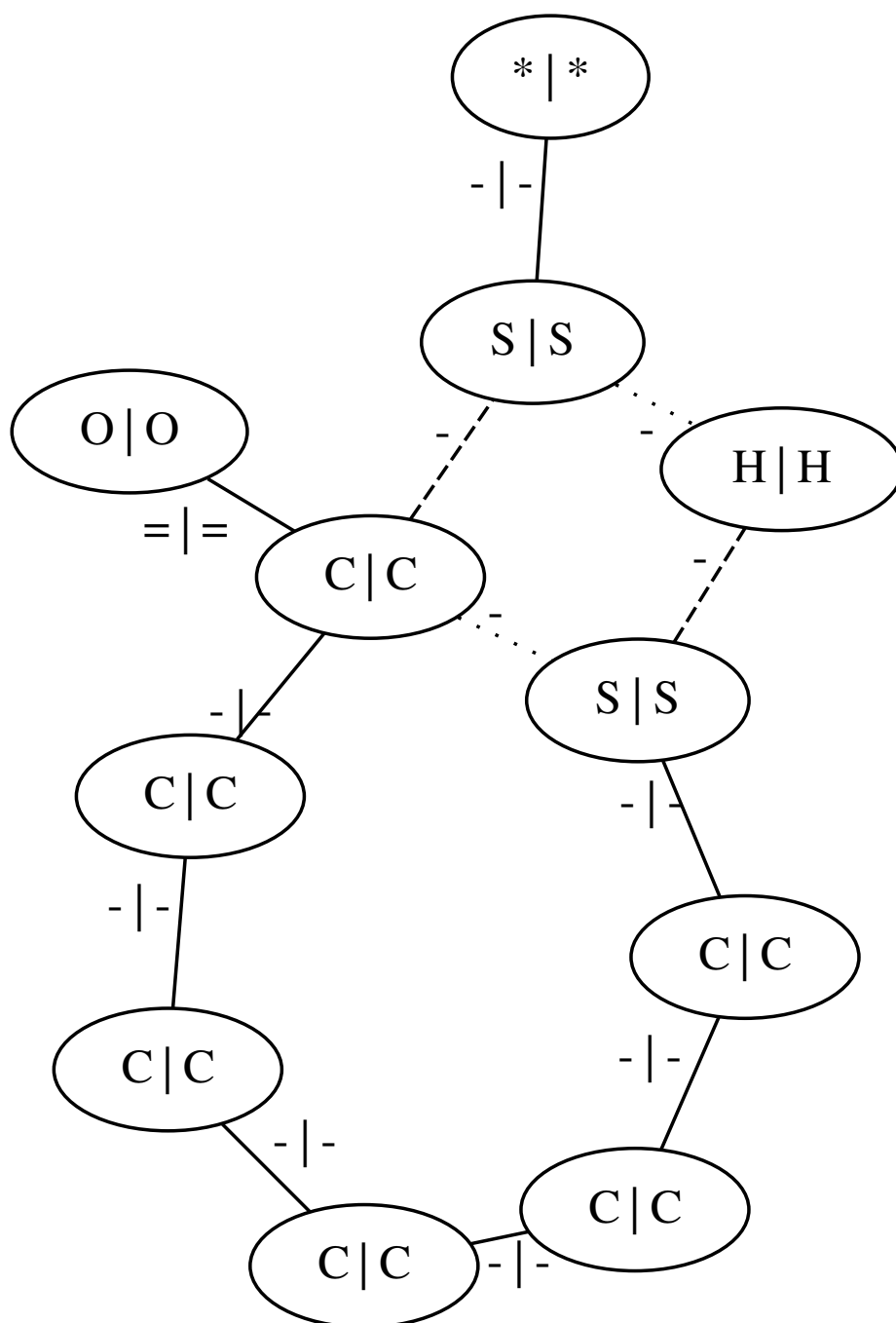
0.0.151 Ring Closure 7 membered S, S



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



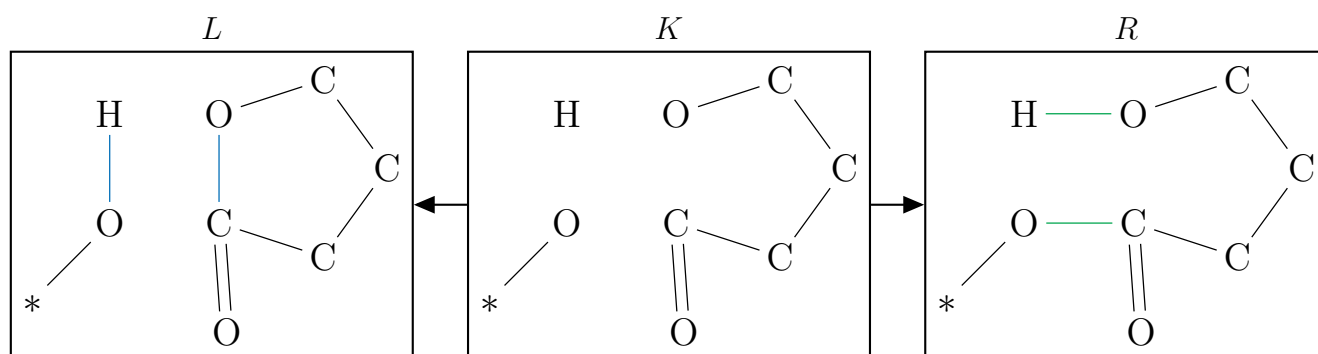
Files: out/751_r_153_11300100_{L, K, R}



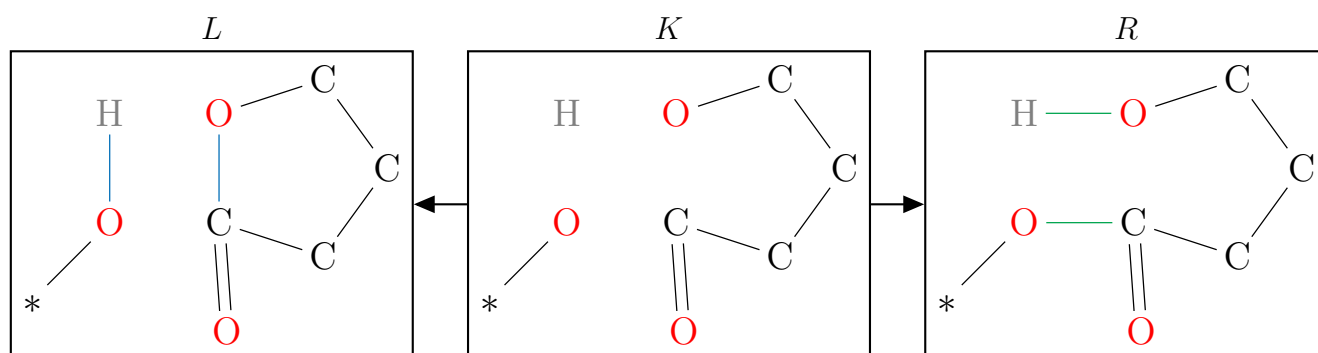
File: out/752_r_153_combined

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

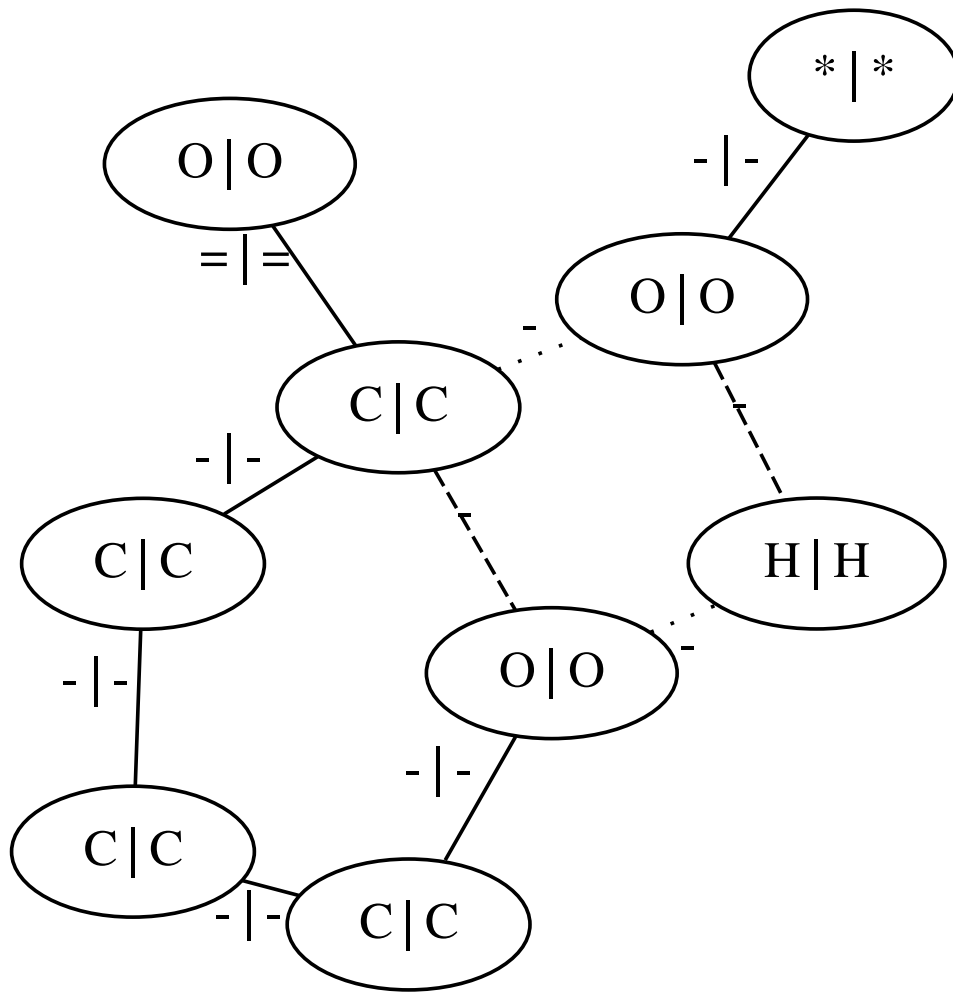
0.0.152 Ring Closure 5 membered, inverse O, O



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



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

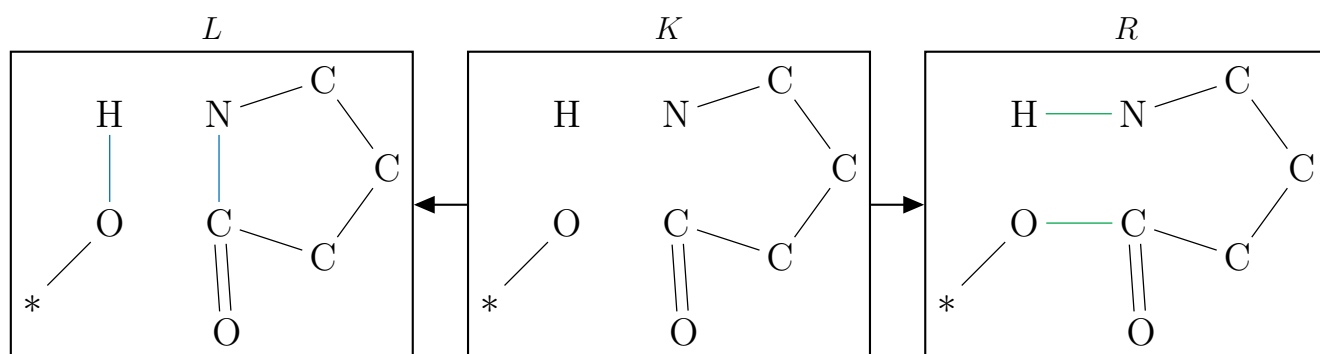


File: out/757_r_154_combined

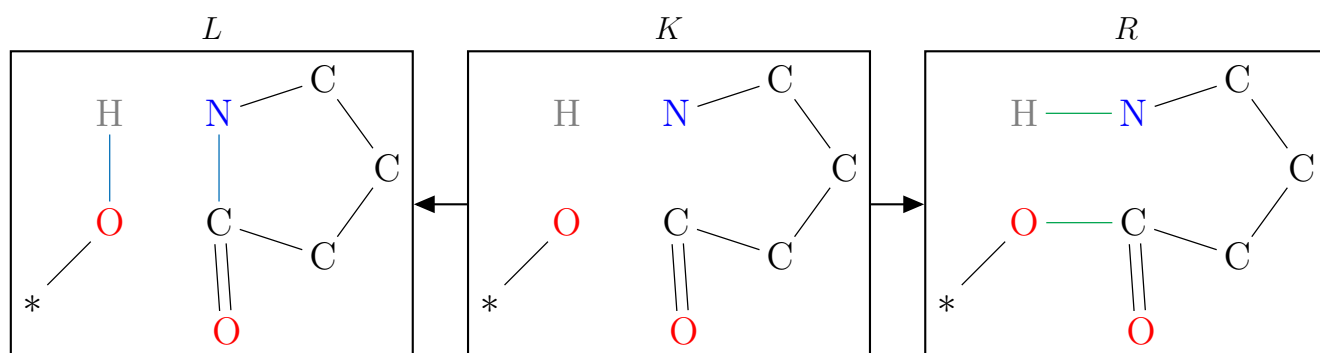
$$\begin{aligned}
 &|\{e \in \text{outEdges}(8) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{ '0' \} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{ '-' \} \\
 &\quad \}| \leq 1
 \end{aligned}$$

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

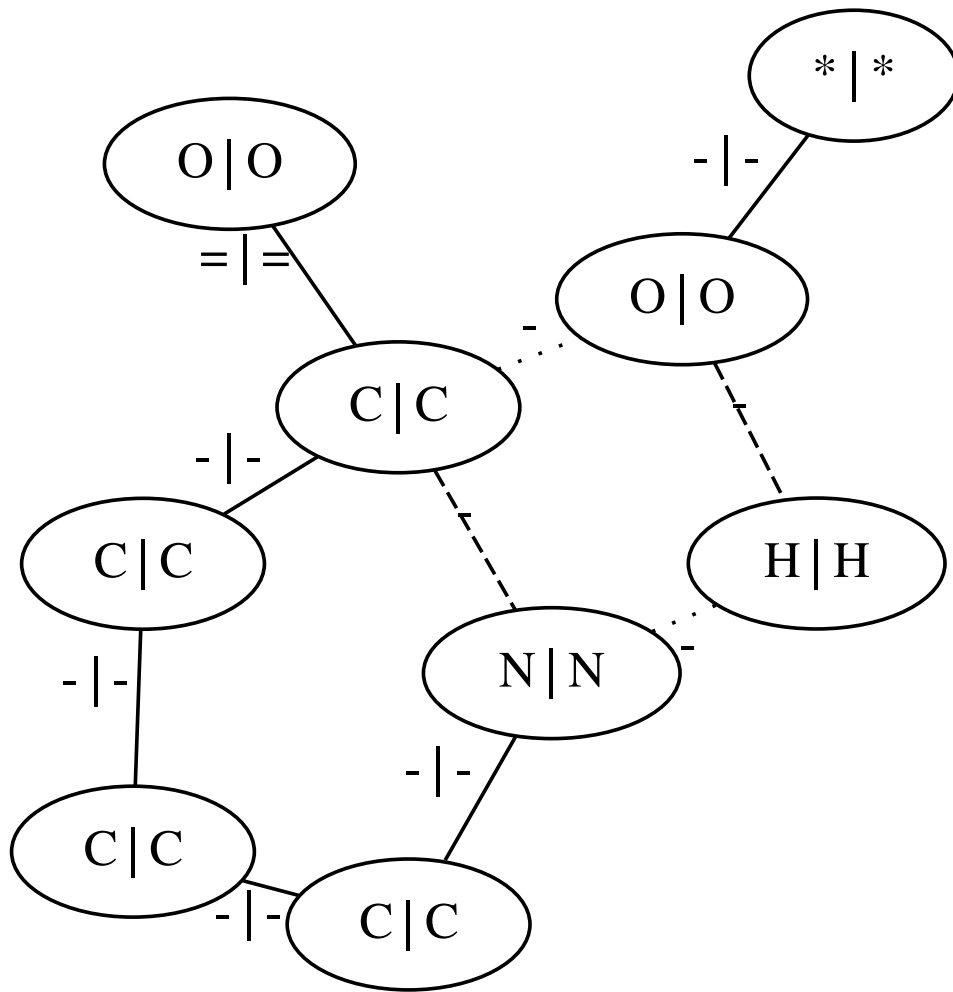
0.0.153 Ring Closure 5 membered, inverse O, N



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



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

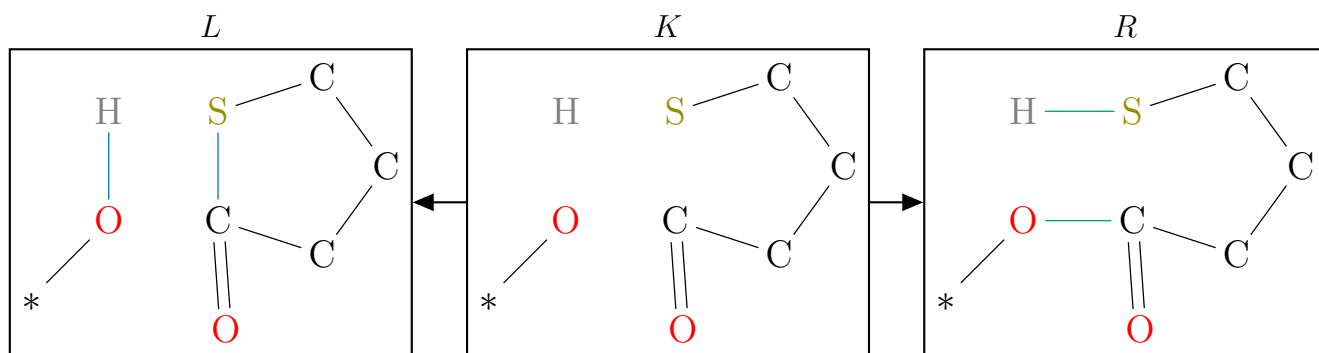
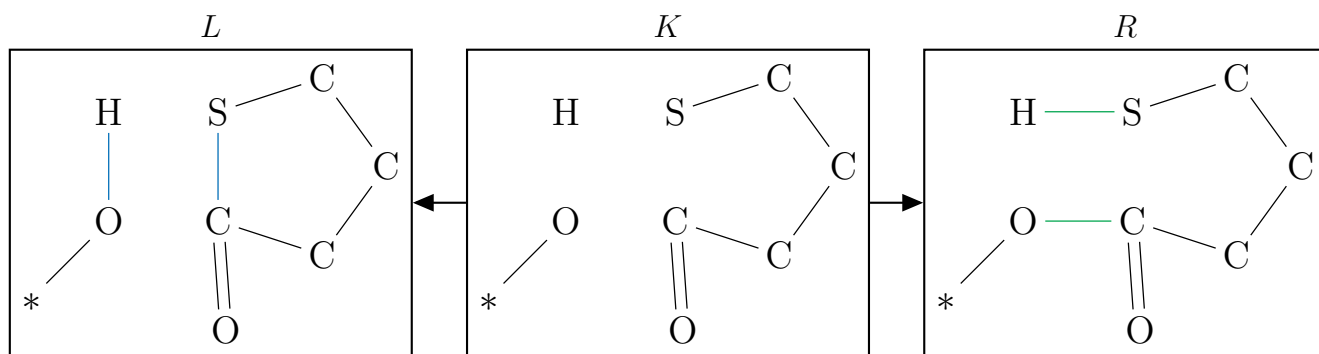


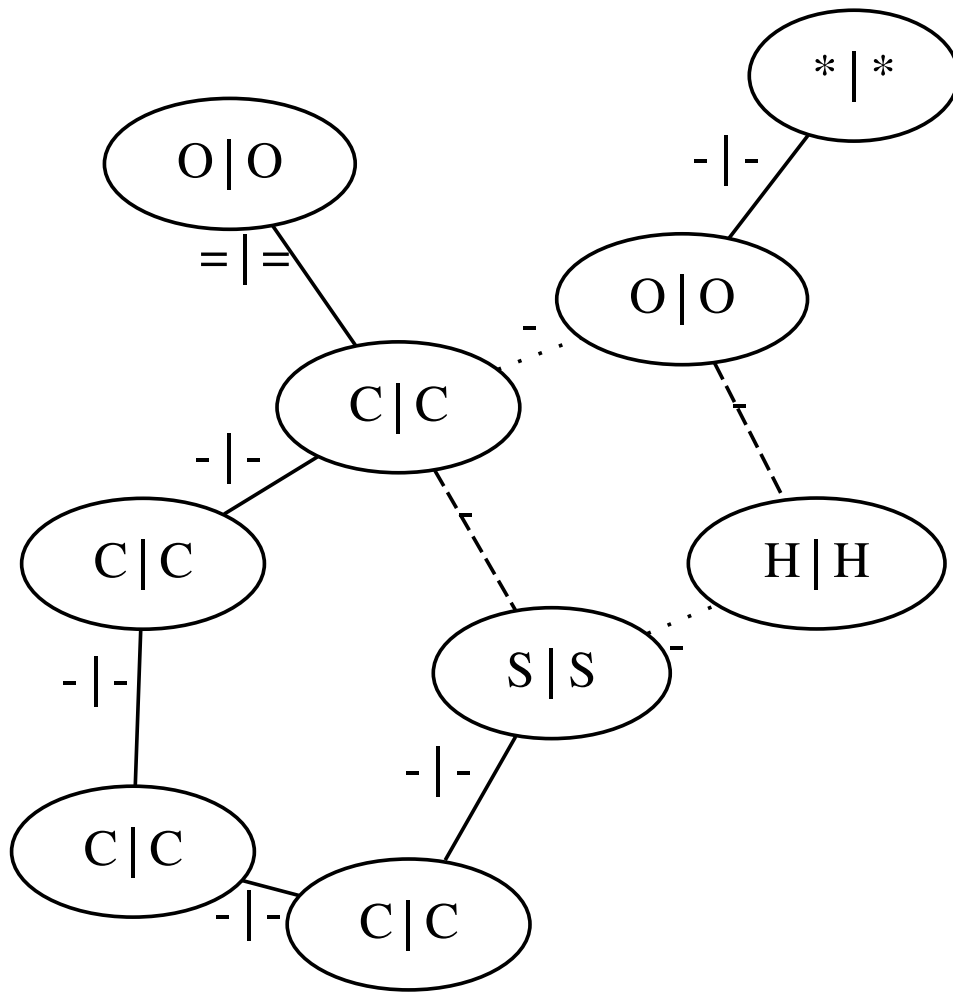
File: out/762_r_155_combined

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

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

0.0.154 Ring Closure 5 membered, inverse O, S



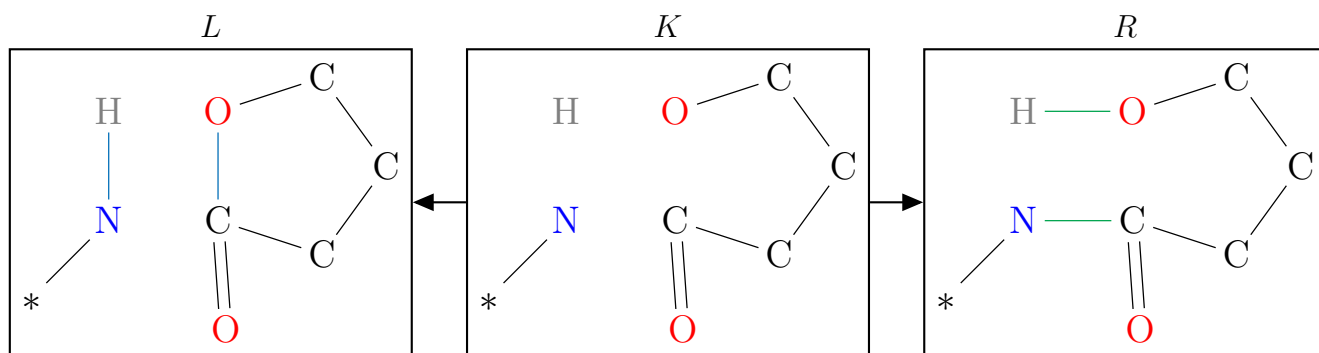
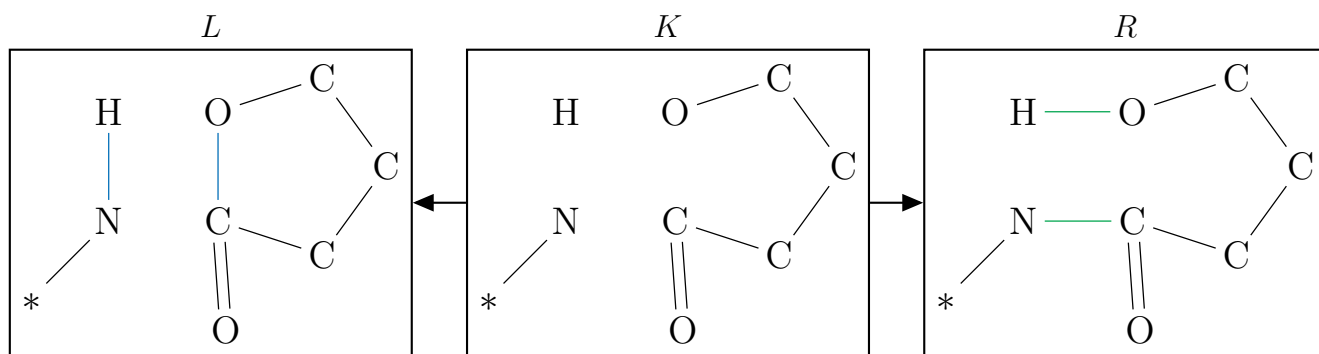


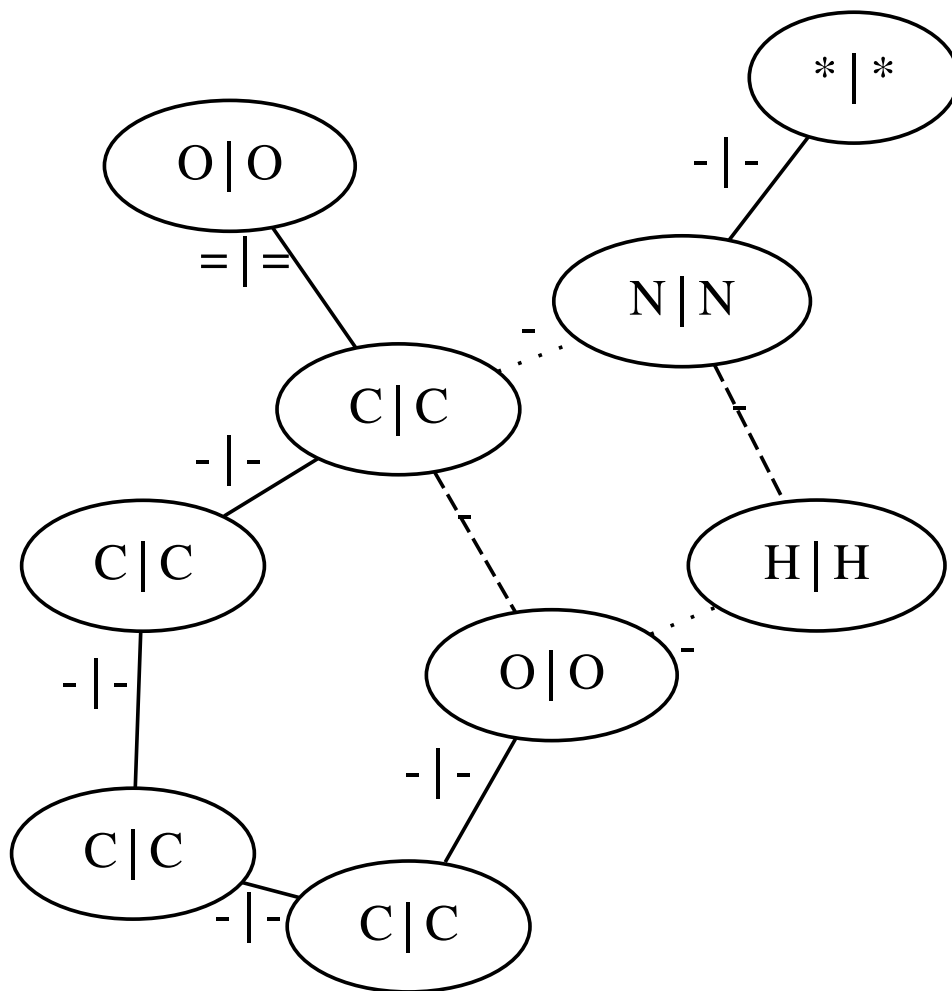
File: out/767_r_156_combined

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

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

0.0.155 Ring Closure 5 membered, inverse N, O

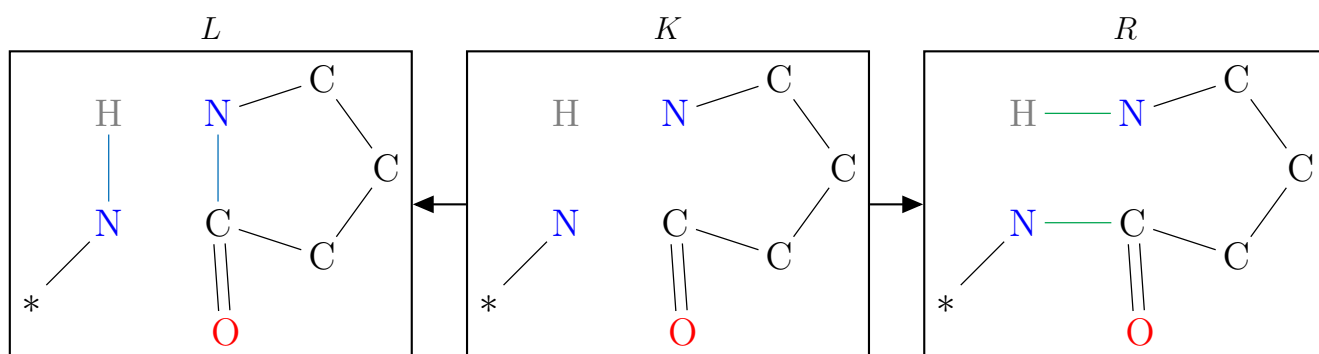
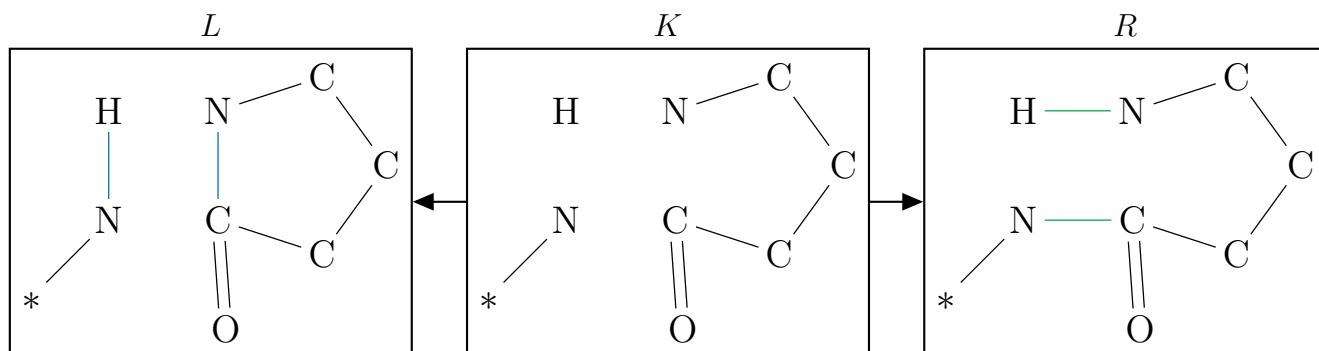




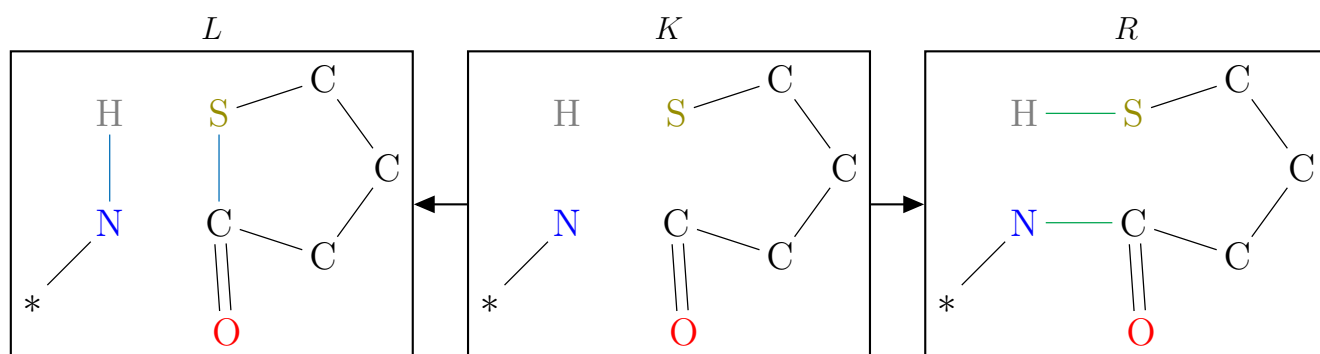
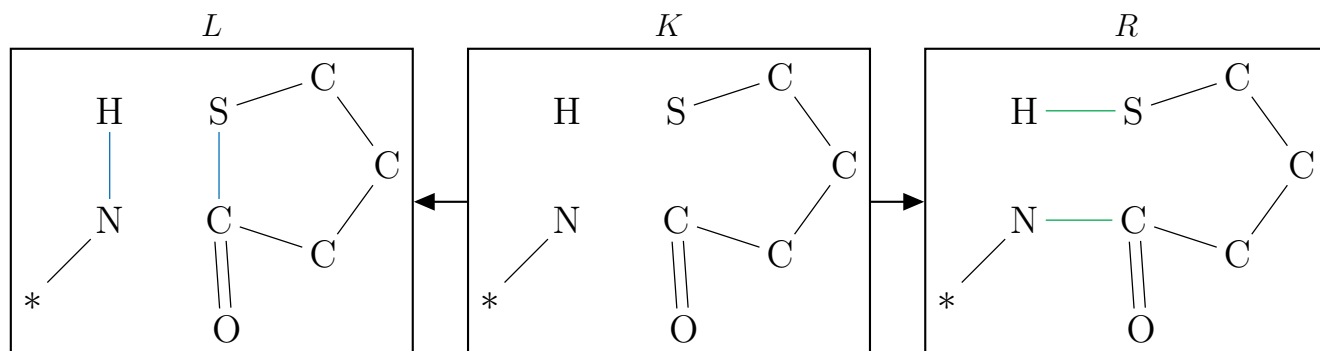
File: out/772_r_157_combined

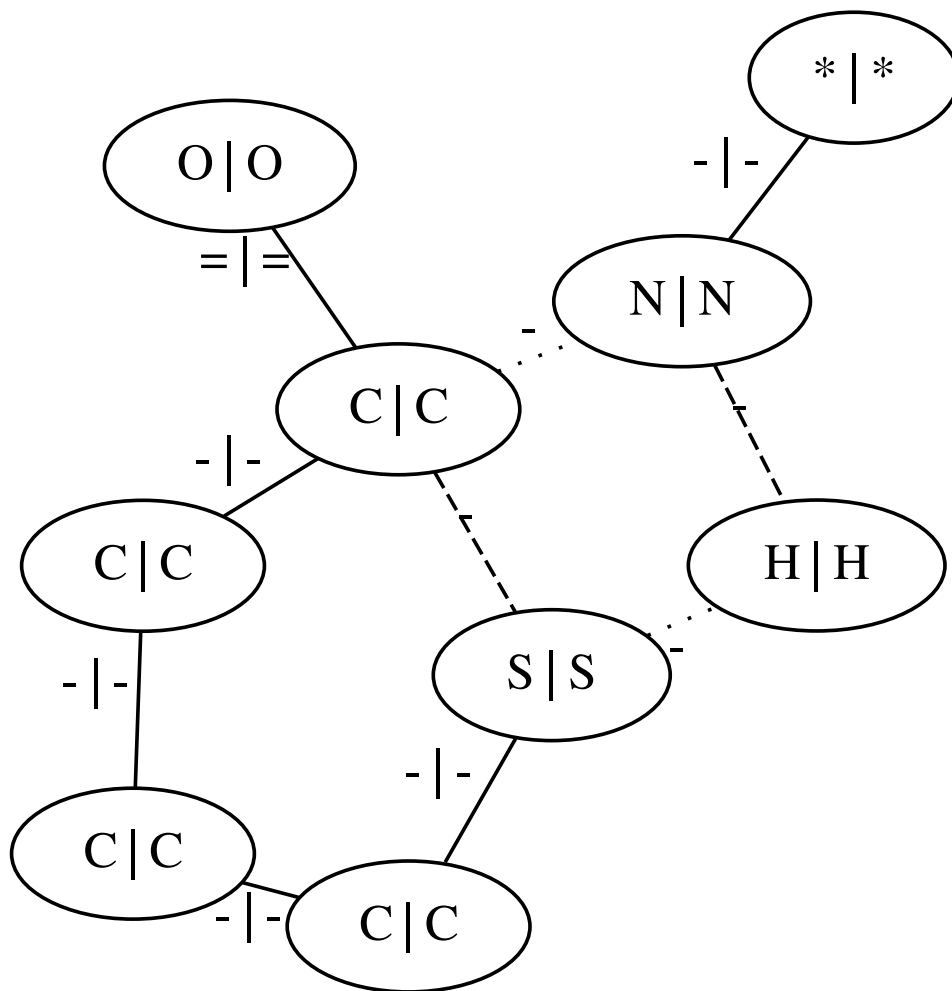
$$\begin{aligned}
 & |\{e \in \text{outEdges}(8) \mid \\
 & \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 & \quad \wedge \\
 & \quad \text{label}(e) \in \{'-\'} \\
 & \quad \}\} | \leq 1
 \end{aligned}$$

0.0.156 Ring Closure 5 membered, inverse N, N



0.0.157 Ring Closure 5 membered, inverse N, S

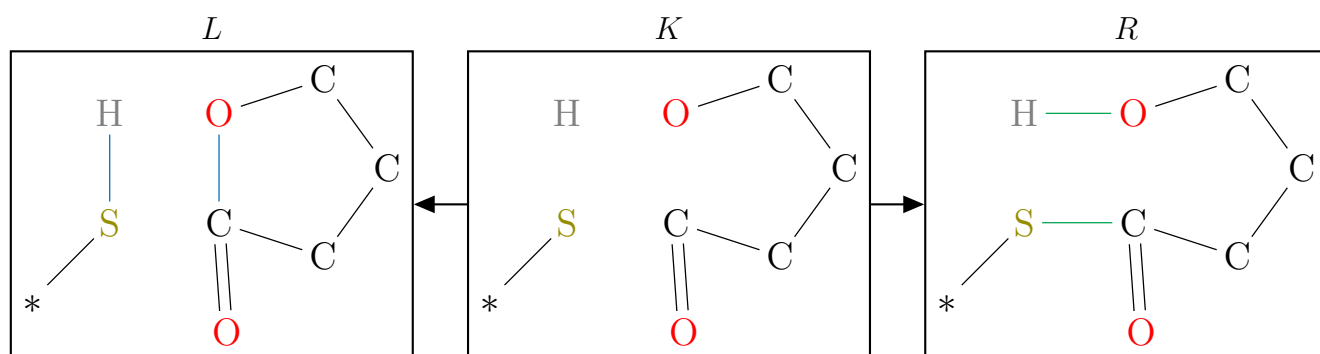
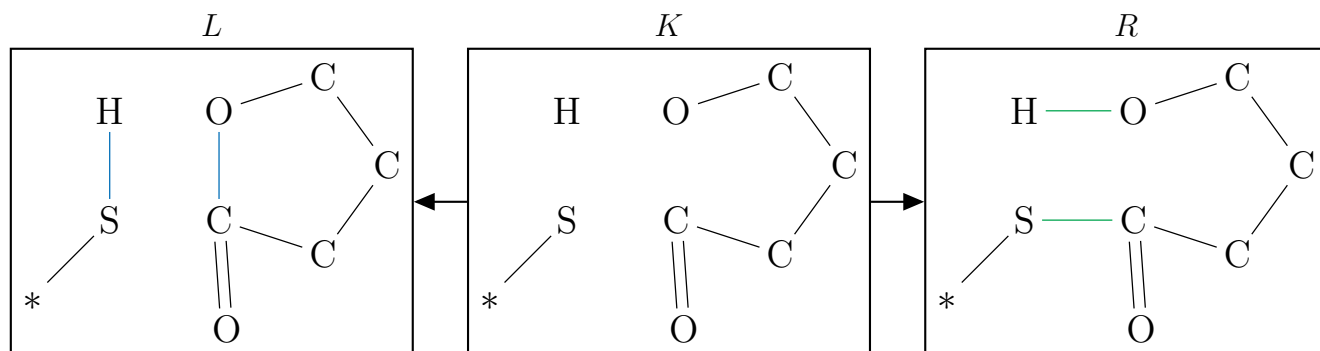


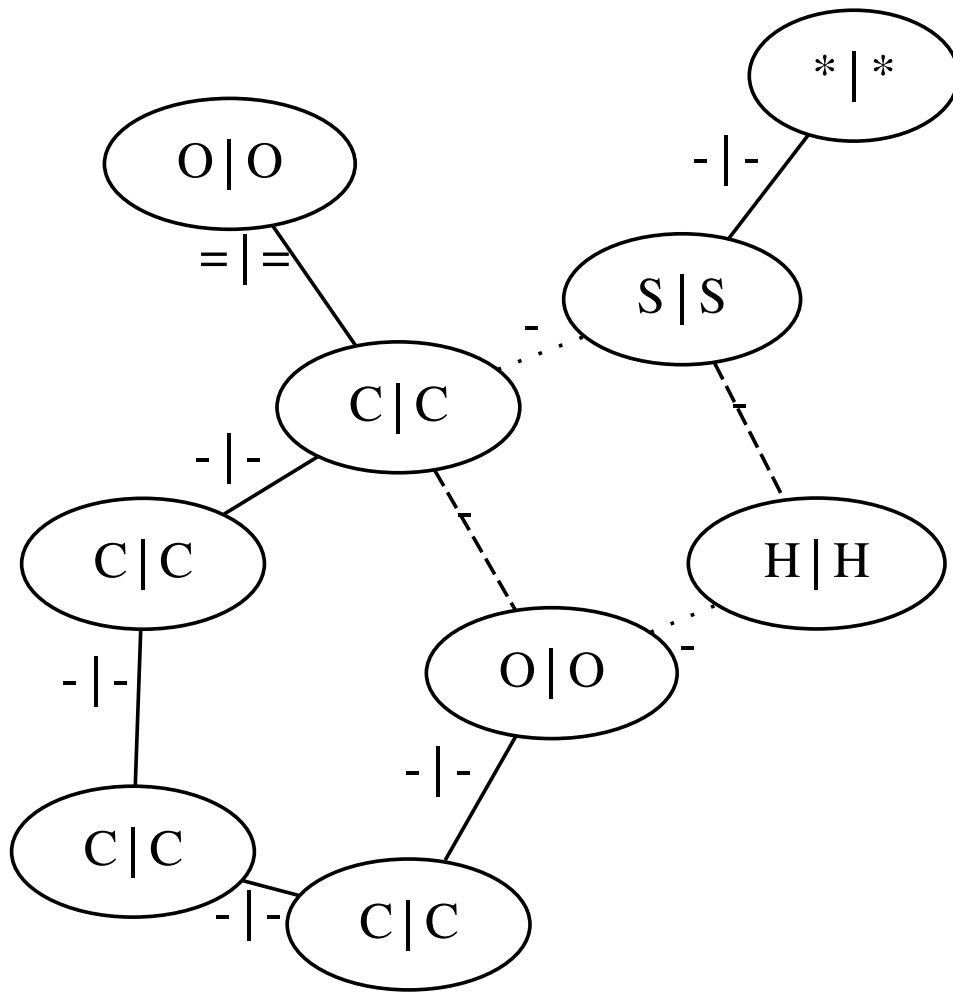


File: out/782_r_159_combined

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

0.0.158 Ring Closure 5 membered, inverse S, O

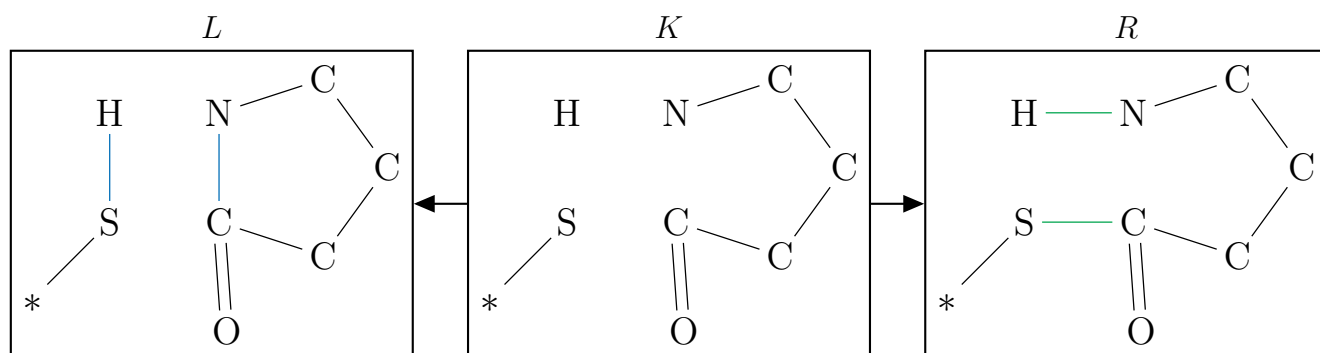




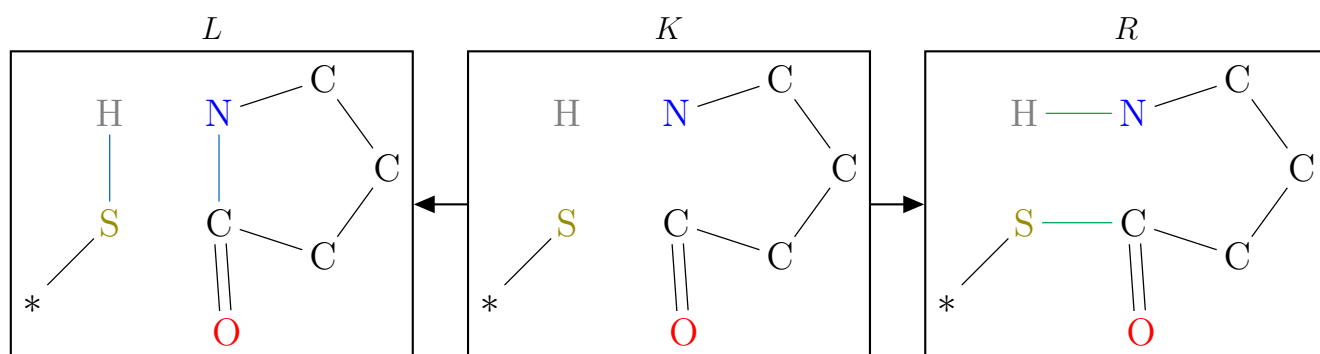
File: out/787_r_160_combined

$|\{e \in \text{outEdges}(8) \mid$
 $\text{label}(\text{target}(e)) \in \{'0'\}$
 \wedge
 $\text{label}(e) \in \{'-\'}\}$
 $\}| \leq 1$

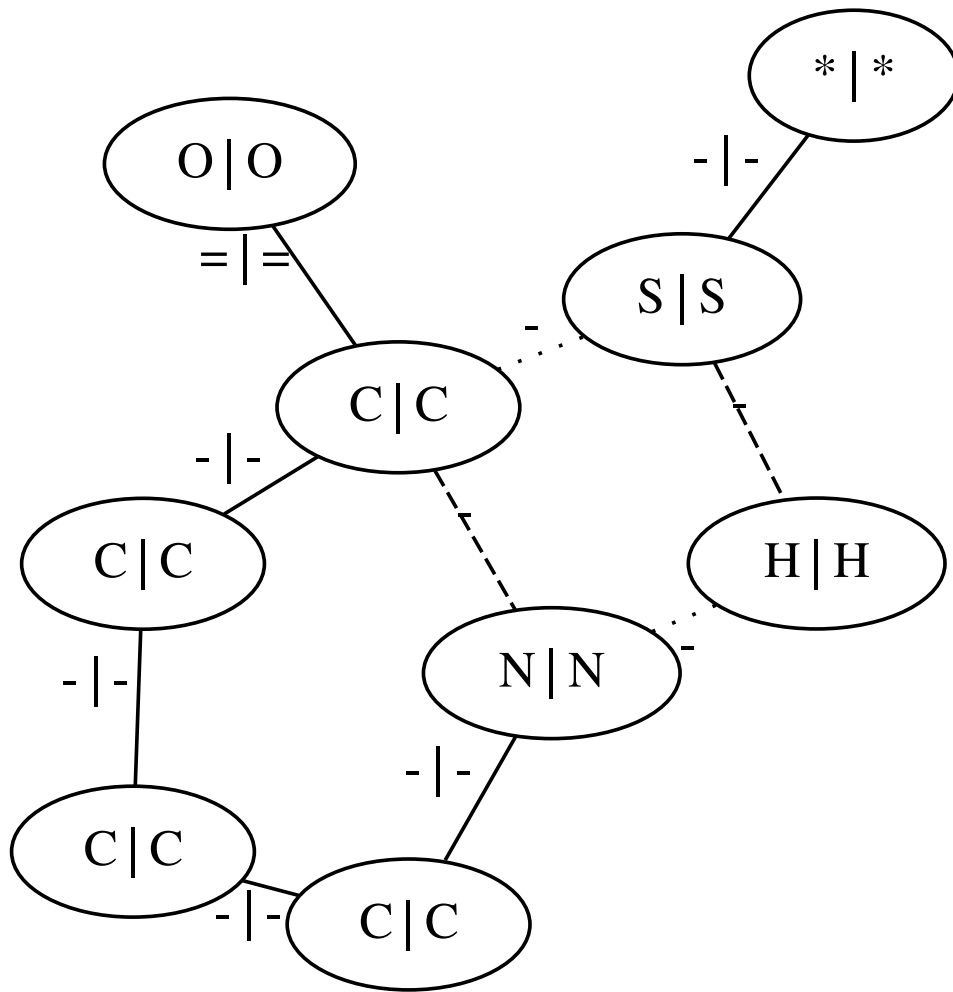
0.0.159 Ring Closure 5 membered, inverse S, N



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



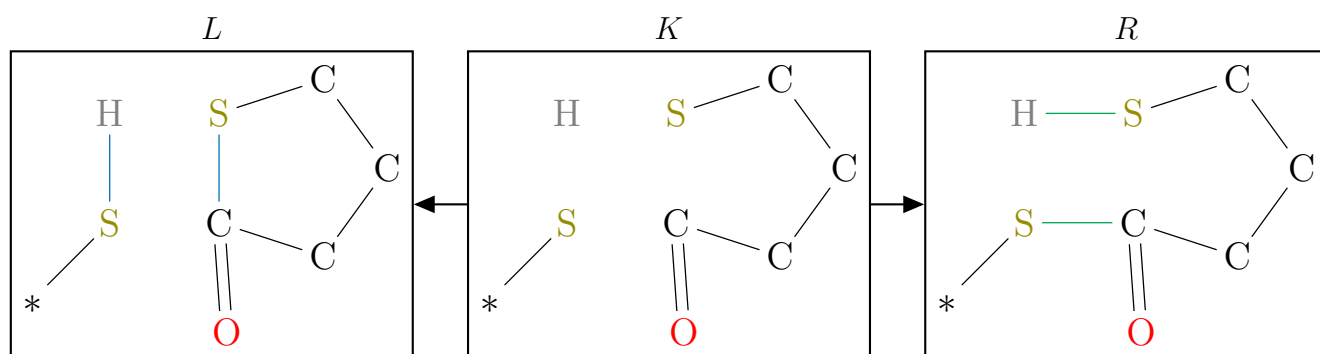
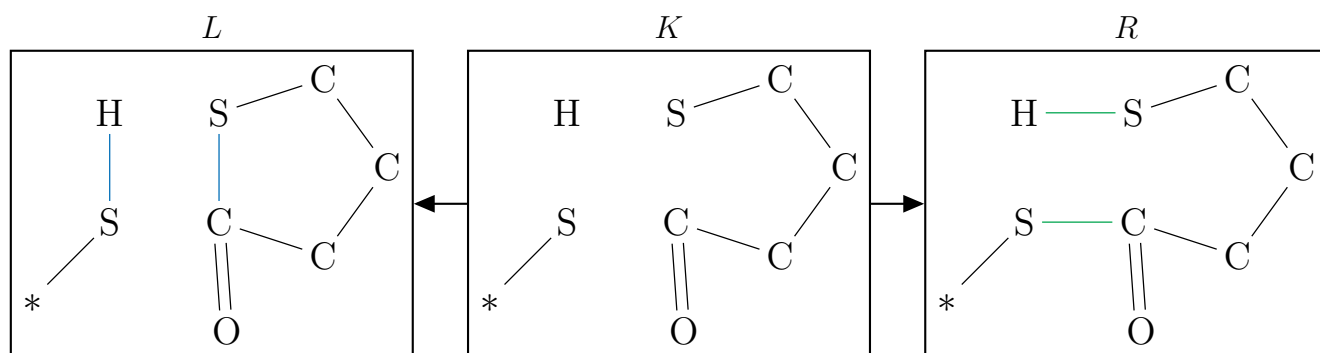
Files: out/791_r_161_11300100_{L, K, R}

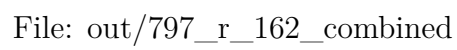


File: out/792_r_161_combined

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

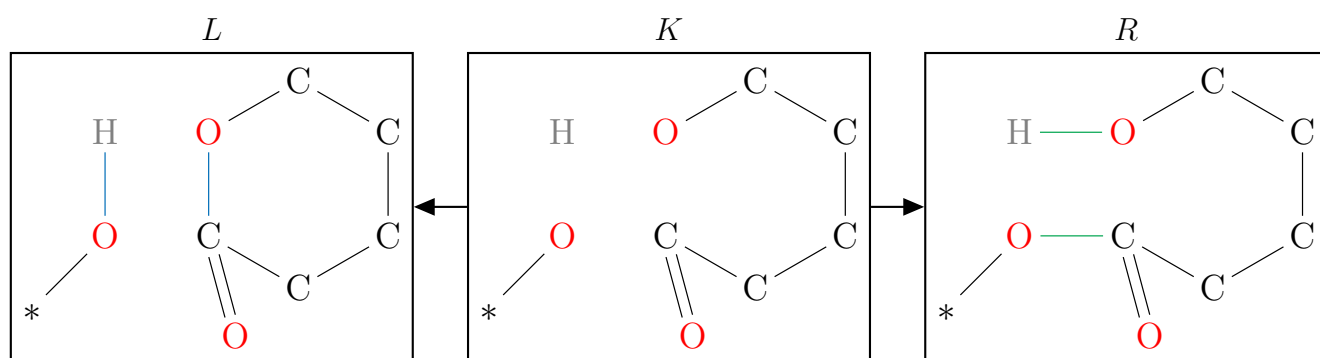
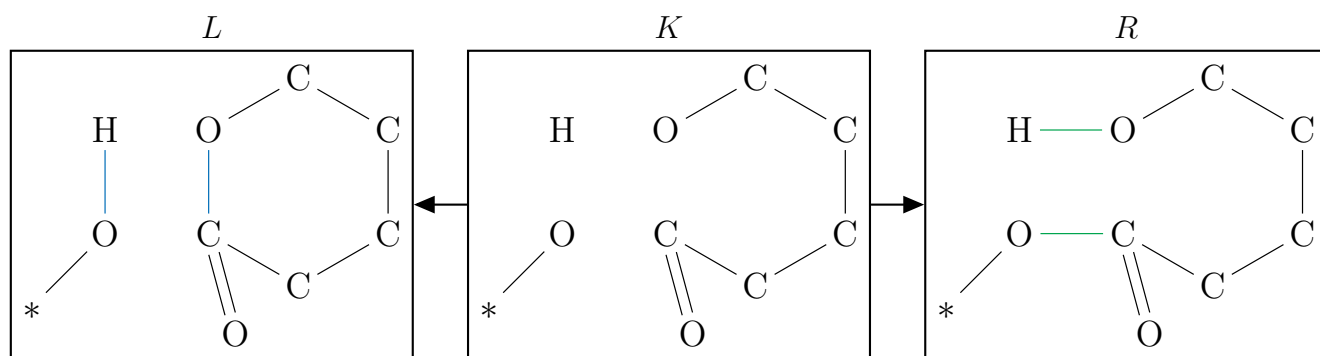
0.0.160 Ring Closure 5 membered, inverse S, S

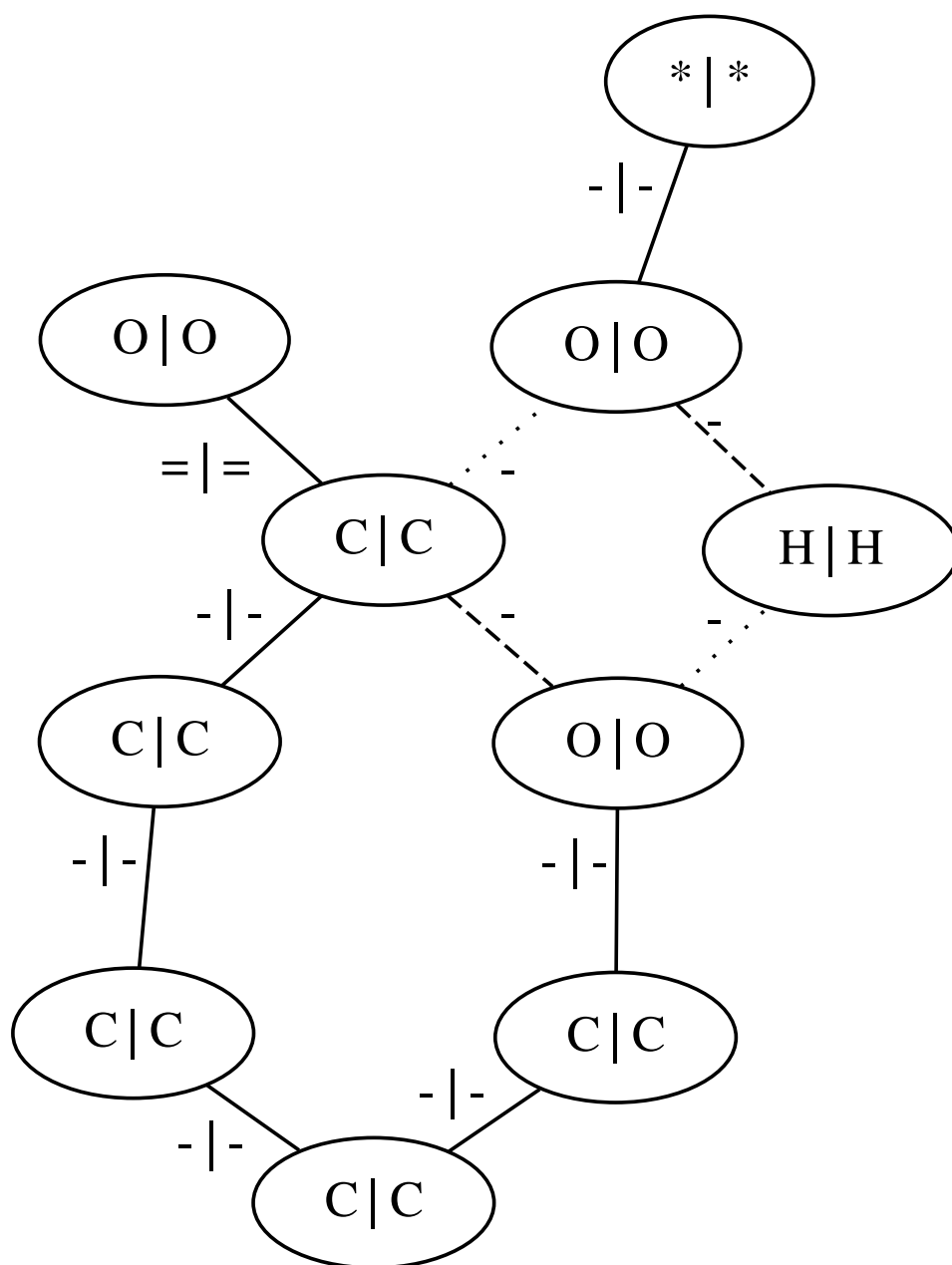




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0.0.161 Ring Closure 6 membered, inverse O, O



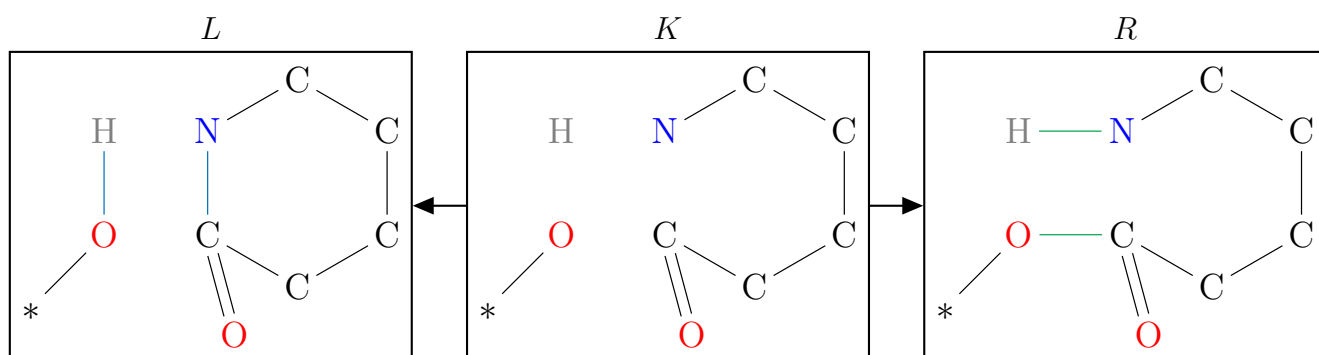
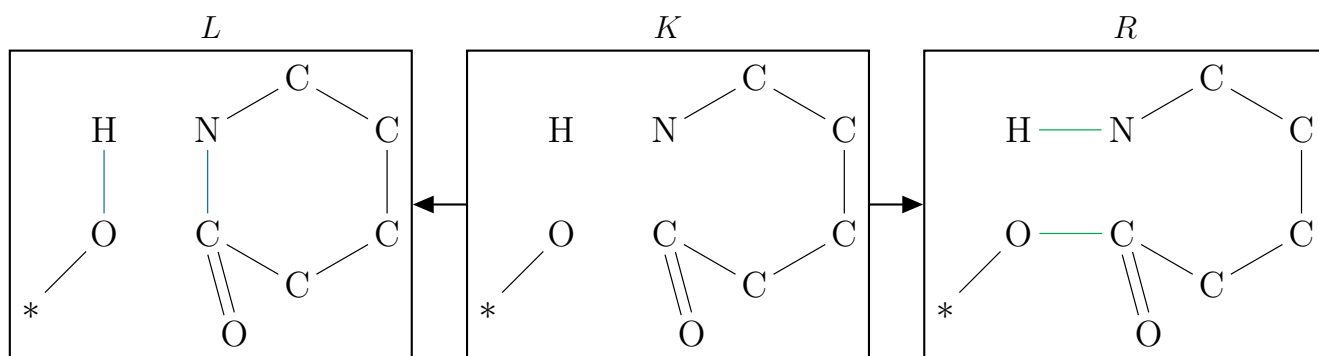


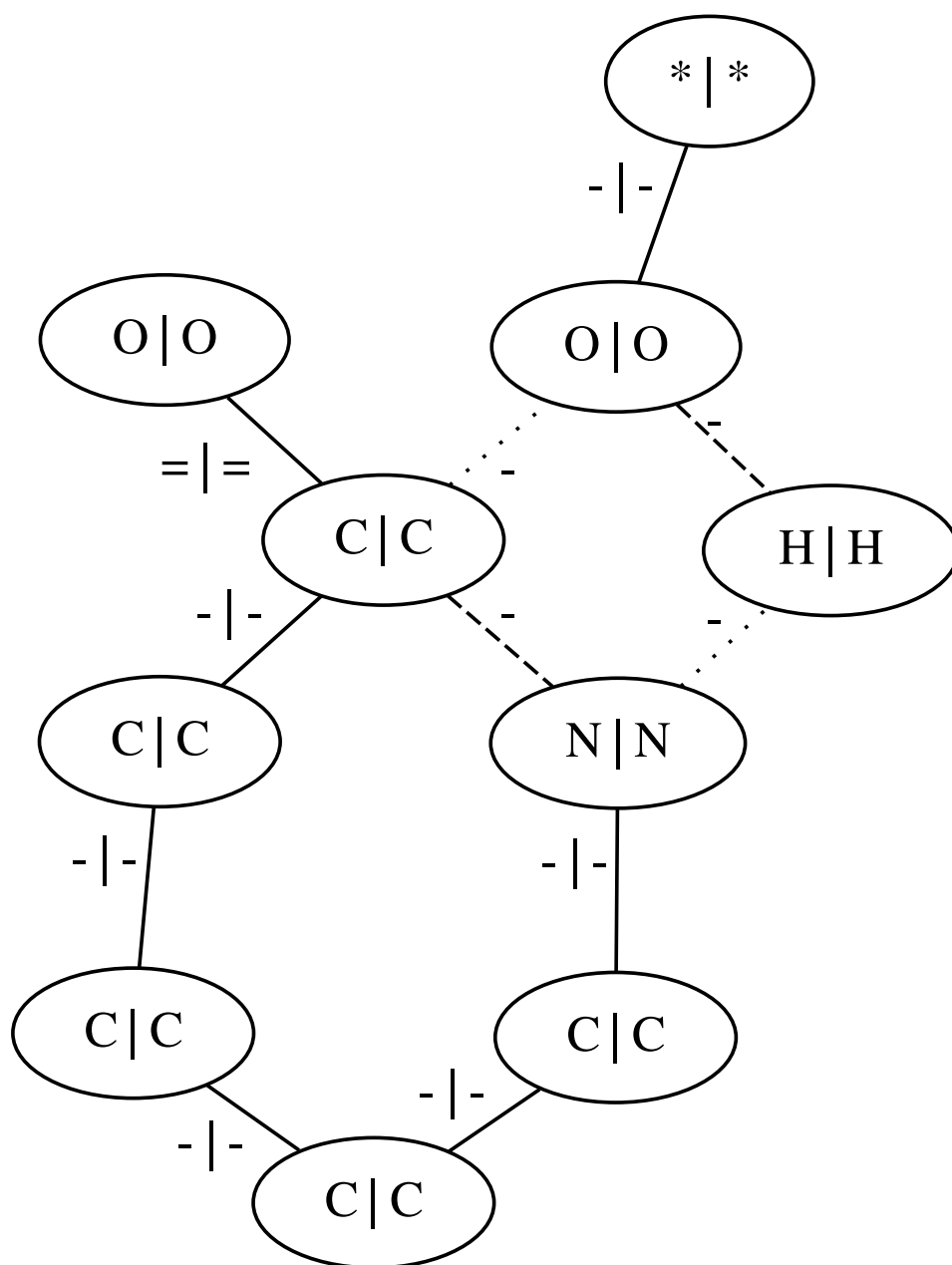
File: out/802_r_163_combined

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

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

0.0.162 Ring Closure 6 membered, inverse O, N



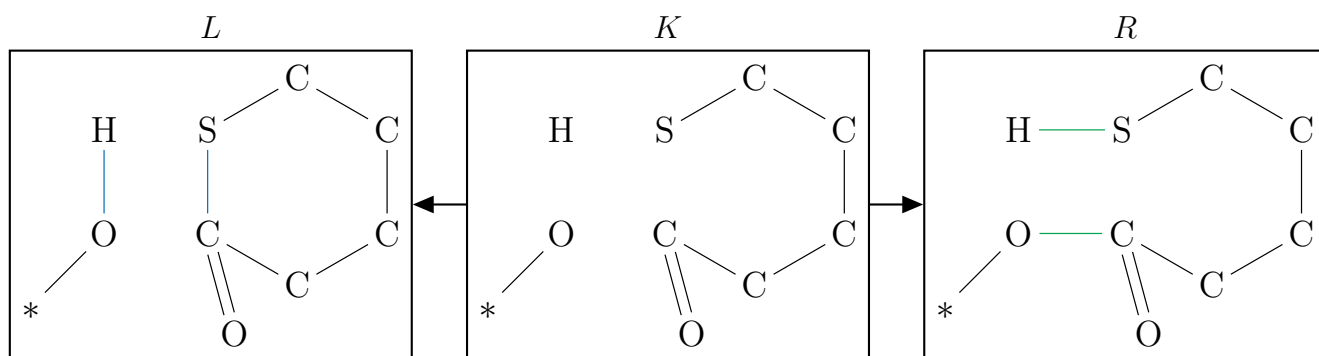


File: out/807_r_164_combined

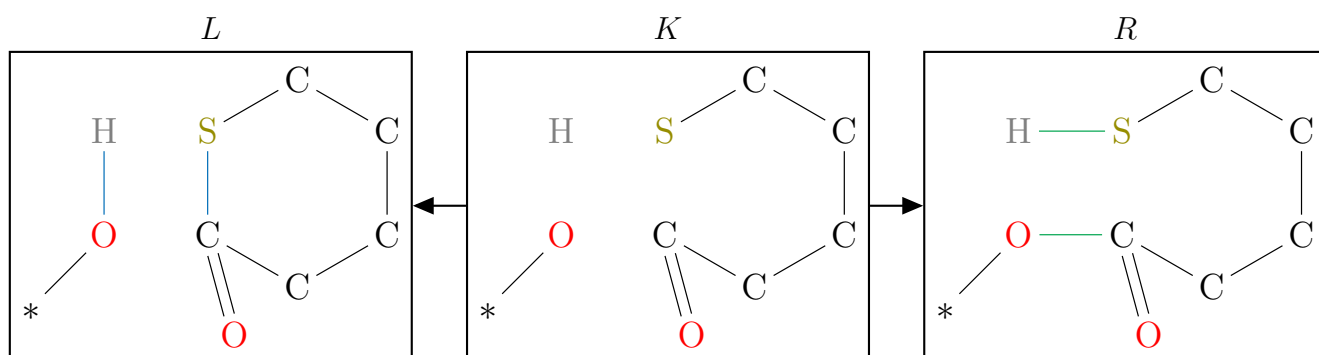
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid \leq 1
\end{aligned}$$

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

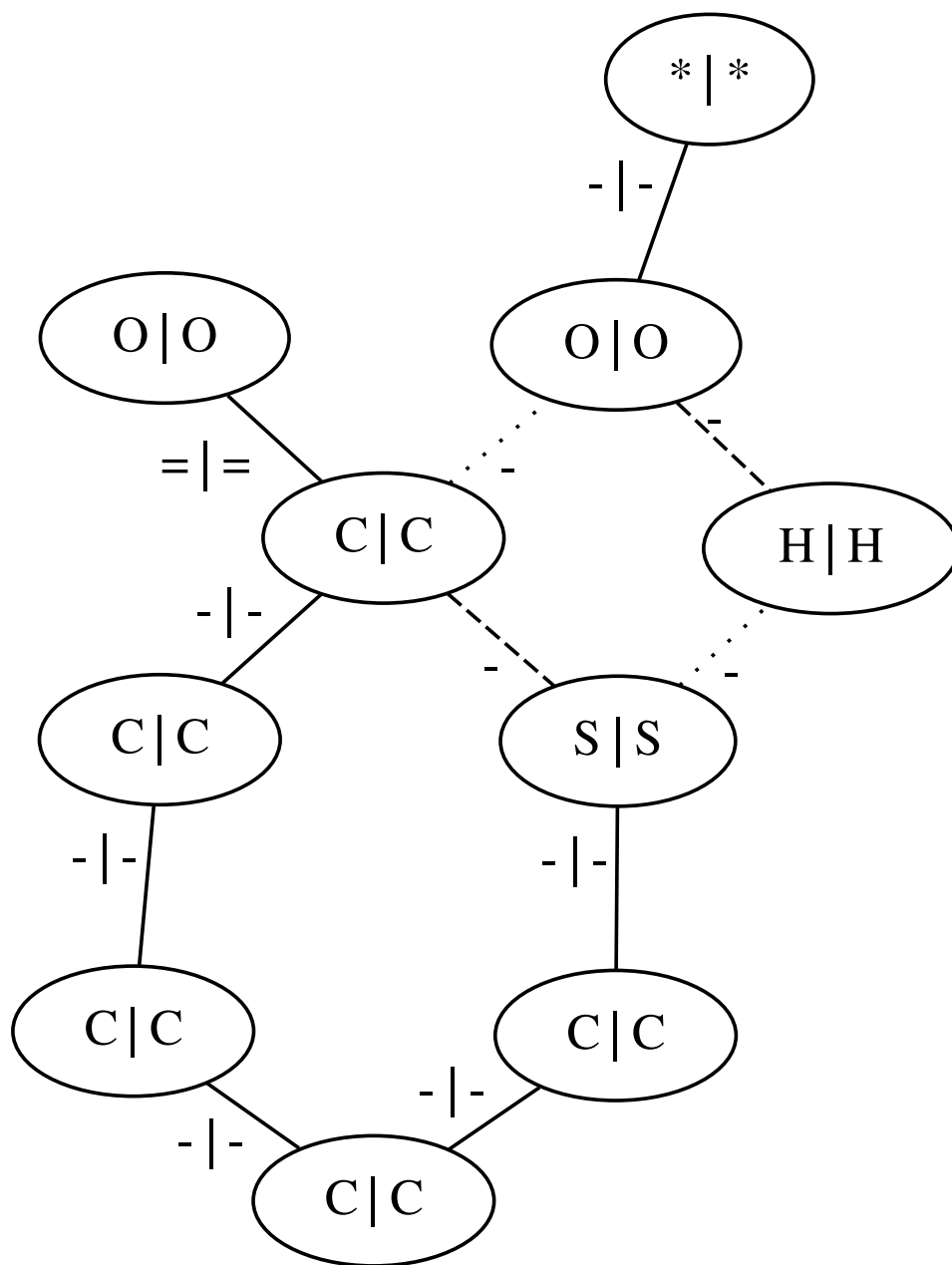
0.0.163 Ring Closure 6 membered, inverse O, S



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



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

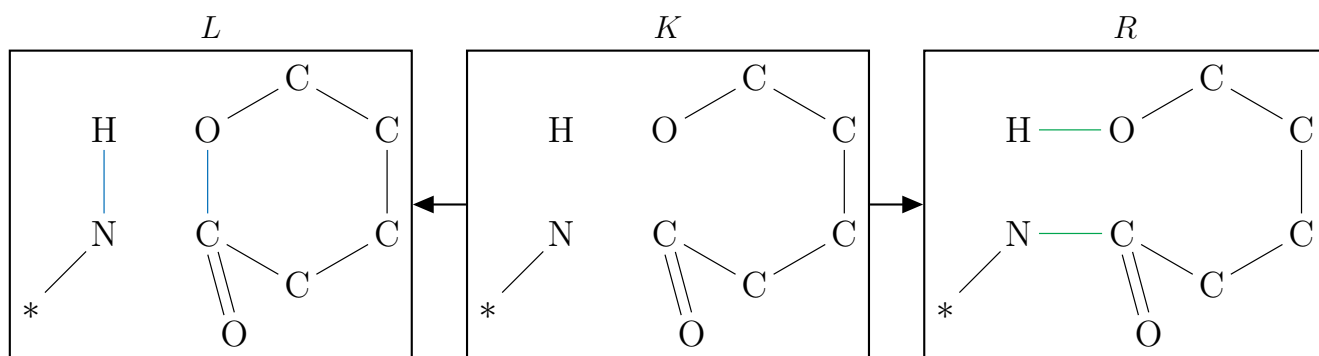


File: out/812_r_165_combined

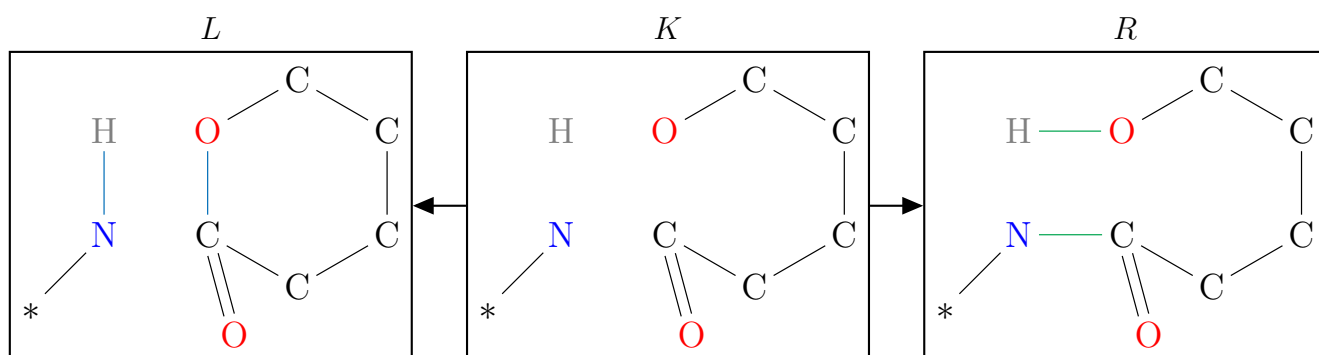
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid \leq 1
\end{aligned}$$

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

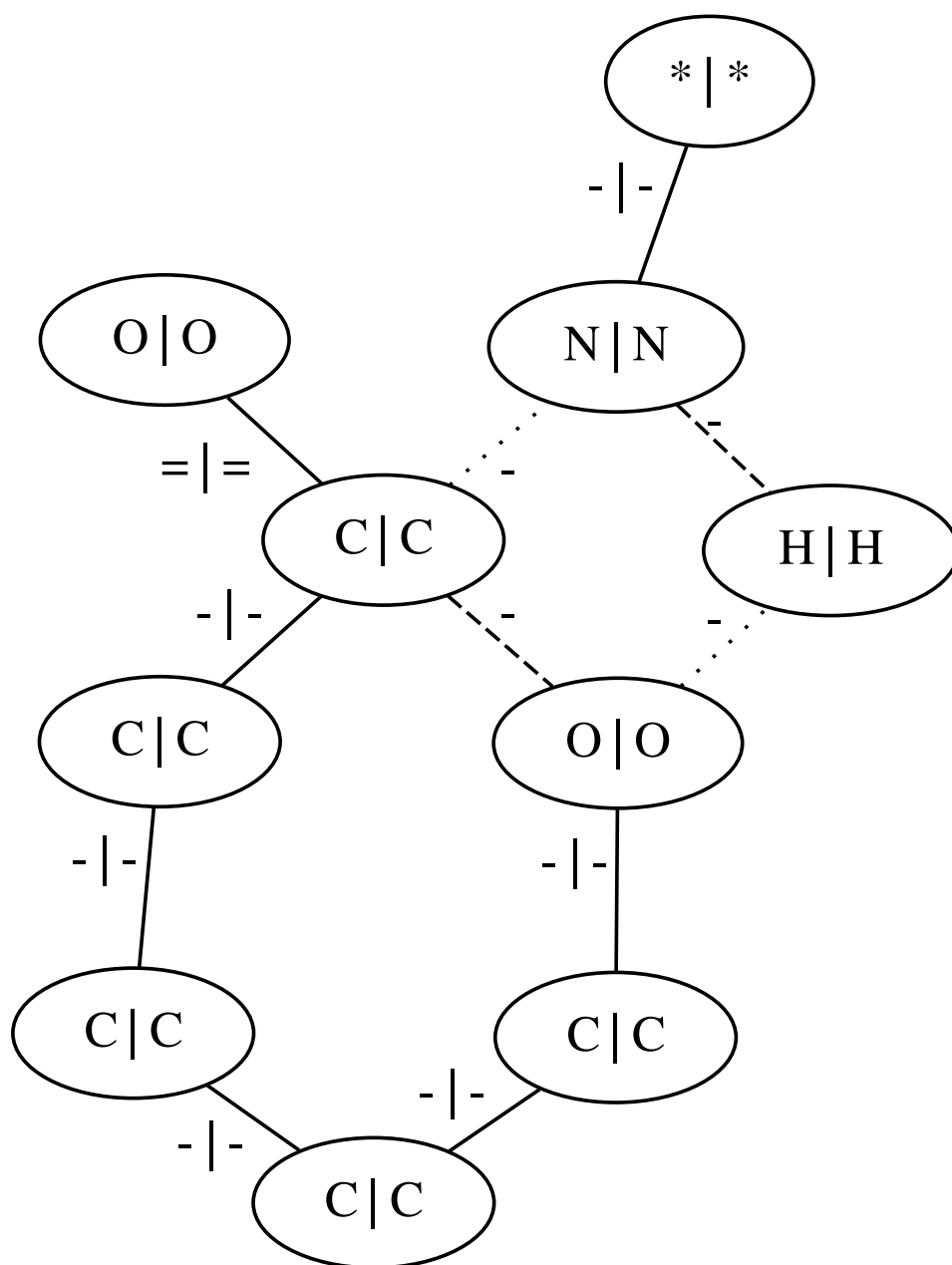
0.0.164 Ring Closure 6 membered, inverse N, O



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



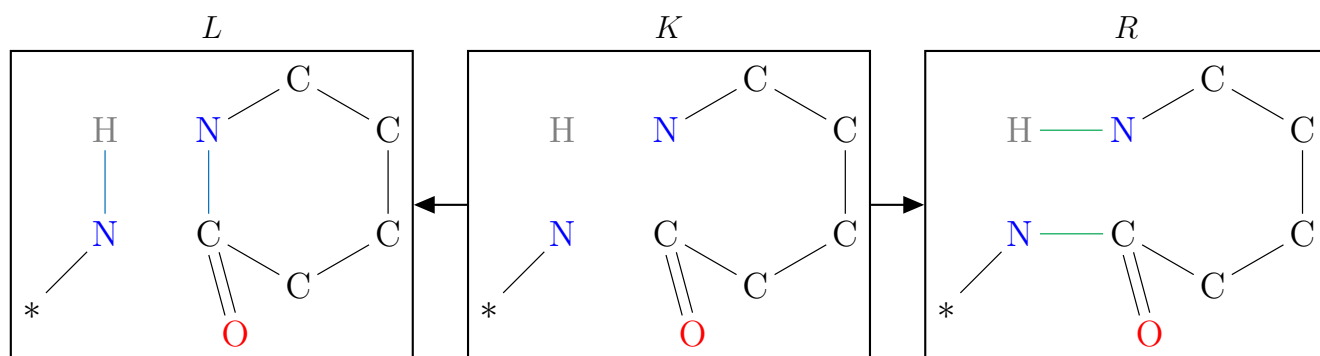
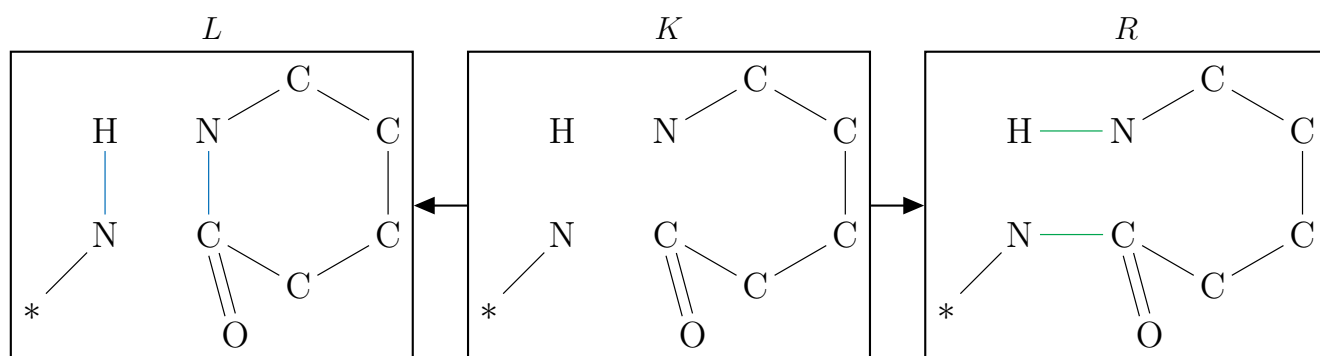
Files: out/816_r_166_11300100_{L, K, R}

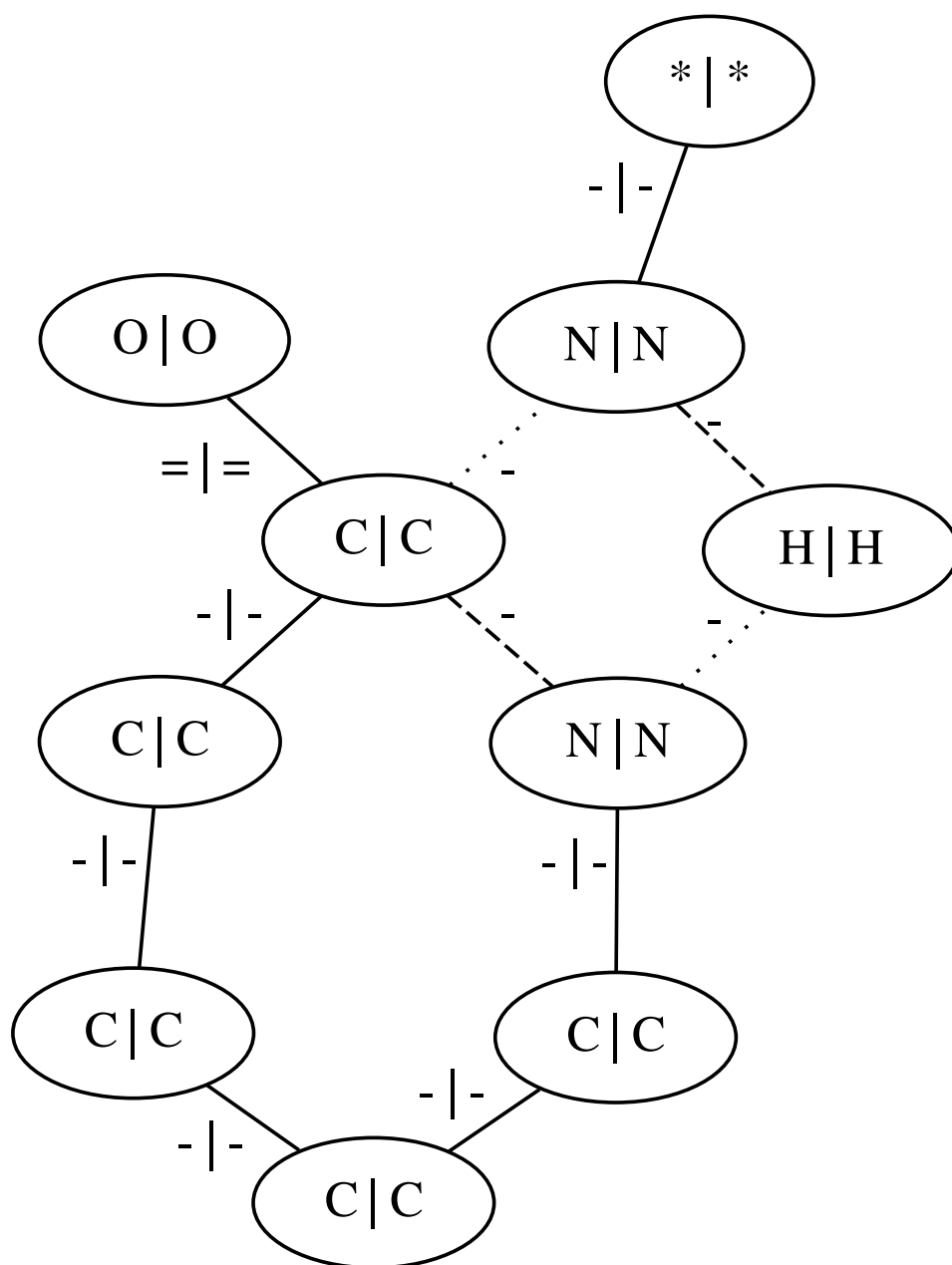


File: out/817_r_166_combined

$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \} | \leq 1
\end{aligned}$$

0.0.165 Ring Closure 6 membered, inverse N, N

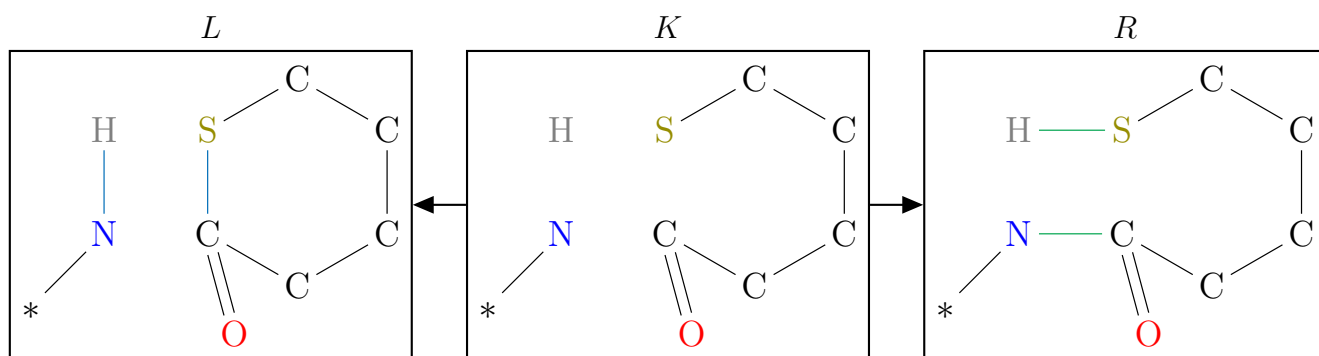
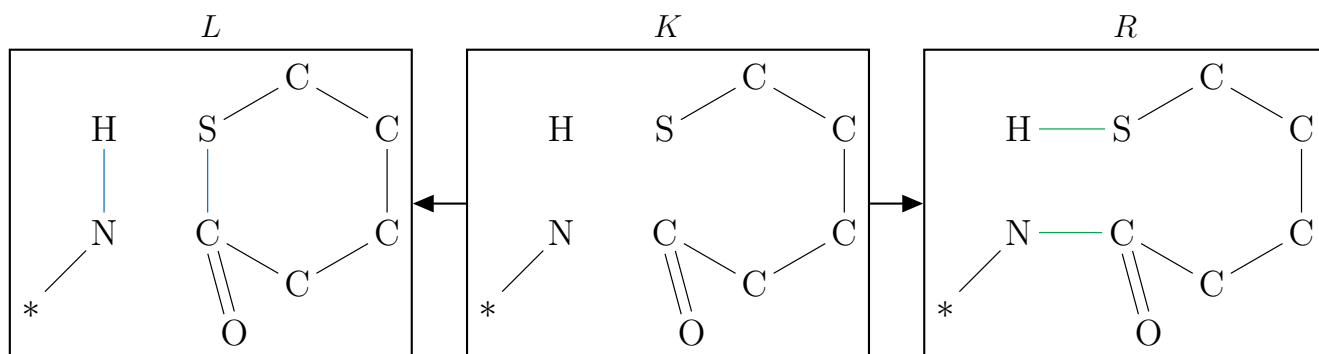


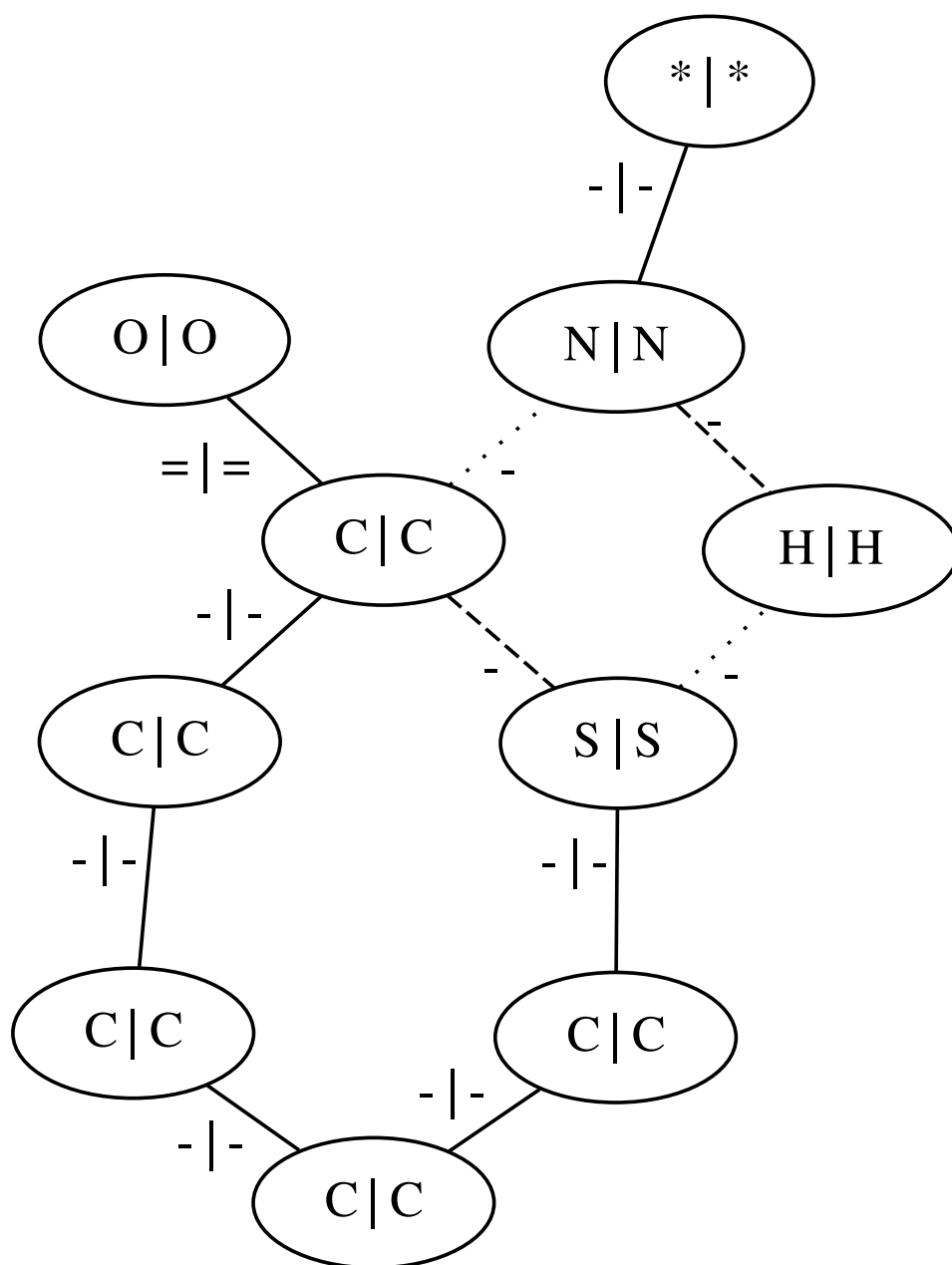


File: out/822_r_167_combined

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

0.0.166 Ring Closure 6 membered, inverse N, S

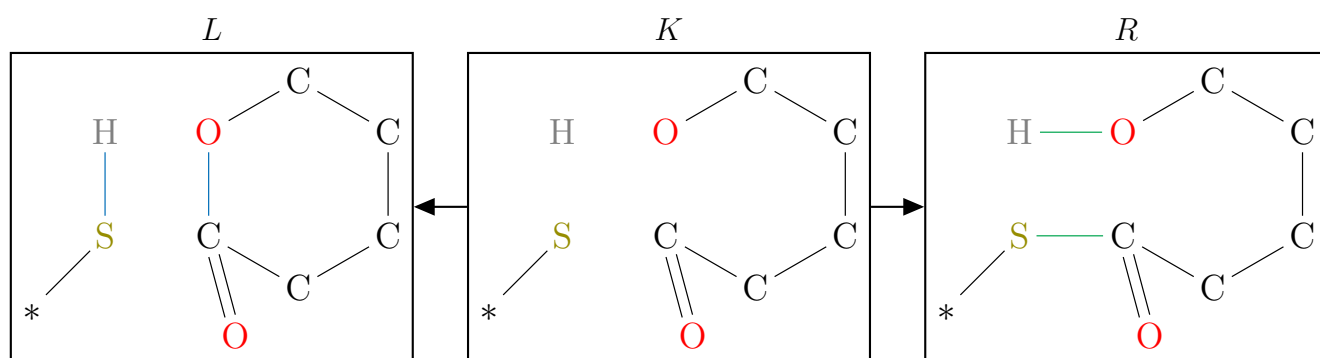
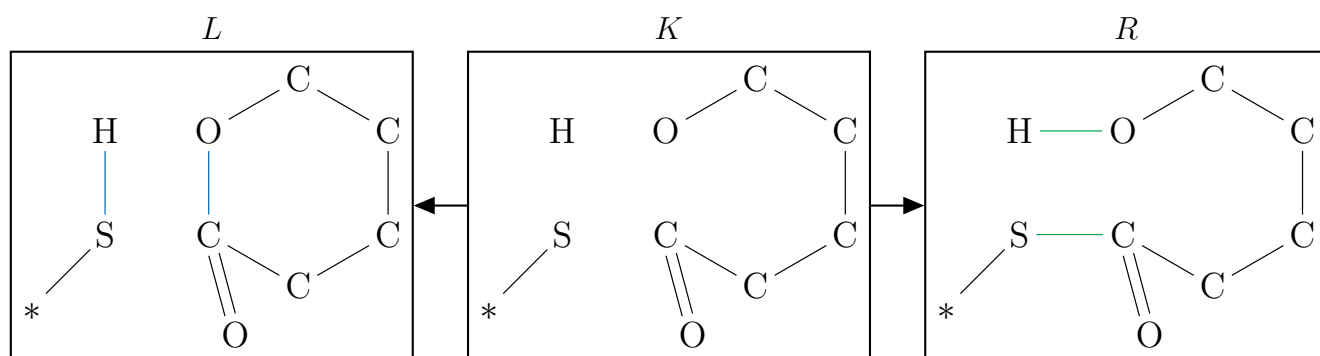


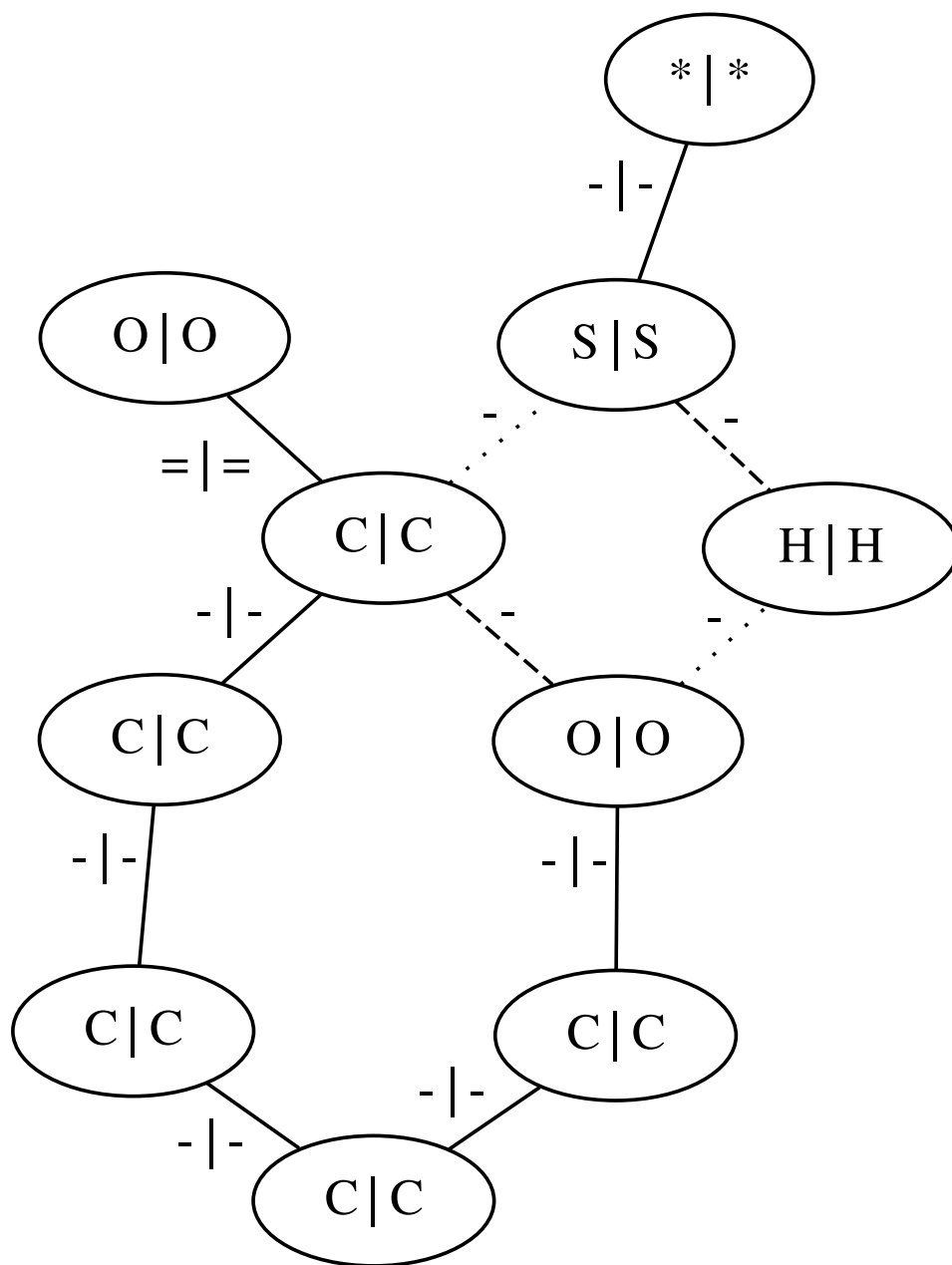


File: out/827_r_168_combined

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

0.0.167 Ring Closure 6 membered, inverse S, O

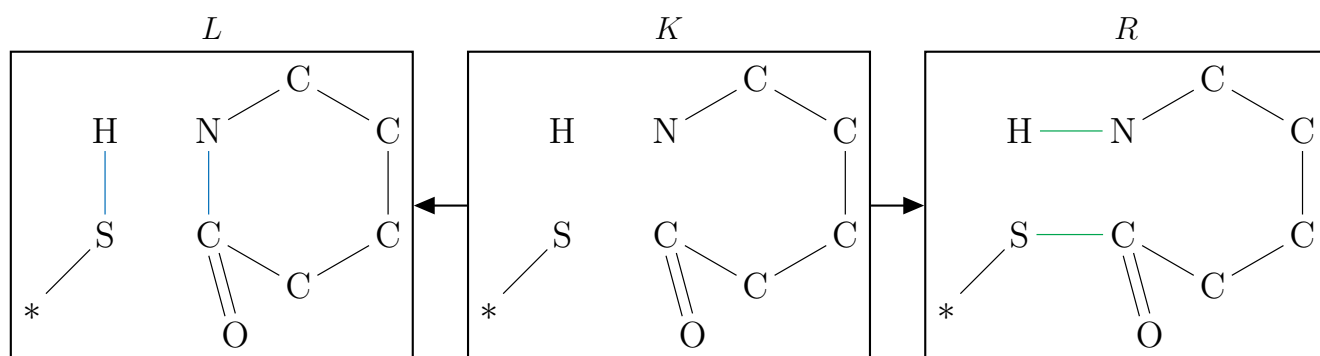




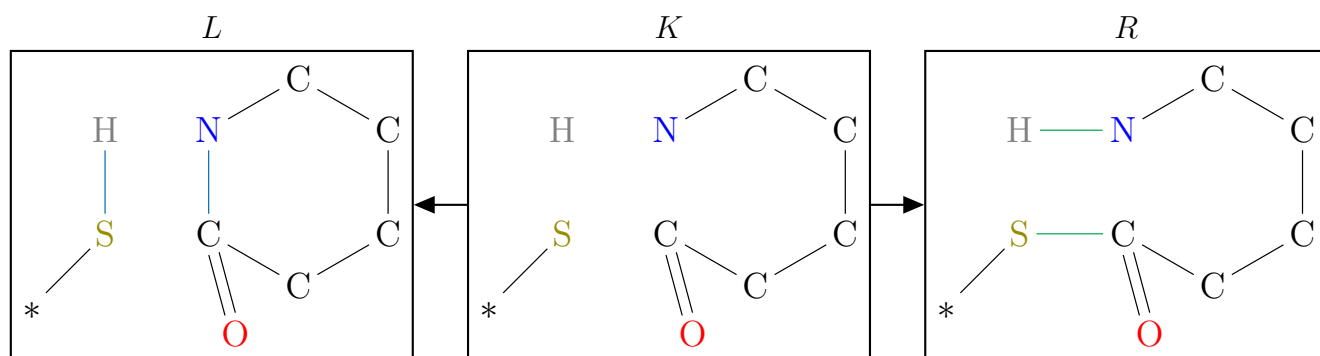
File: out/832_r_169_combined

$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| \leq 1
\end{aligned}$$

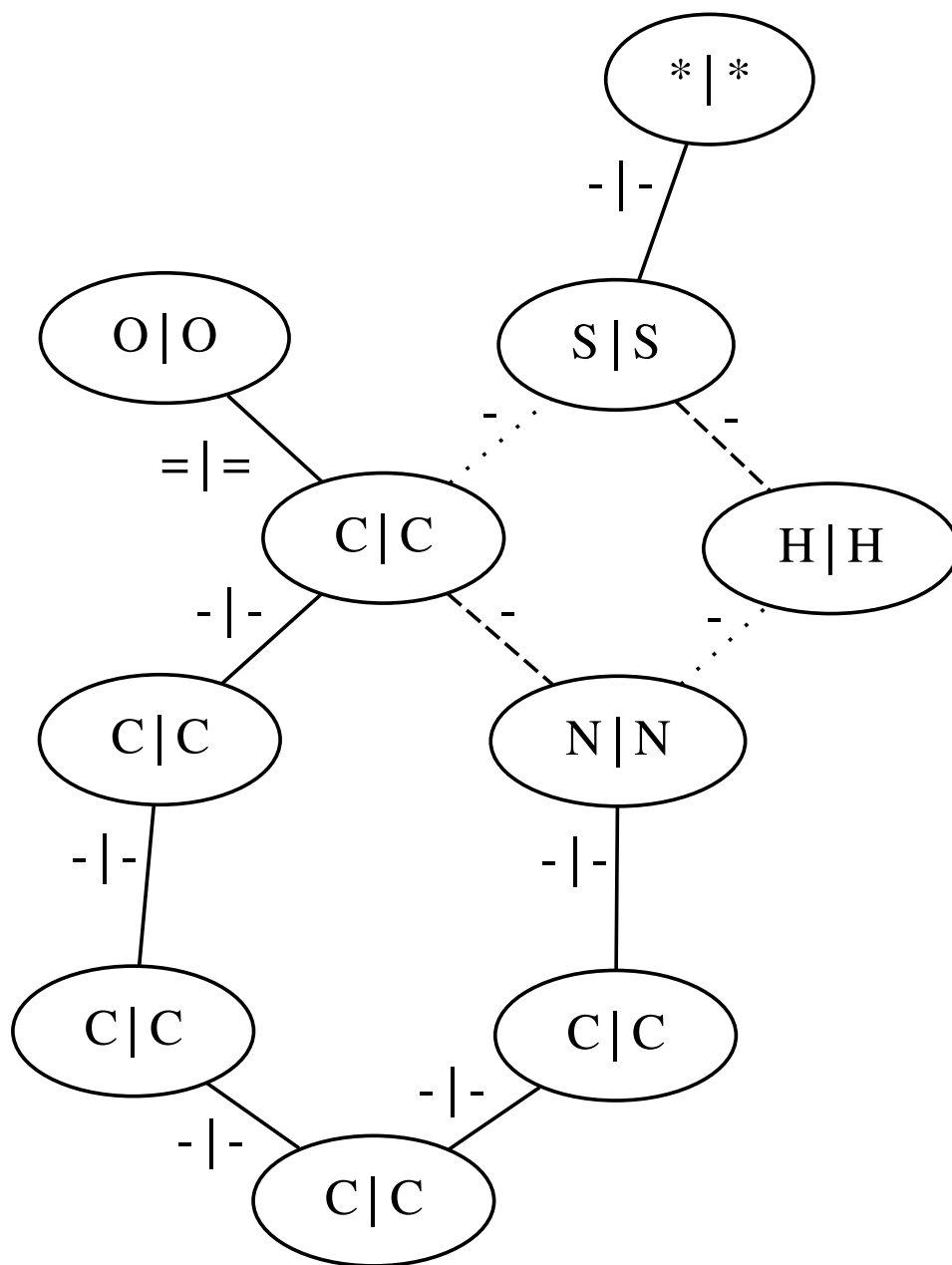
0.0.168 Ring Closure 6 membered, inverse S, N



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



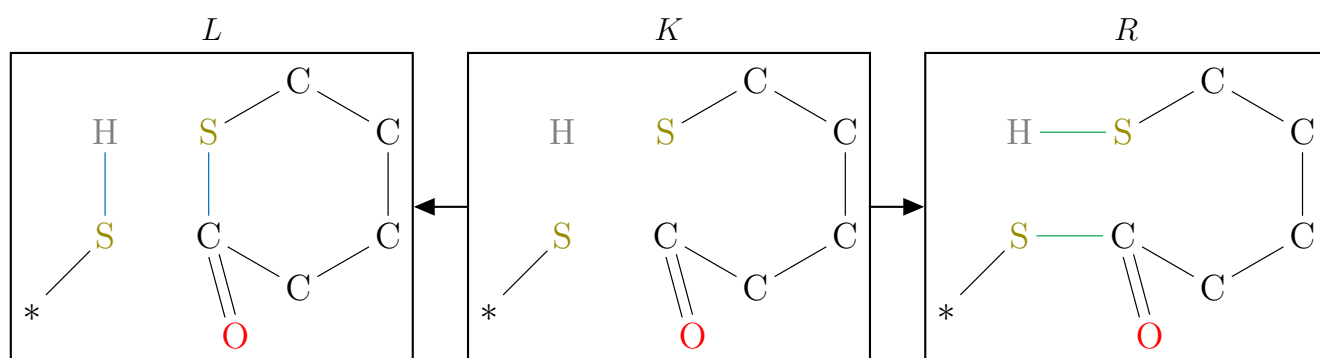
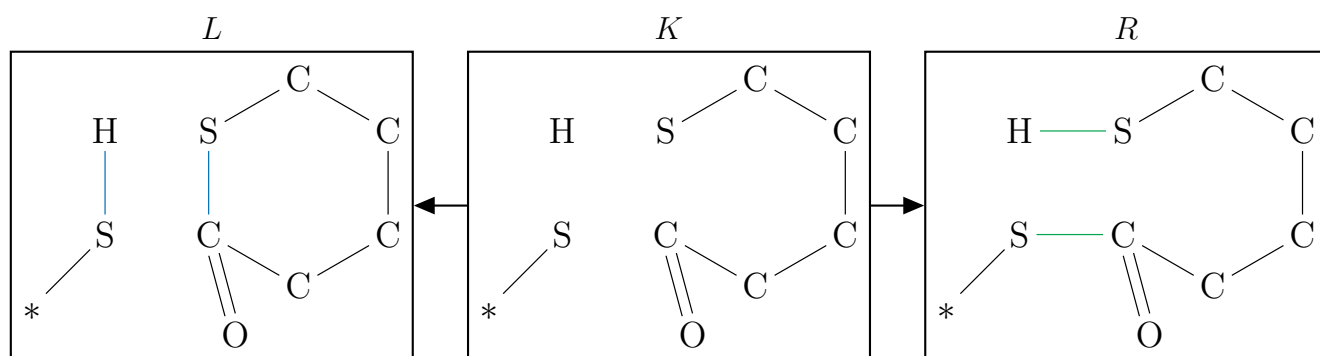
Files: out/836_r_170_11300100_{L, K, R}

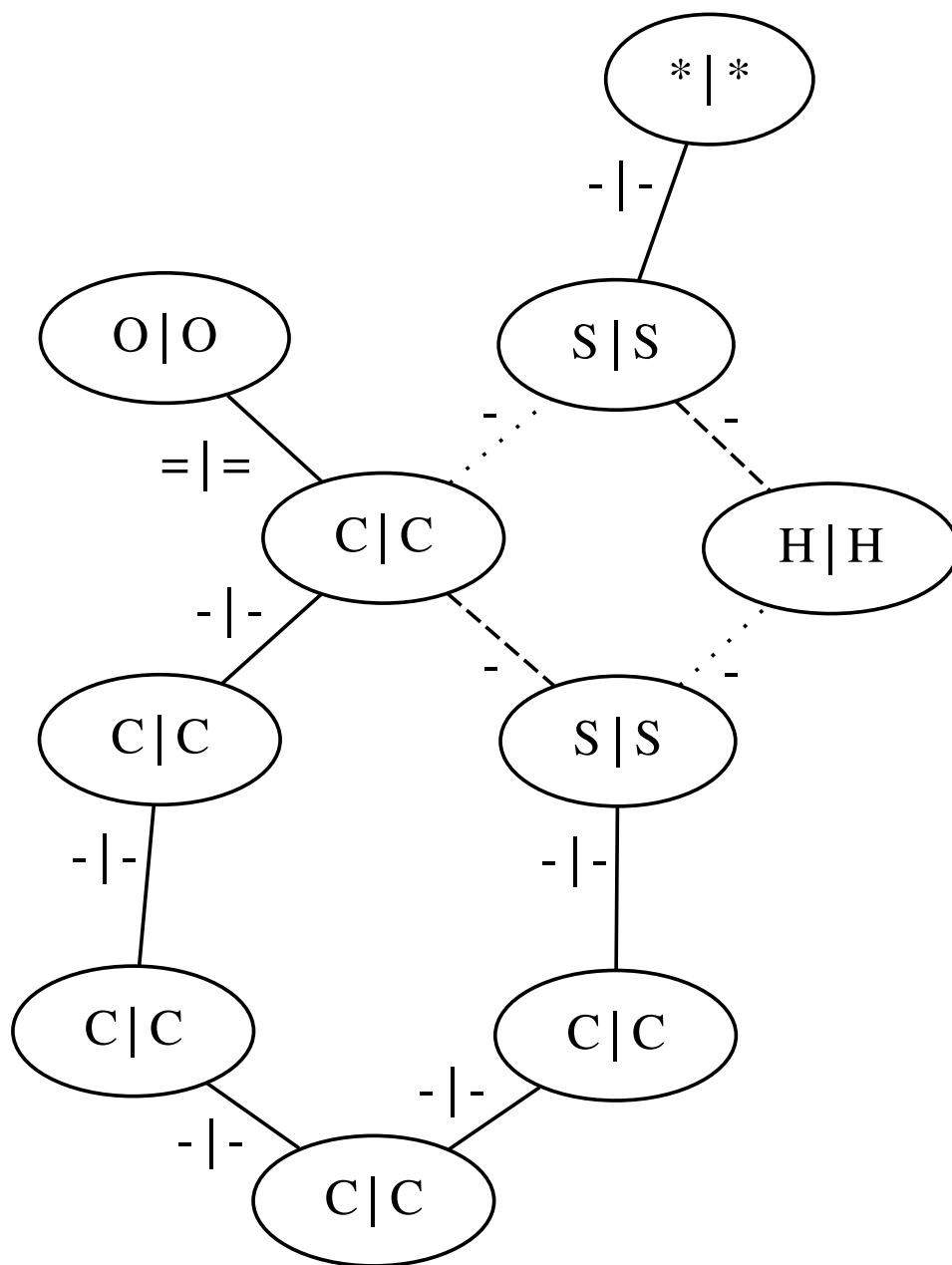


File: out/837_r_170_combined

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

0.0.169 Ring Closure 6 membered, inverse S, S

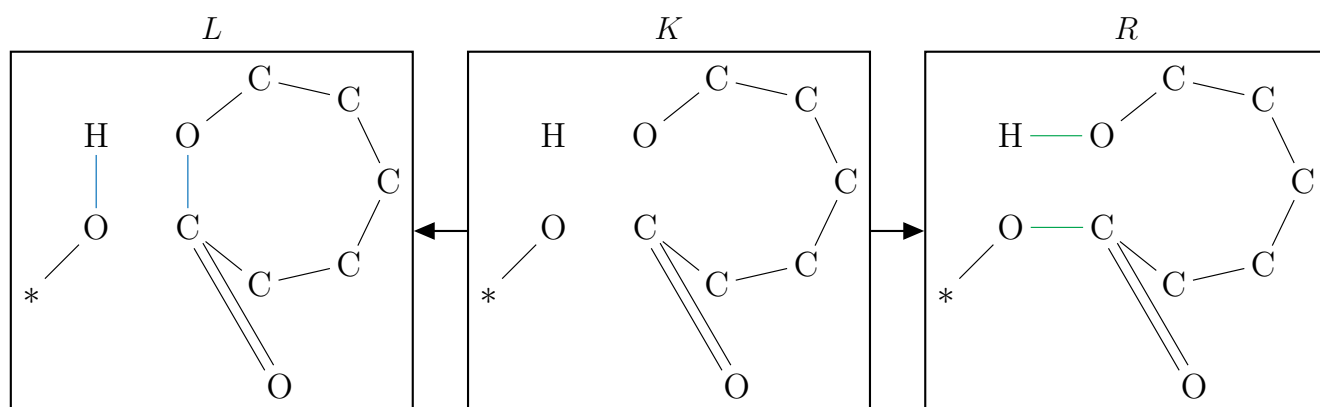




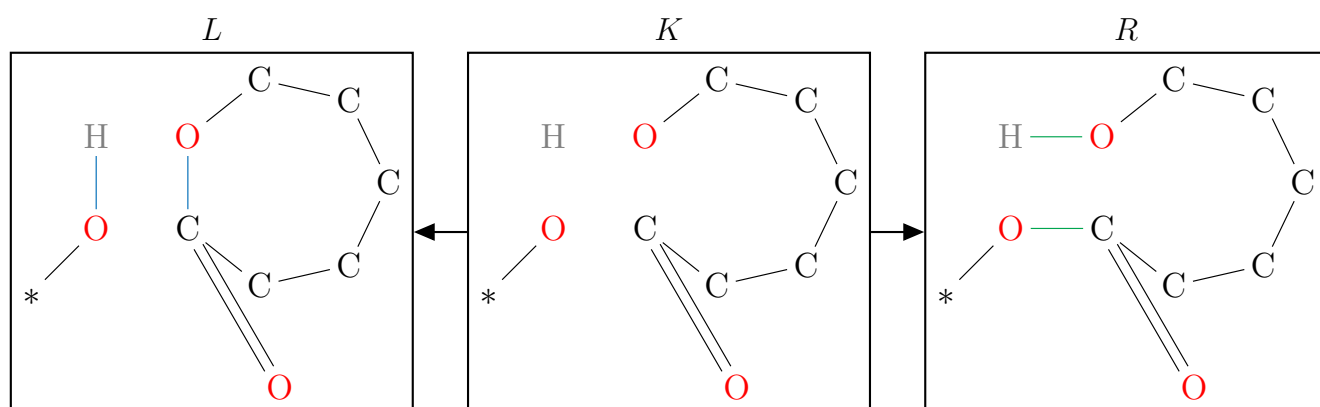
File: out/842_r_171_combined

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

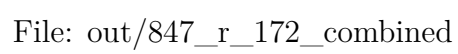
0.0.170 Ring Closure 7 membered, inverse O, O



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



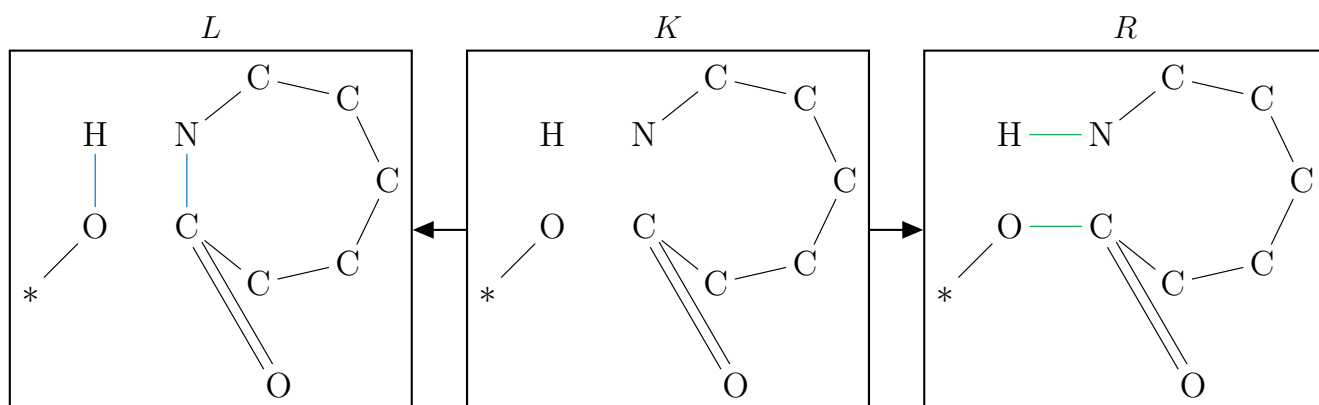
Files: out/846_r_172_11300100_{L, K, R}



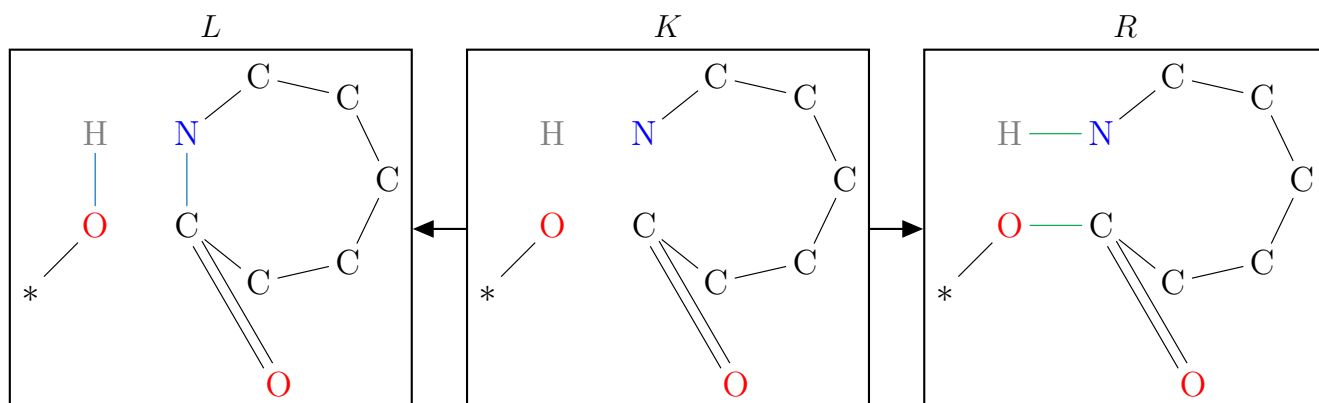
$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\} \leq 1
\end{aligned}$$

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

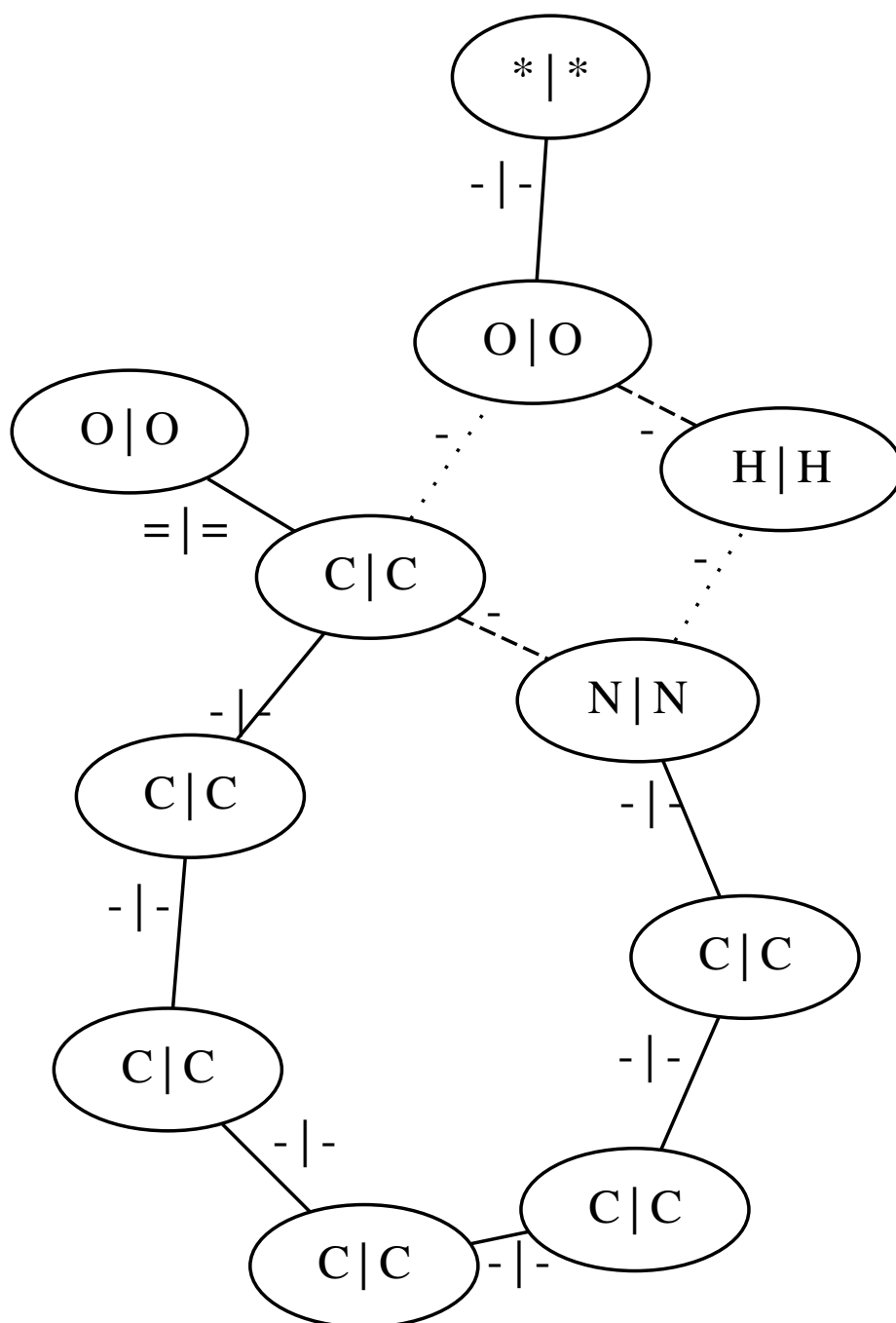
0.0.171 Ring Closure 7 membered, inverse O, N



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



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

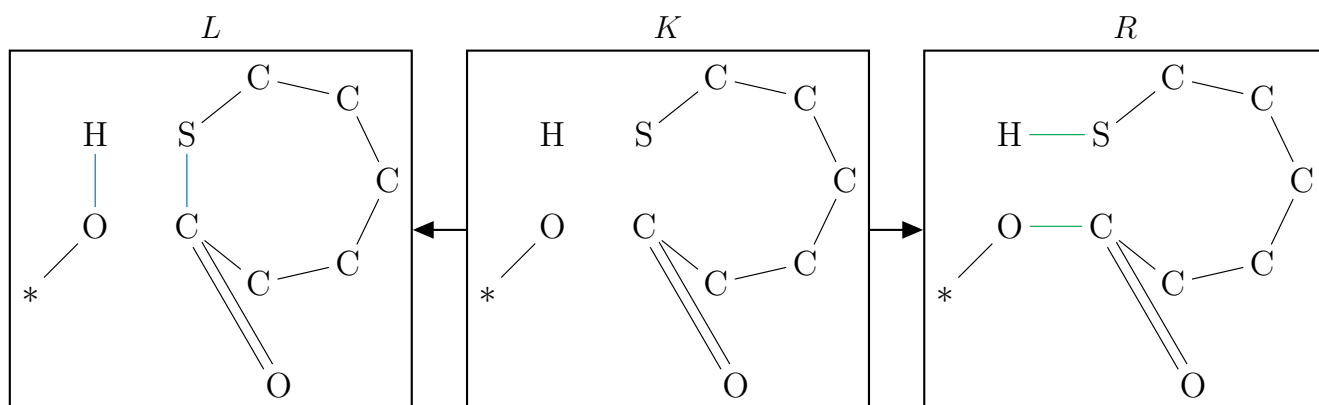


File: out/852_r_173_combined

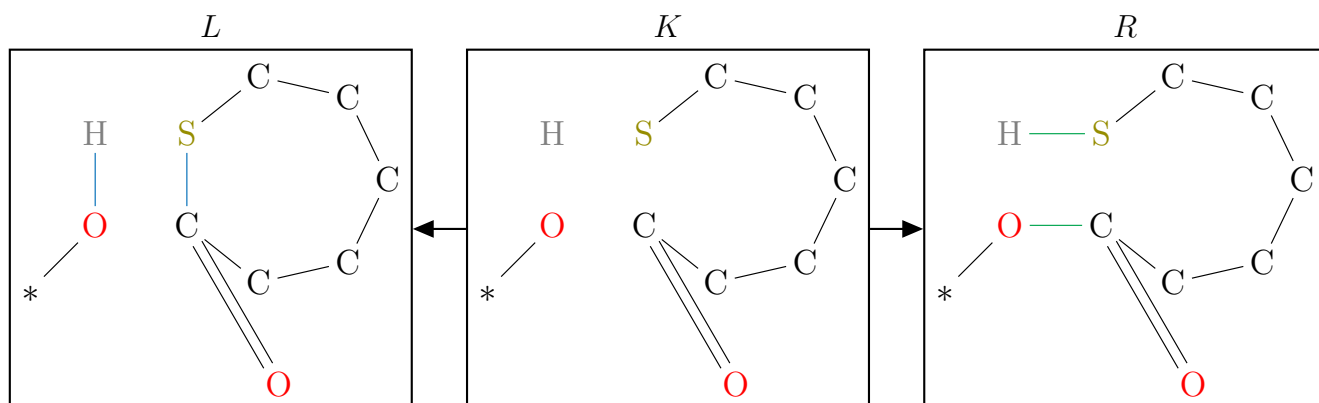
$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\} \leq 1
\end{aligned}$$

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

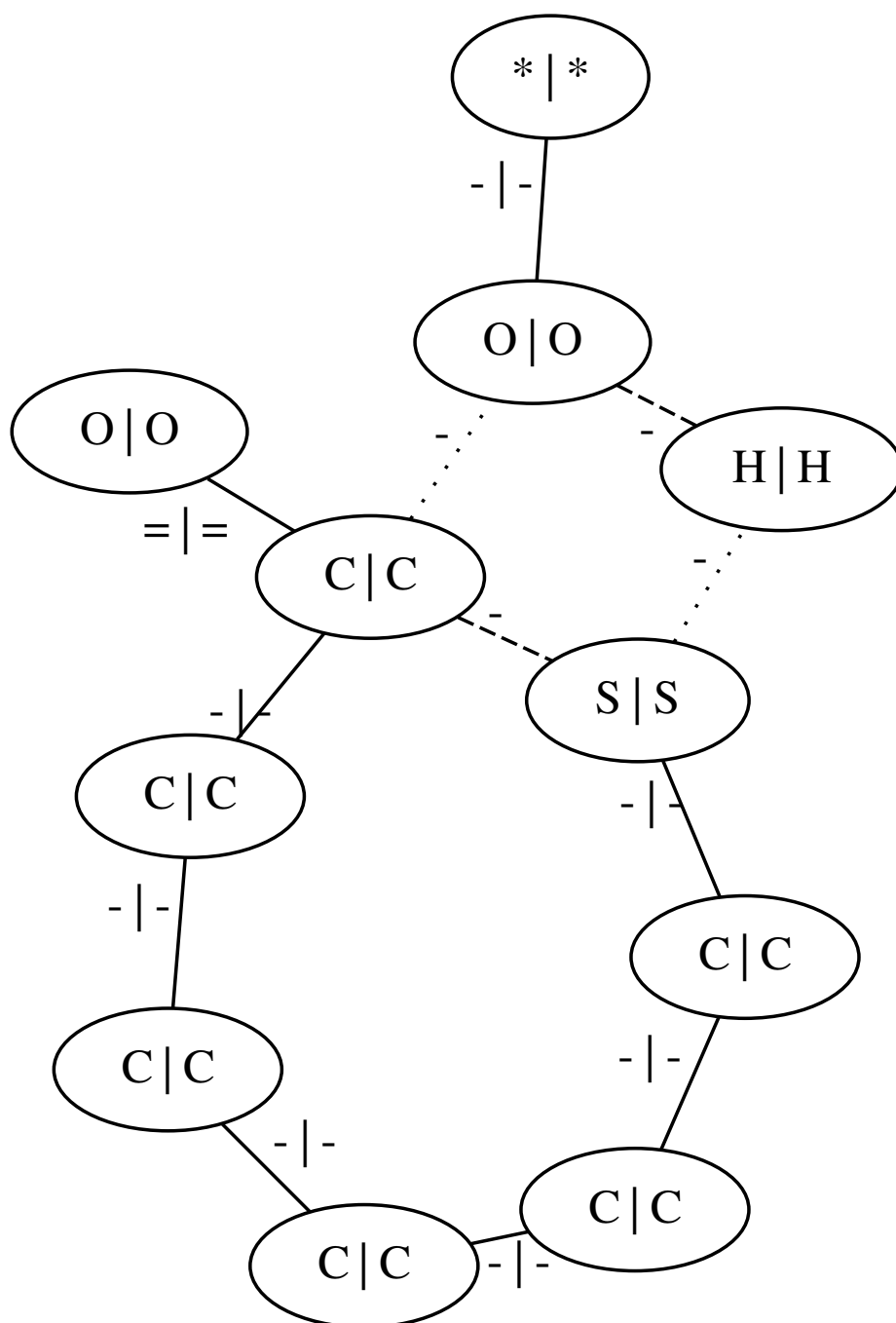
0.0.172 Ring Closure 7 membered, inverse O, S



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



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

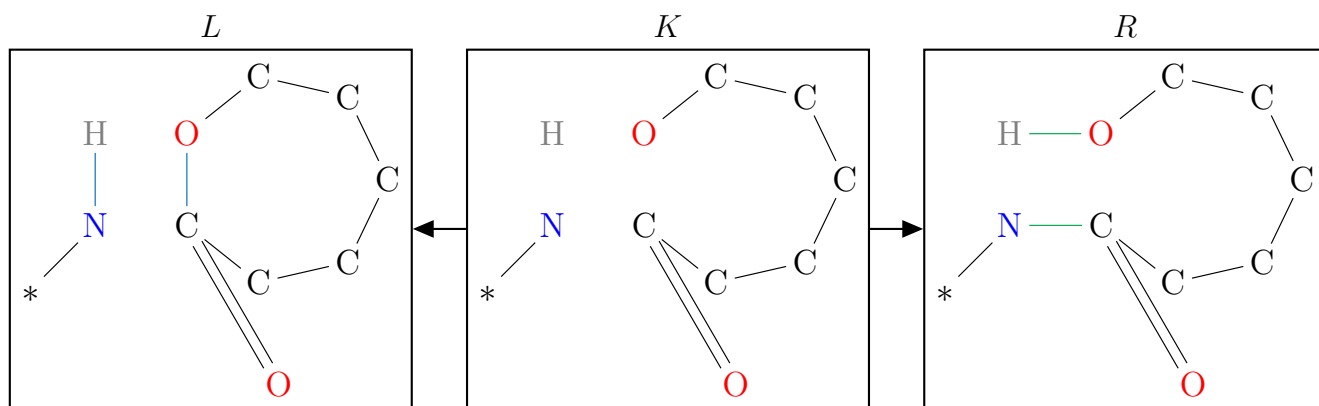
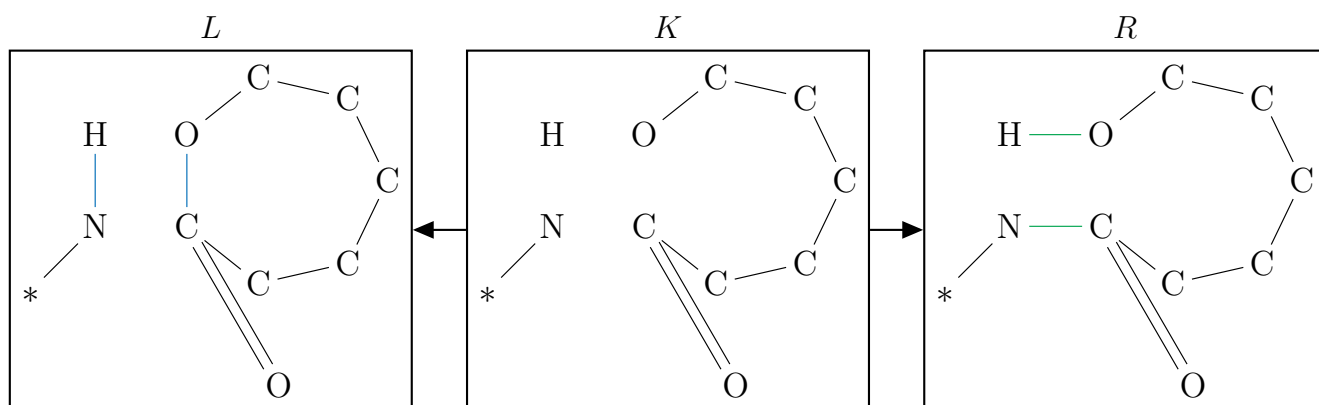


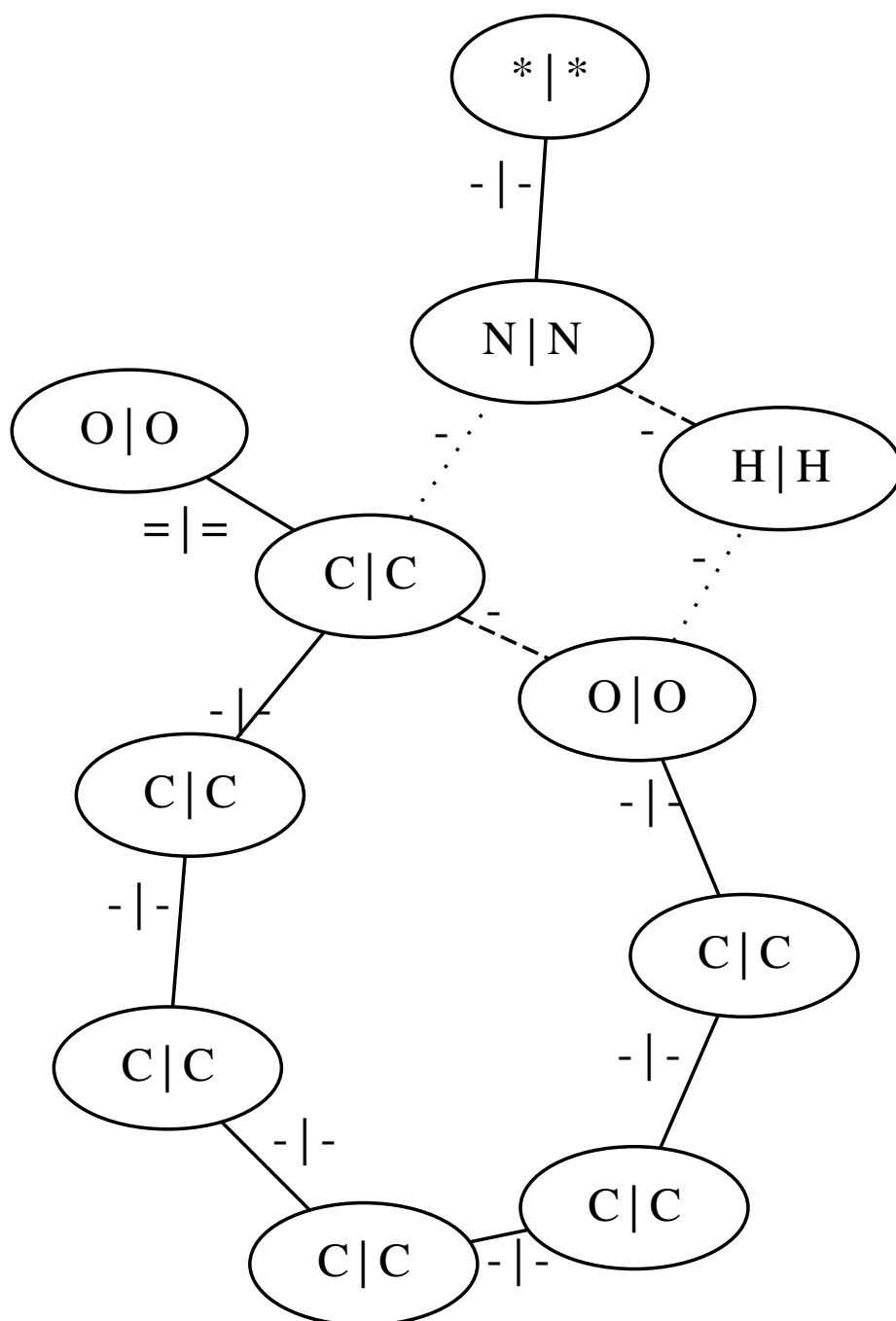
File: out/857_r_174_combined

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

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

0.0.173 Ring Closure 7 membered, inverse N, O

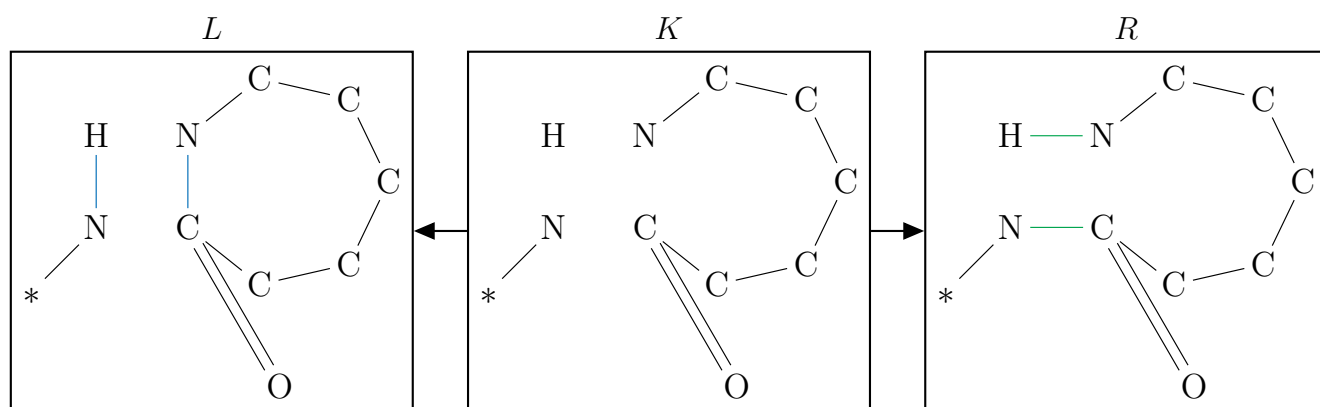




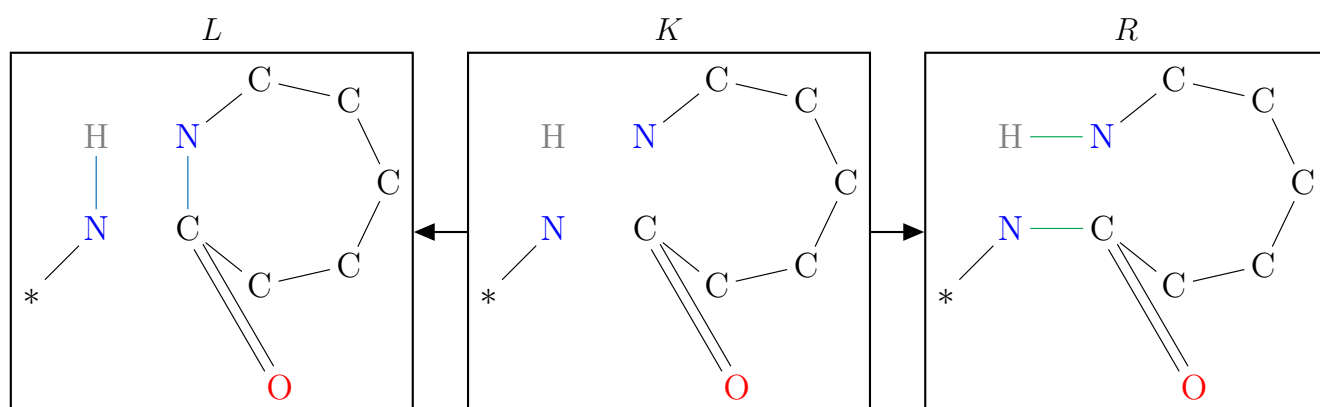
File: out/862_r_175_combined

$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| \leq 1
\end{aligned}$$

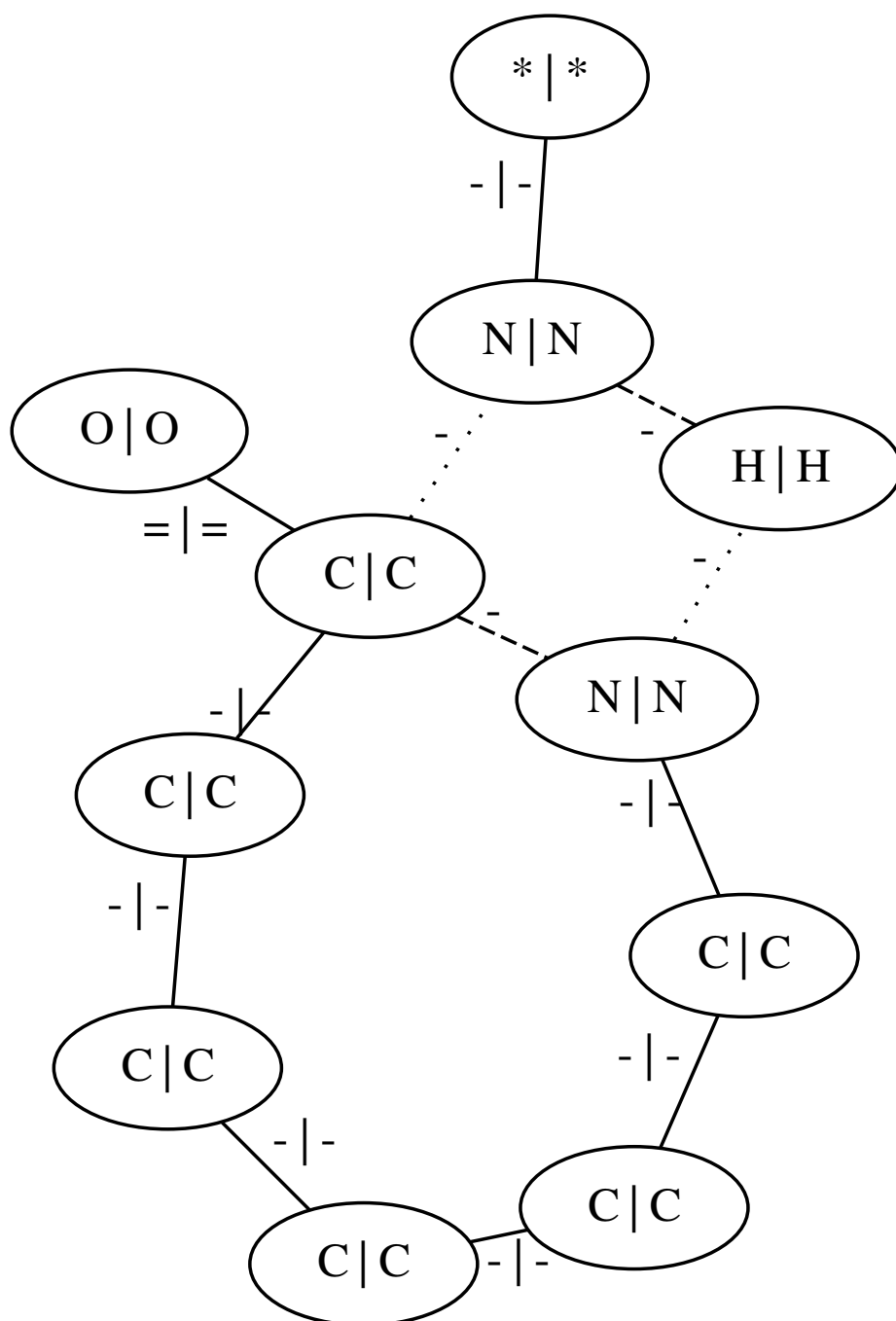
0.0.174 Ring Closure 7 membered, inverse N, N



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



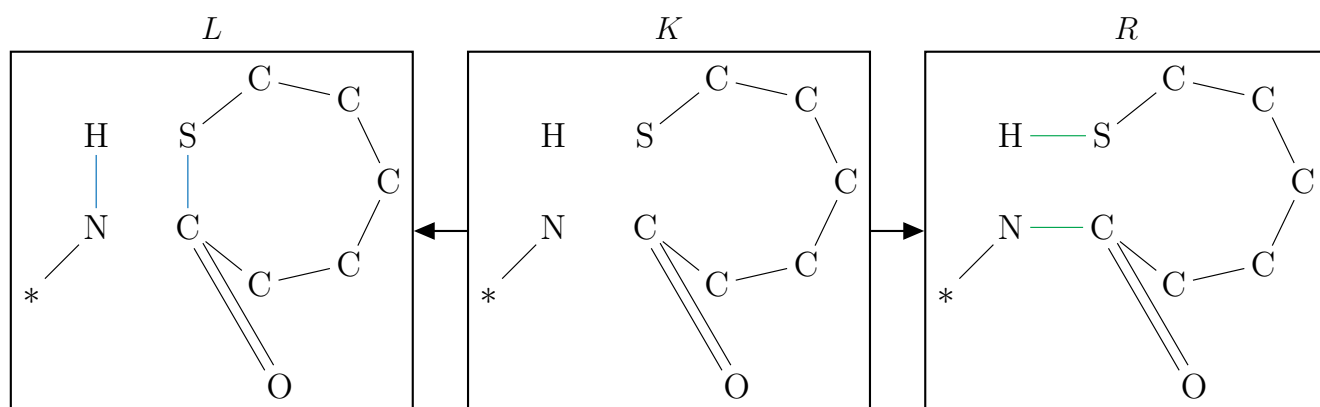
Files: out/866_r_176_11300100_{L, K, R}



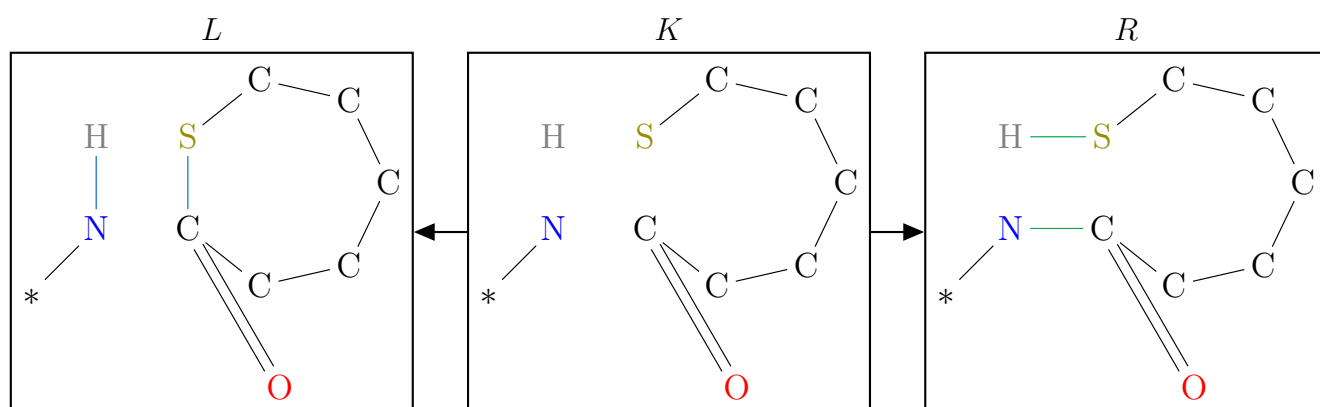
File: out/867_r_176_combined

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

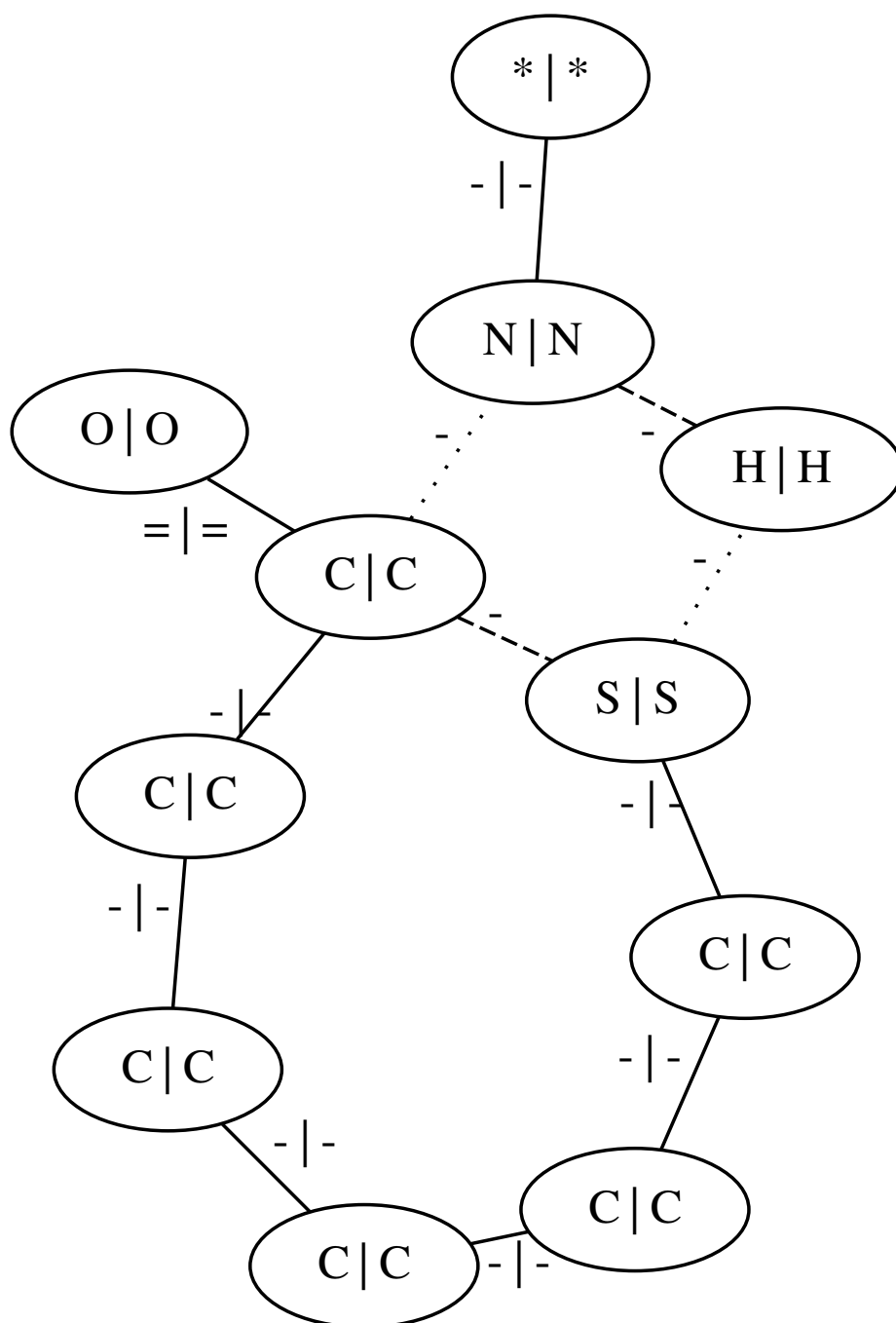
0.0.175 Ring Closure 7 membered, inverse N, S



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



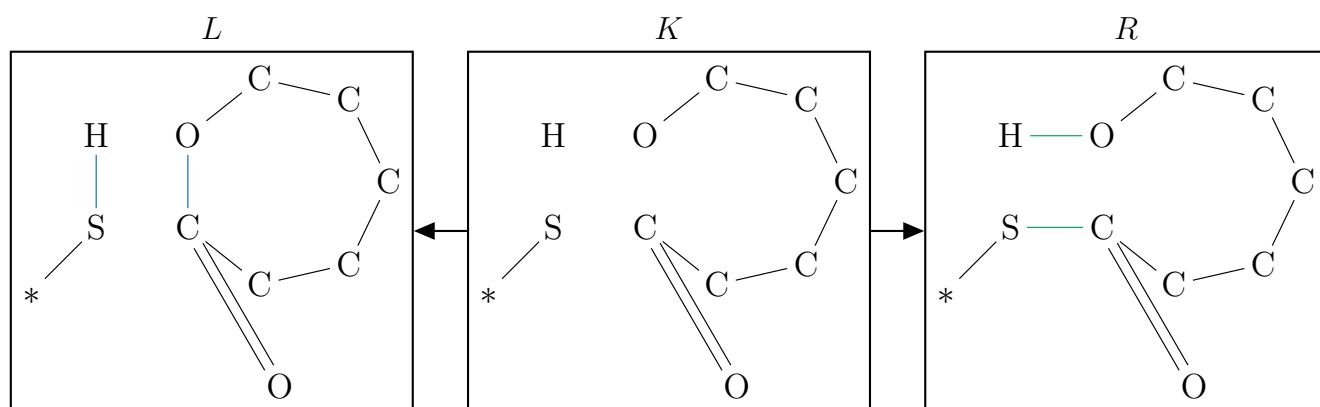
Files: out/871_r_177_11300100_{L, K, R}



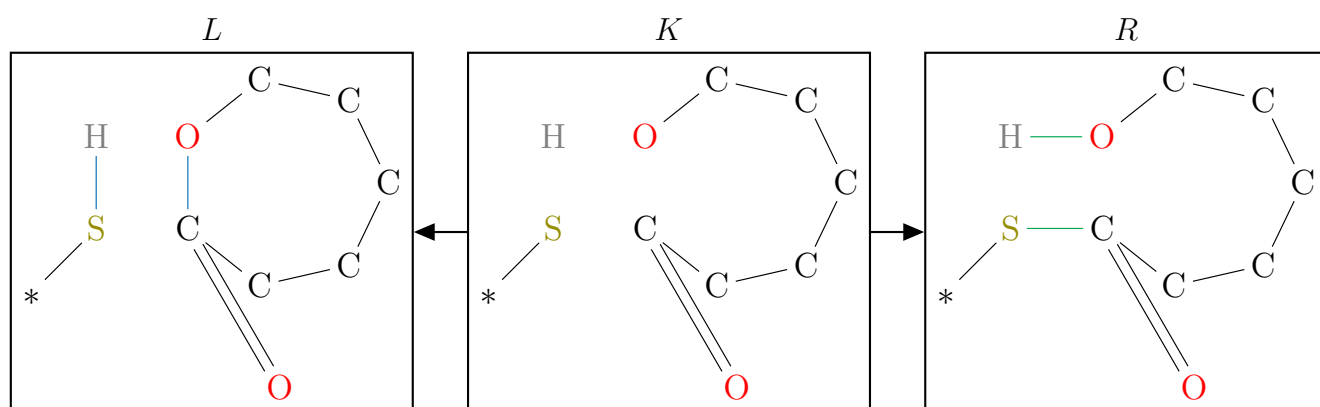
File: out/872_r_177_combined

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

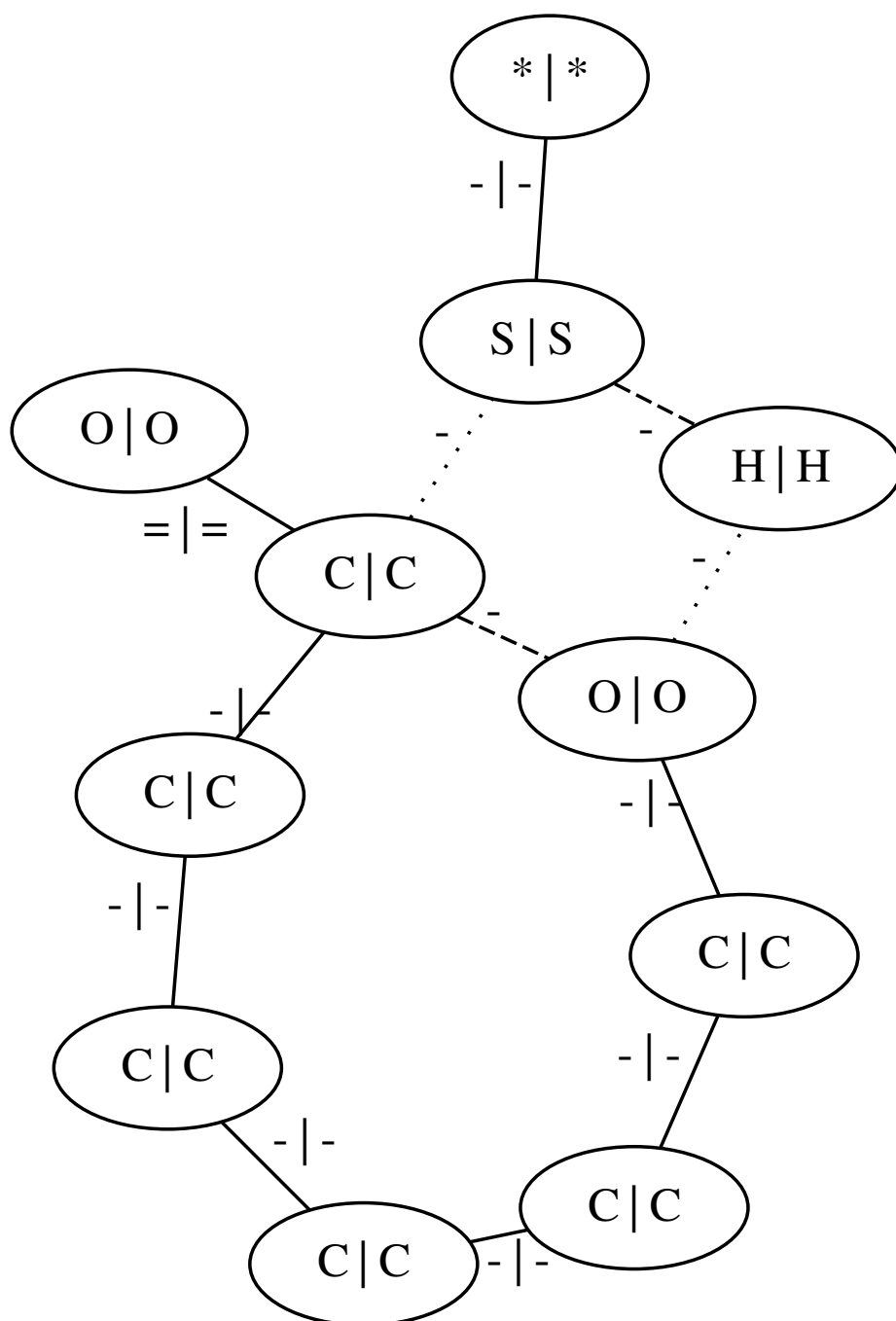
0.0.176 Ring Closure 7 membered, inverse S, O



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



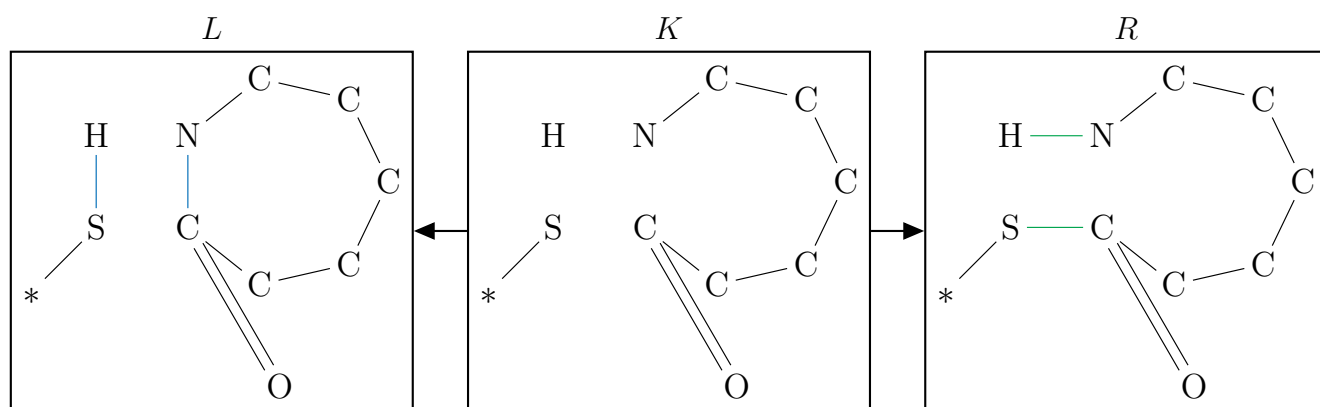
Files: out/876_r_178_11300100_{L, K, R}



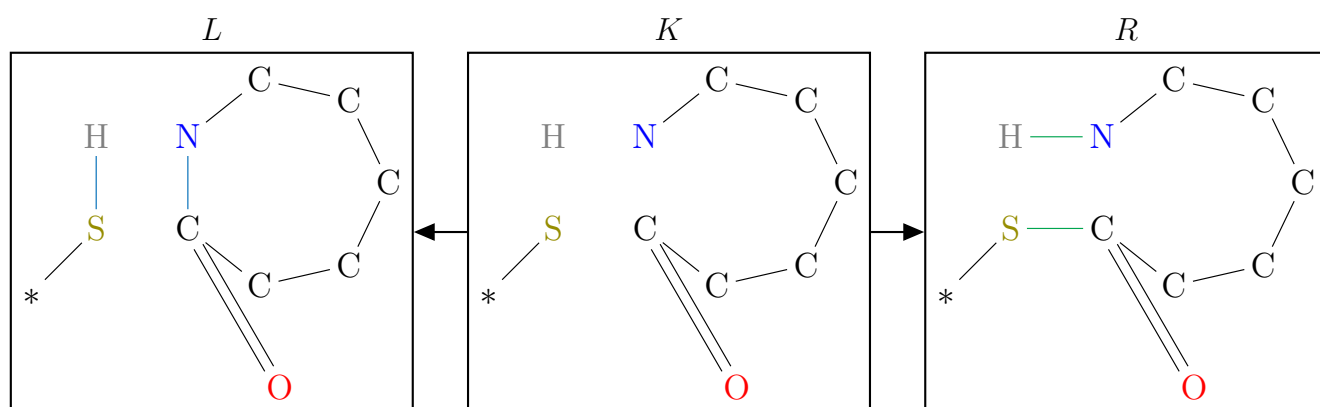
File: out/877_r_178_combined

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

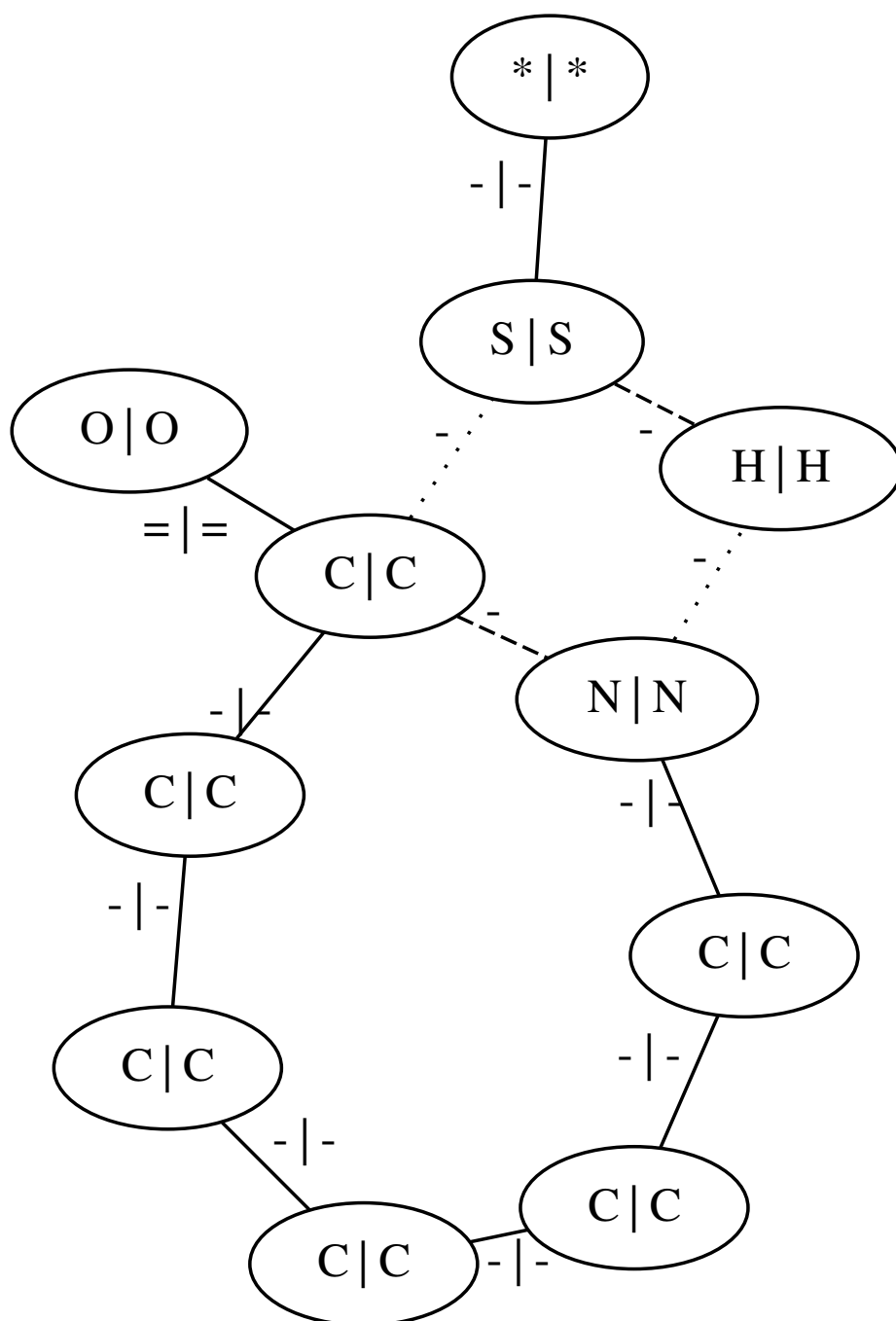
0.0.177 Ring Closure 7 membered, inverse S, N



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



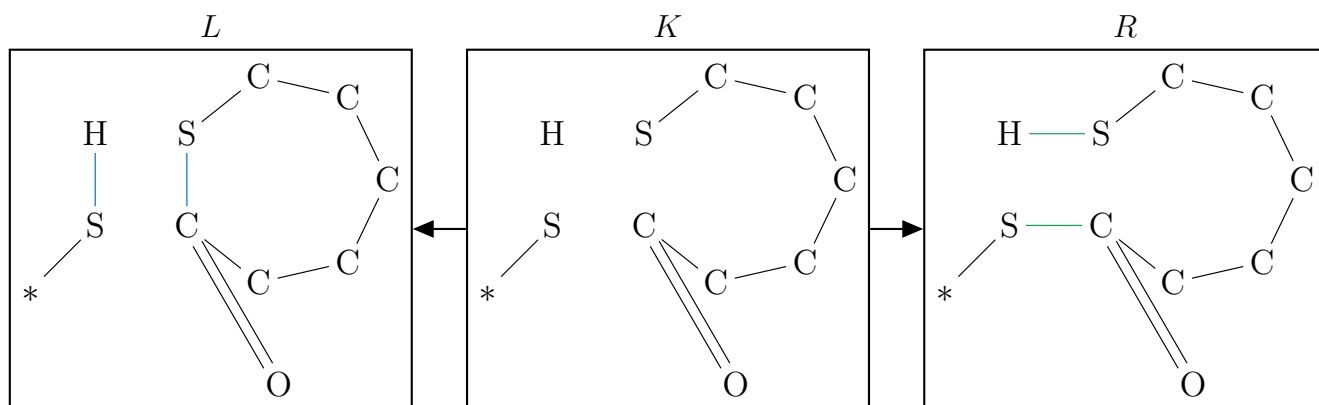
Files: out/881_r_179_11300100_{L, K, R}



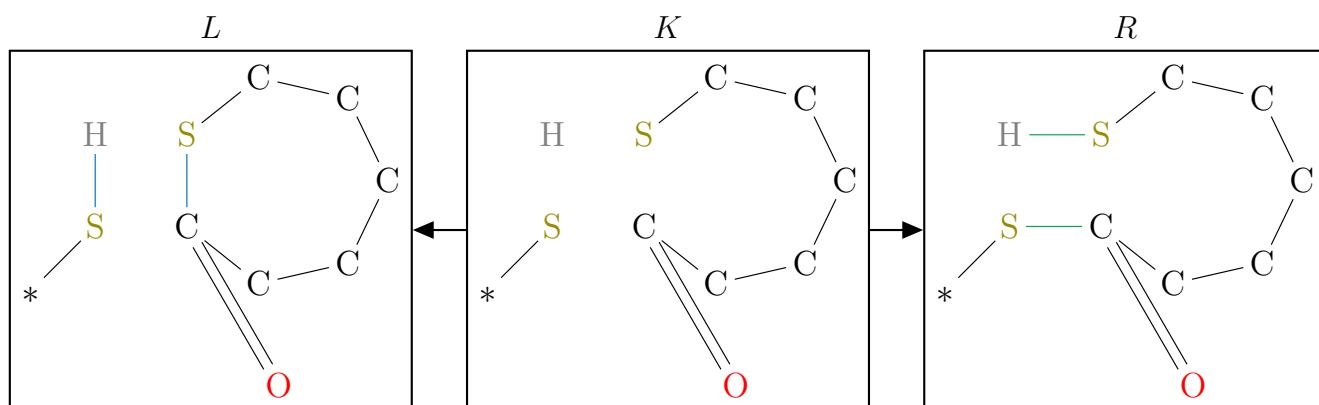
File: out/882_r_179_combined

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

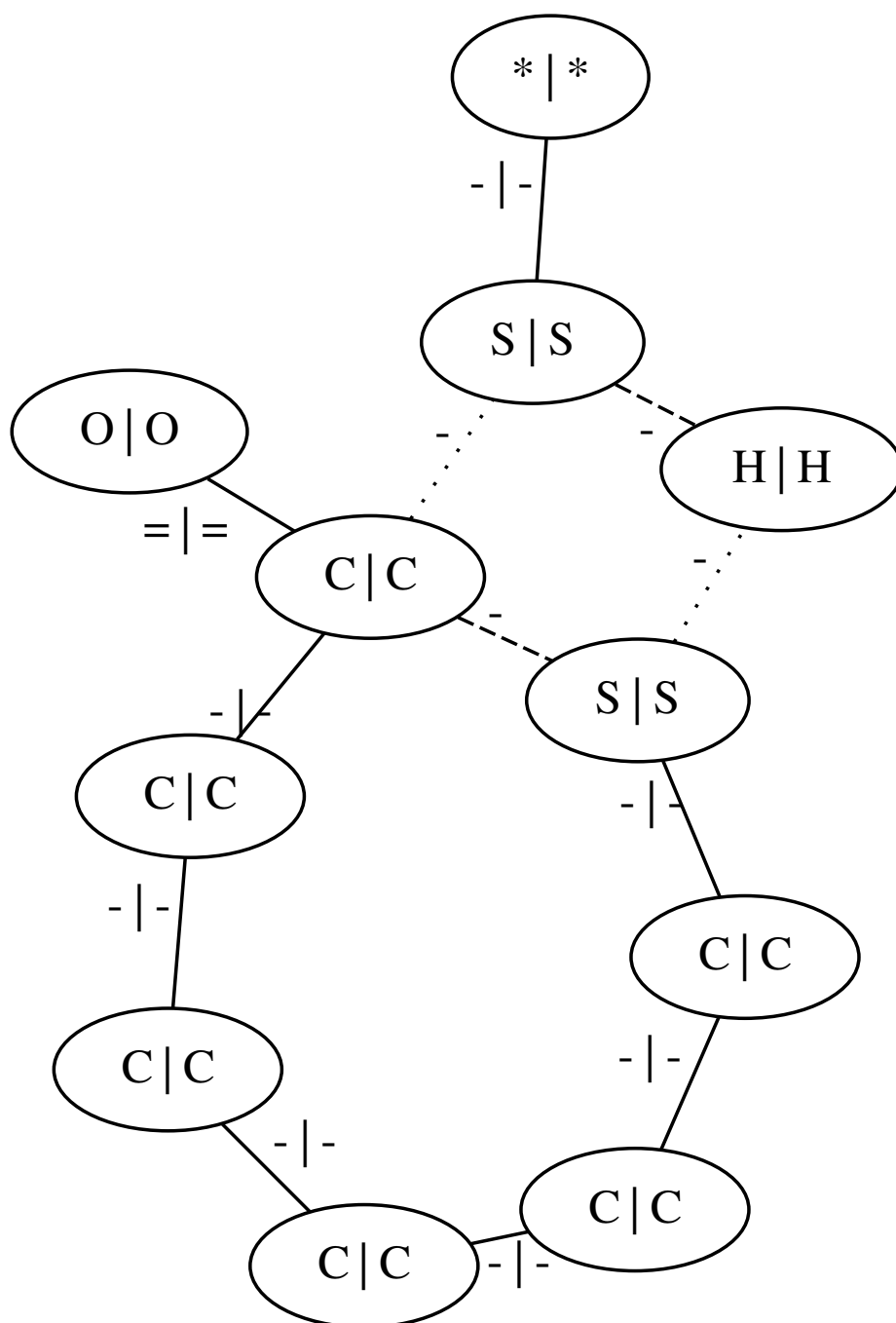
0.0.178 Ring Closure 7 membered, inverse S, S



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



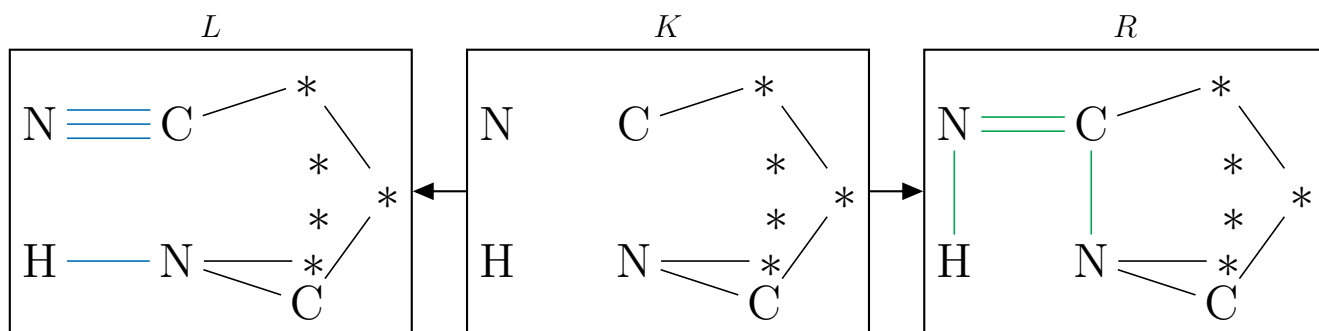
Files: out/886_r_180_11300100_{L, K, R}



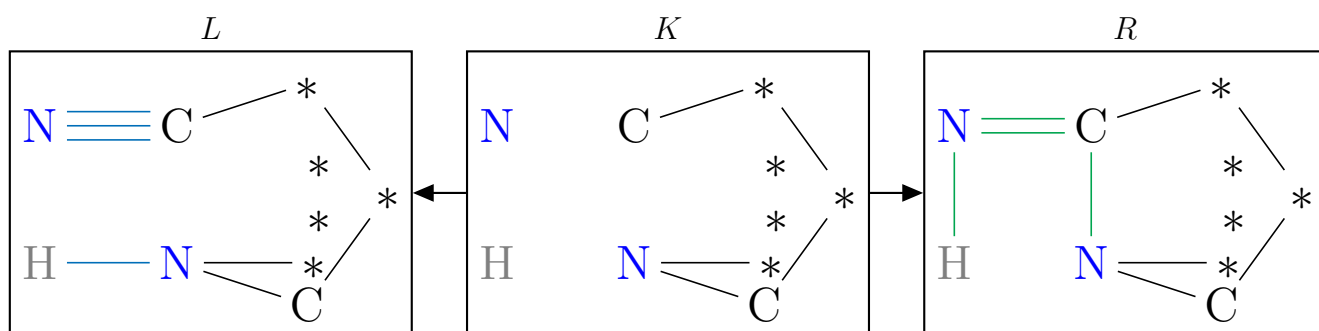
File: out/887_r_180_combined

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

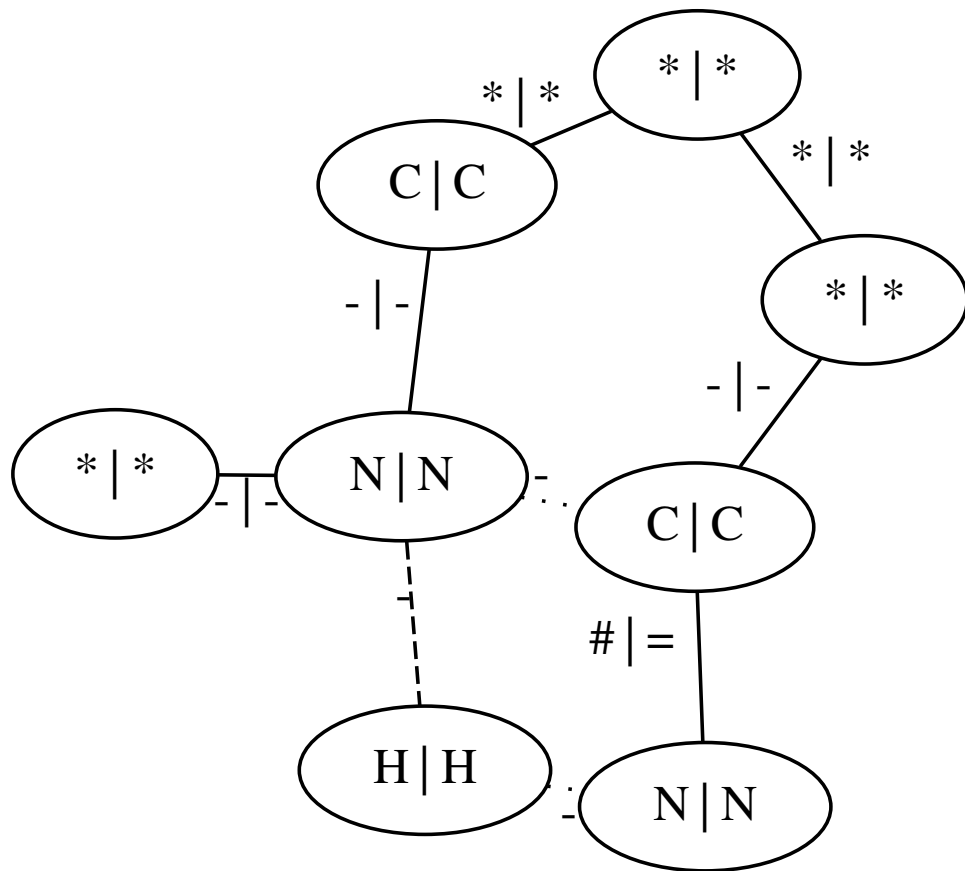
0.0.179 Amine Nitrile Ring Closure 5



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



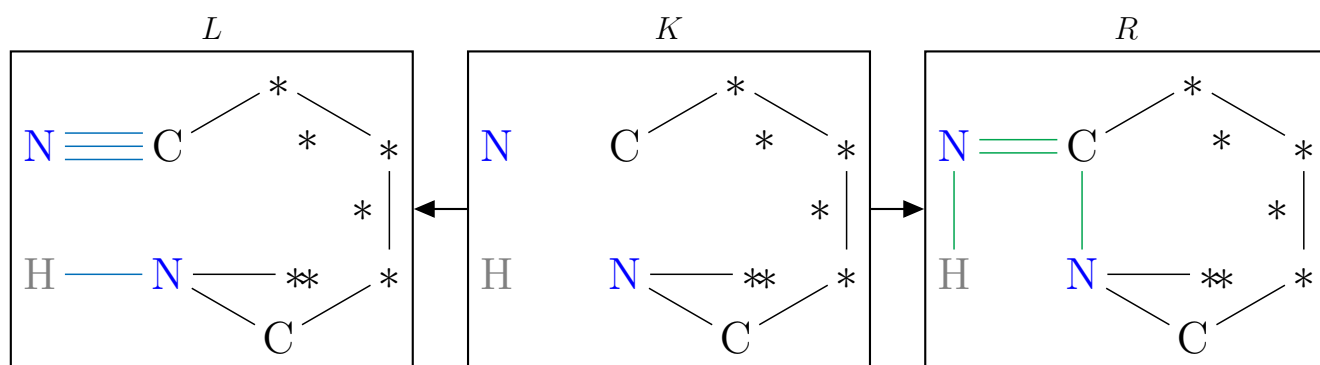
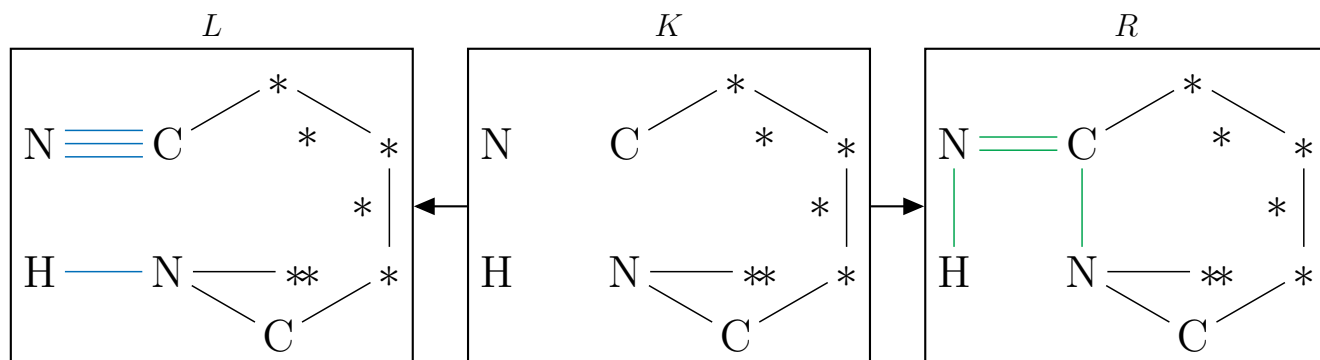
Files: out/891_r_181_11300100_{L, K, R}

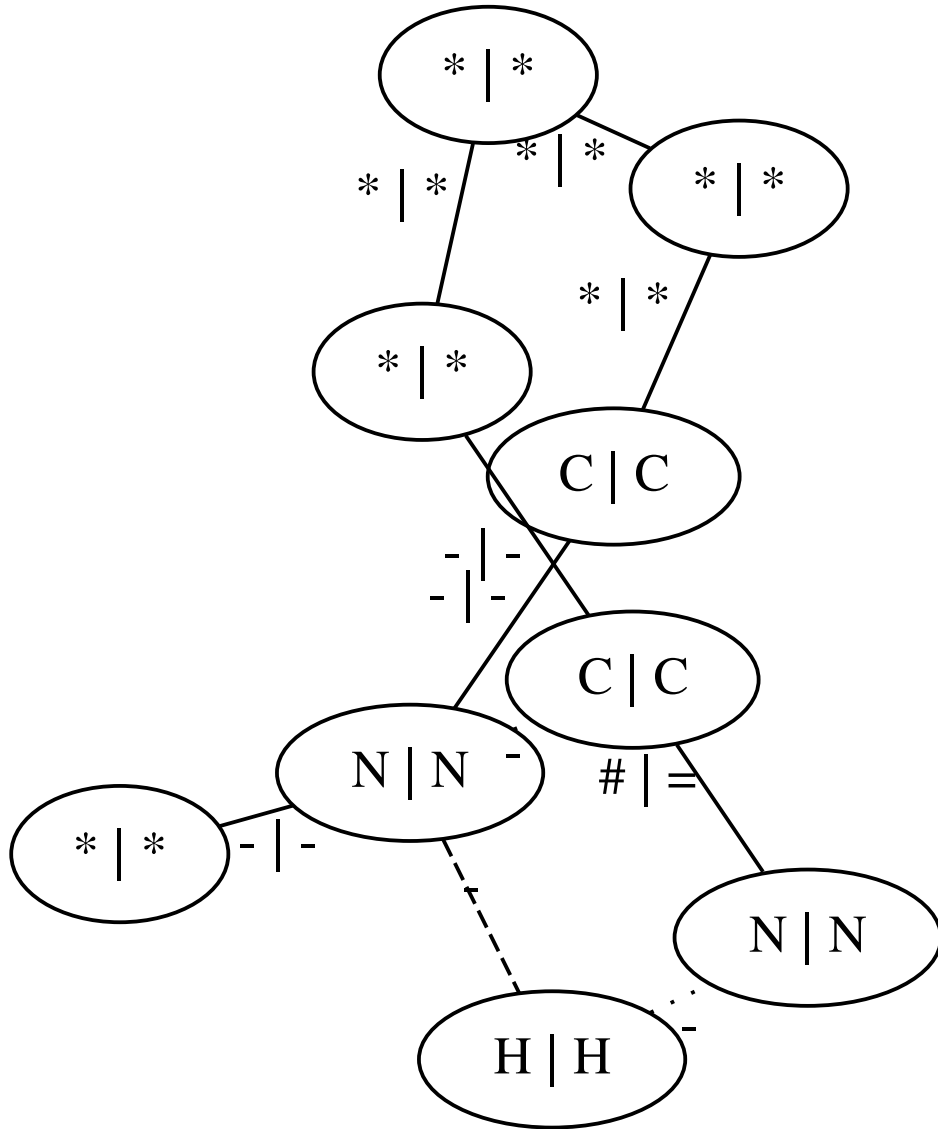


File: out/892_r_181_combined

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

0.0.180 Amine Nitrile Ring Closure 6

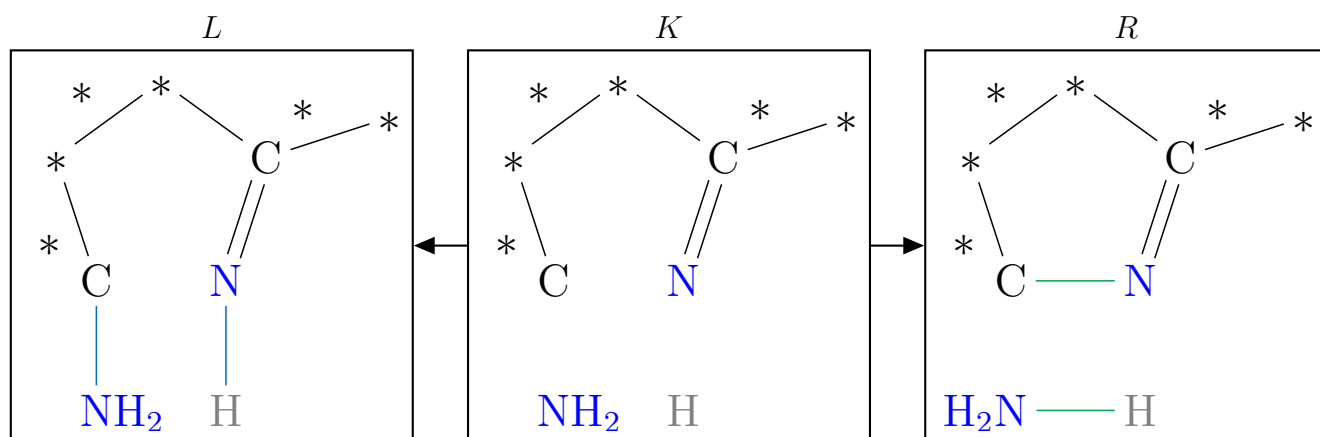
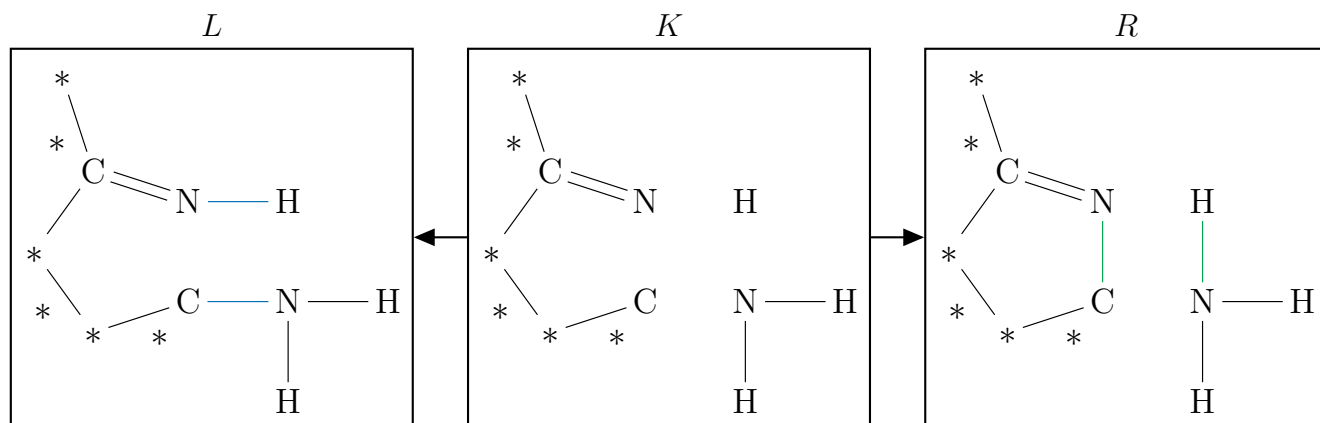


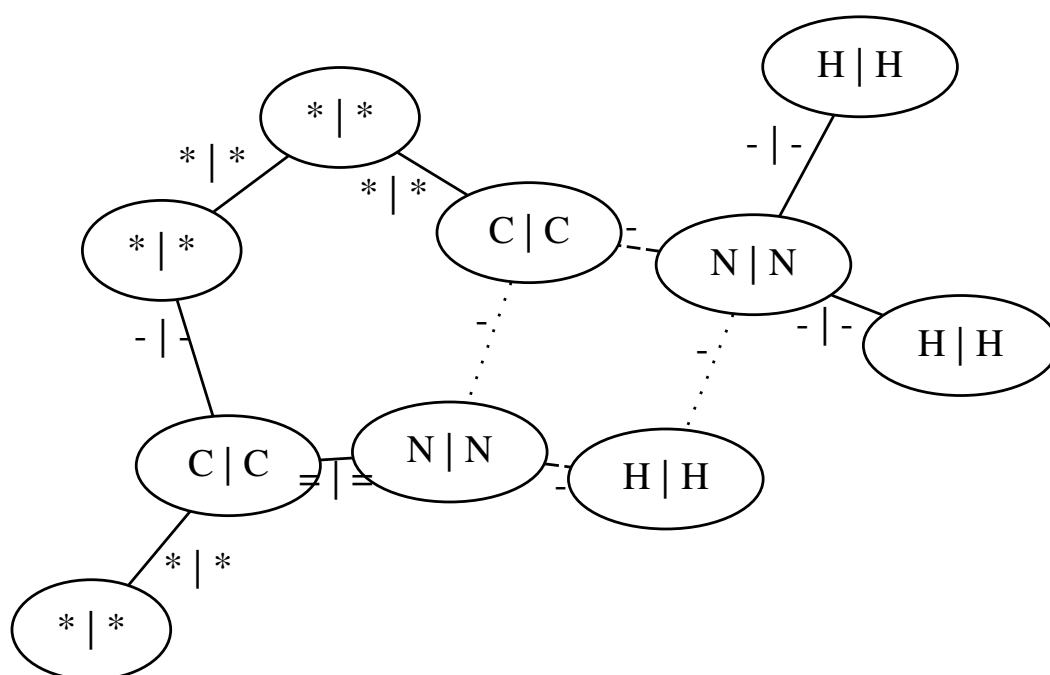


File: out/897_r_182_combined

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

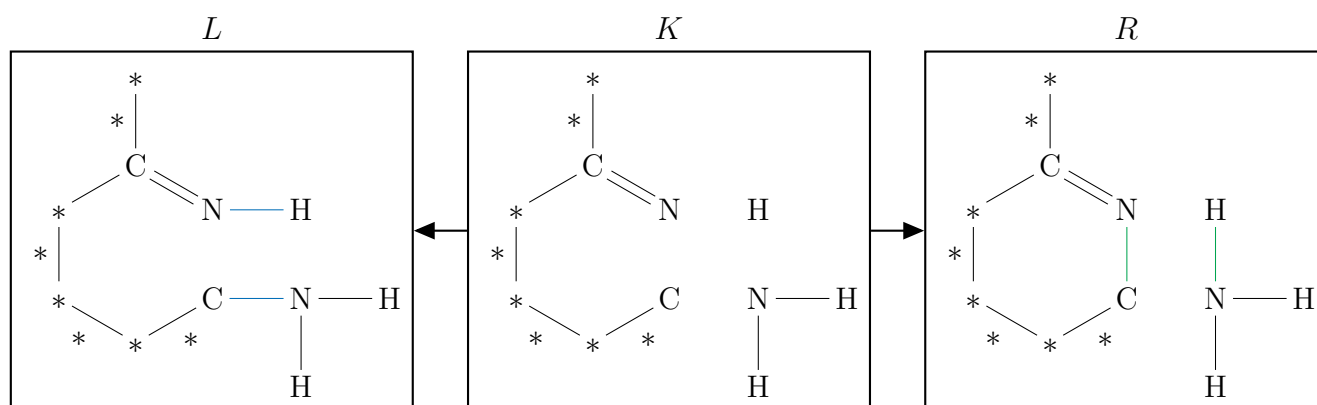
0.0.181 Amine Imine Ring Closure 5



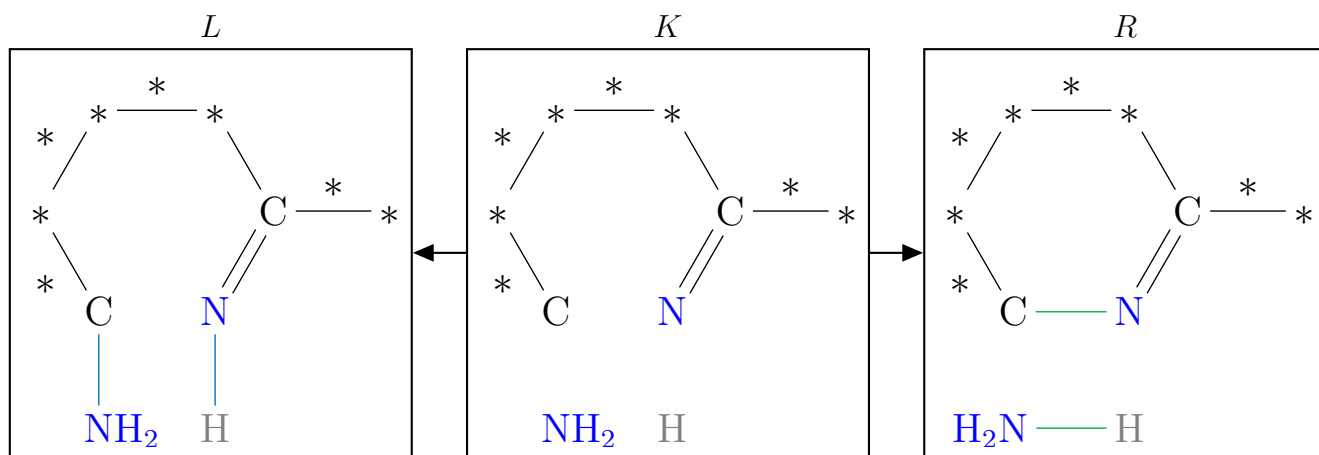


File: out/902_r_183_combined

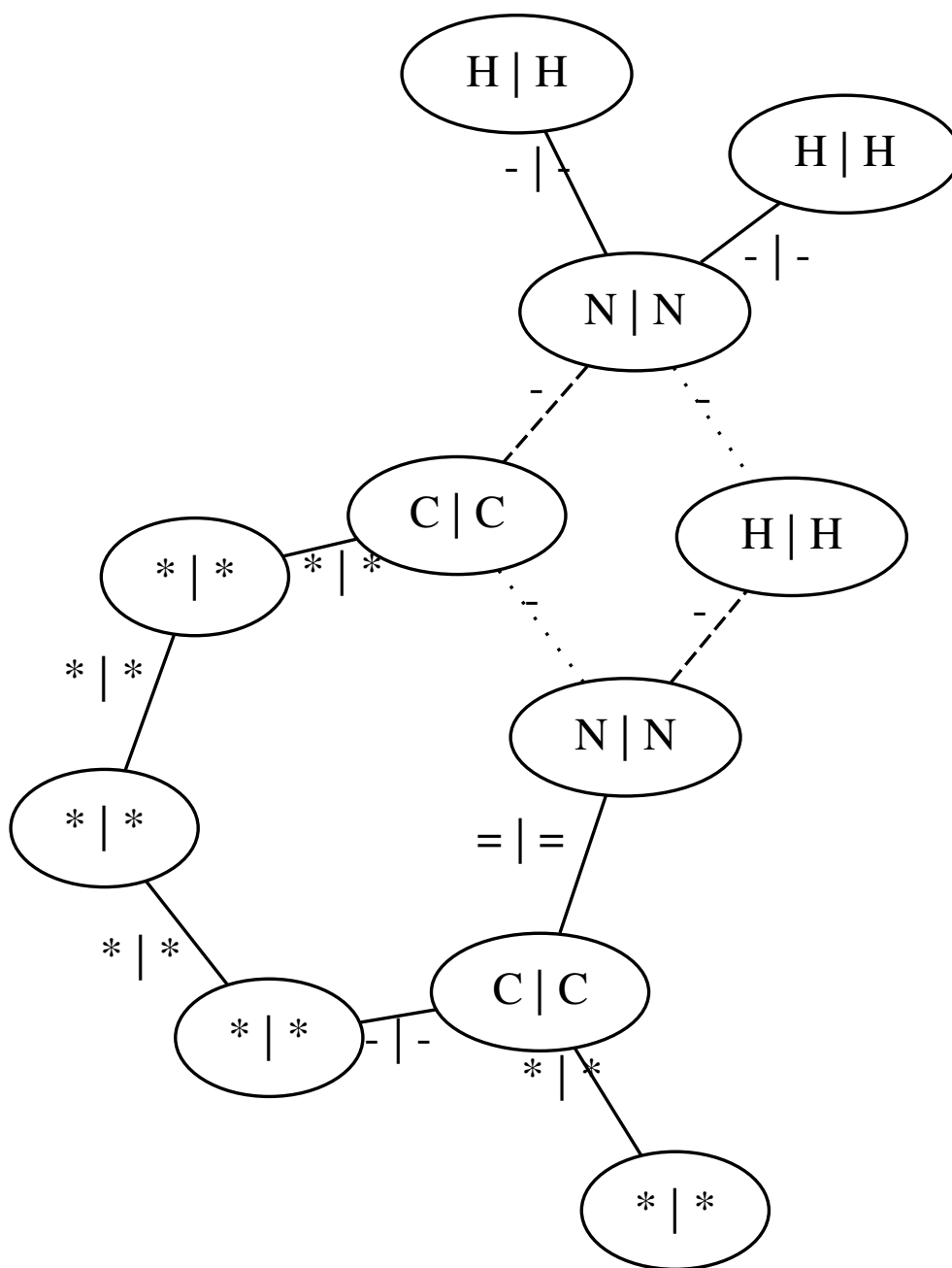
0.0.182 Amine Imine Ring Closure 6



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

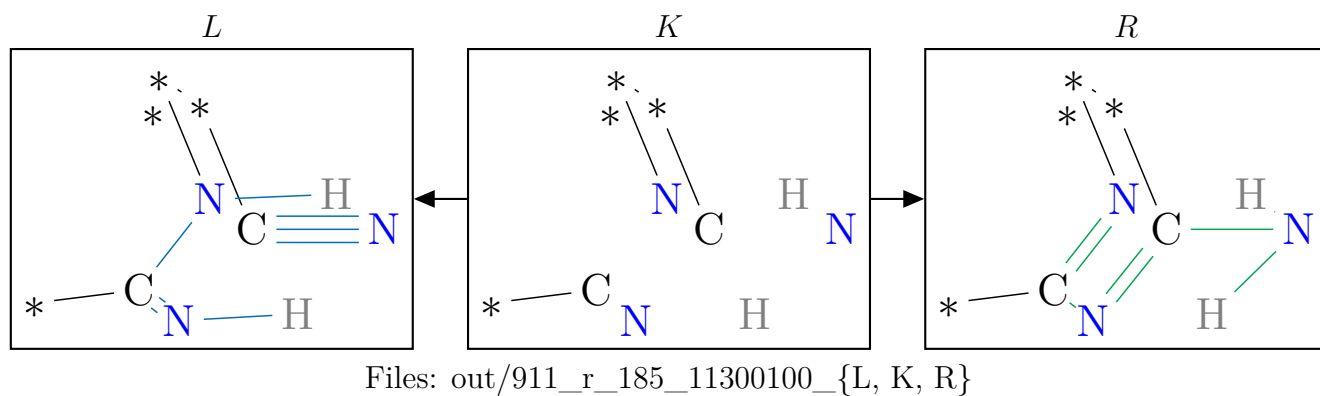
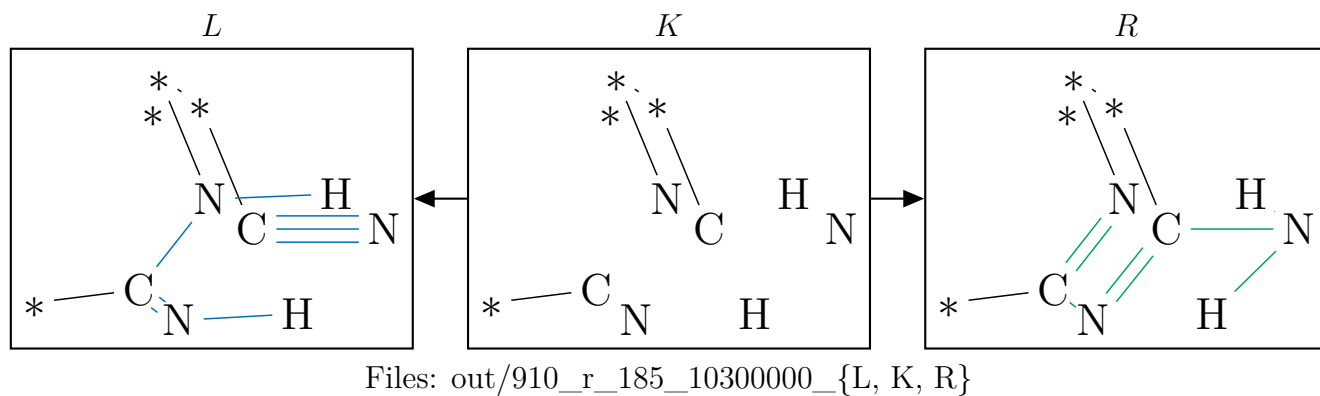


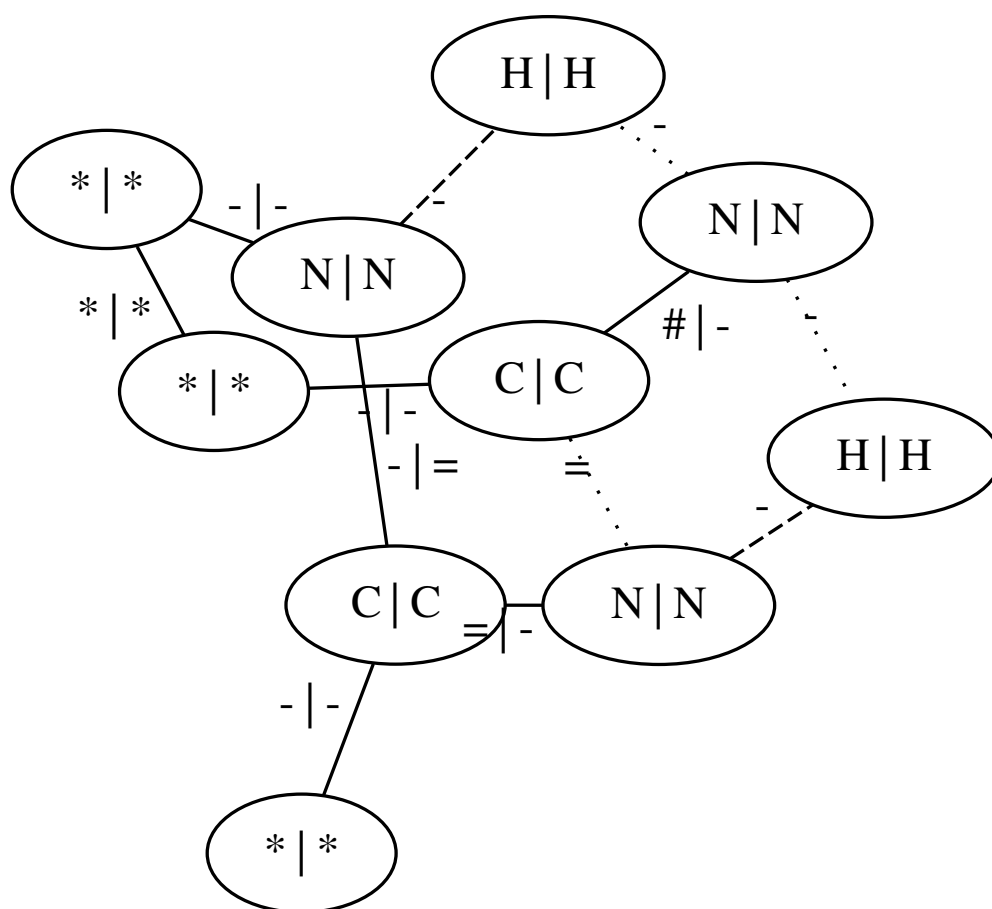
Files: out/906_r_184_11300100_{L, K, R}



File: out/907_r_184_combined

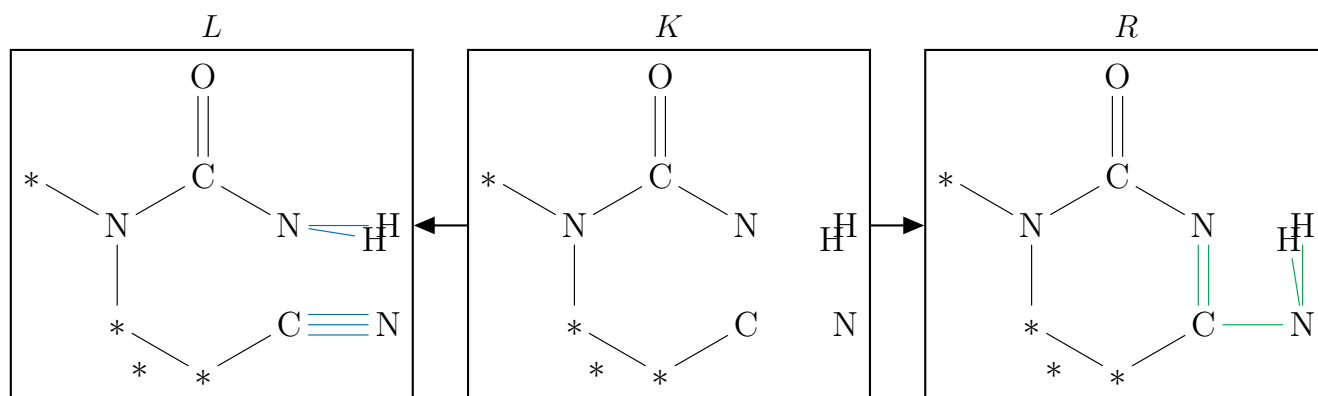
0.0.183 Amidine Nitrile Ring Closure 6



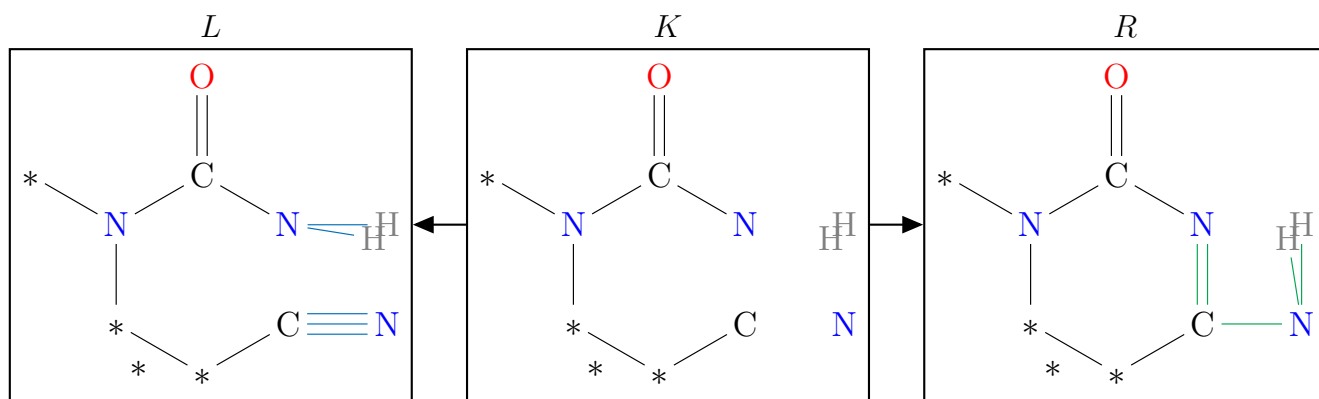


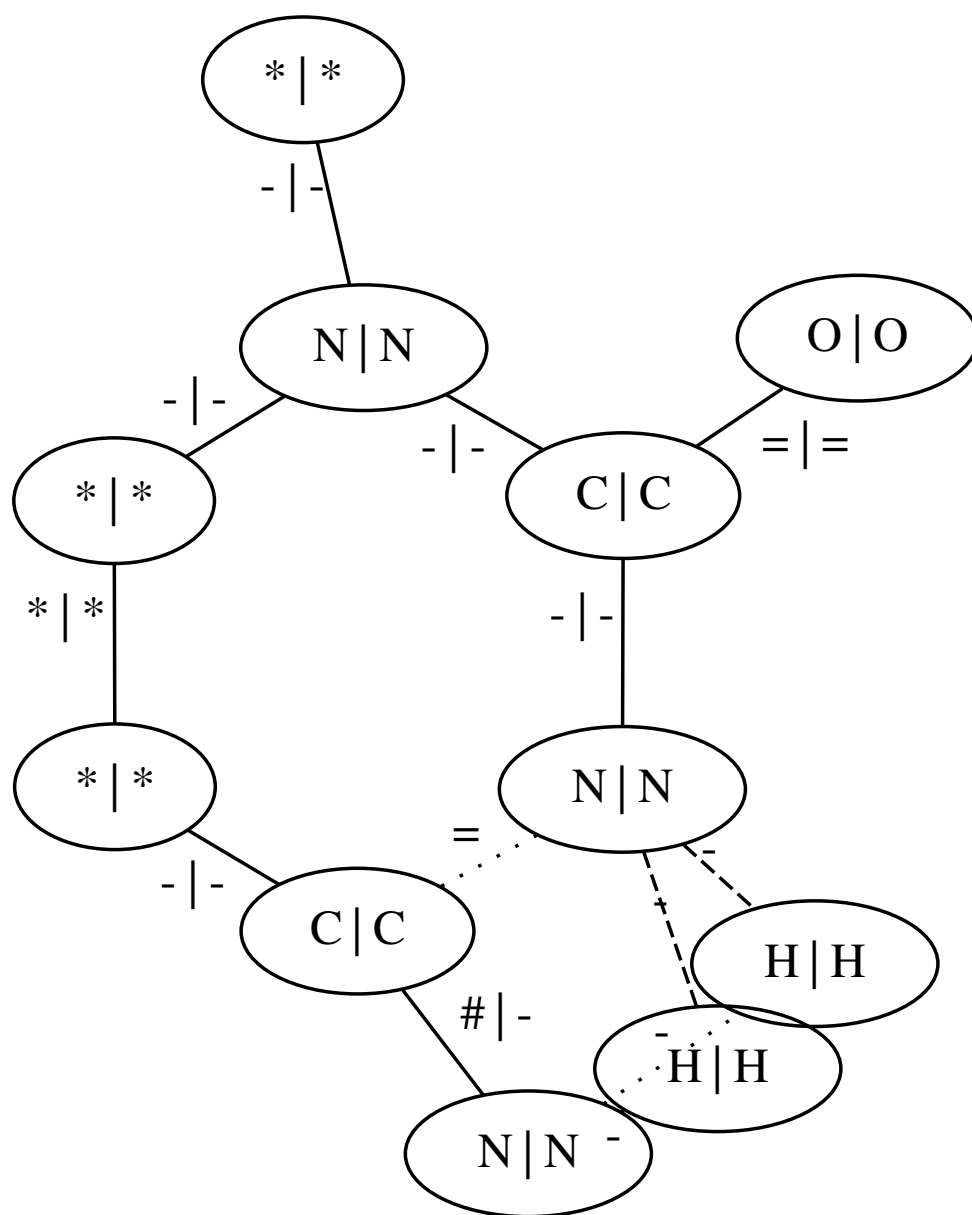
File: out/912_r_185_combined

0.0.184 Amide Nitrile Ring Closure 6



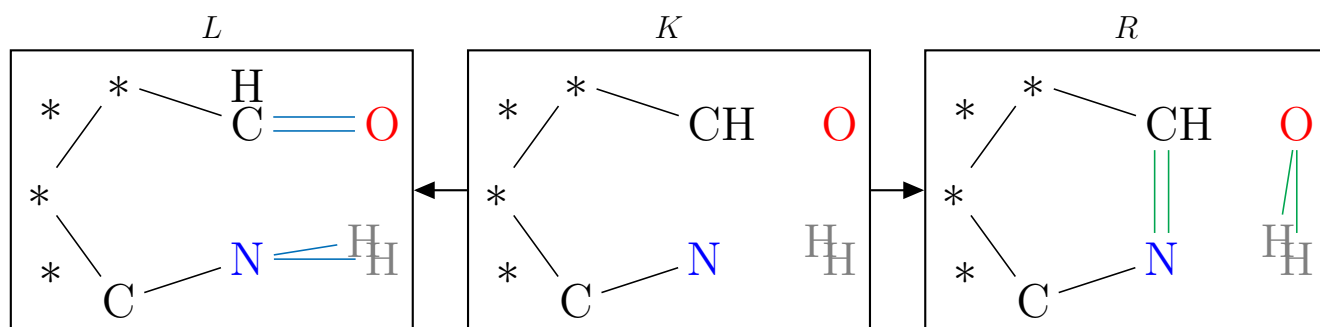
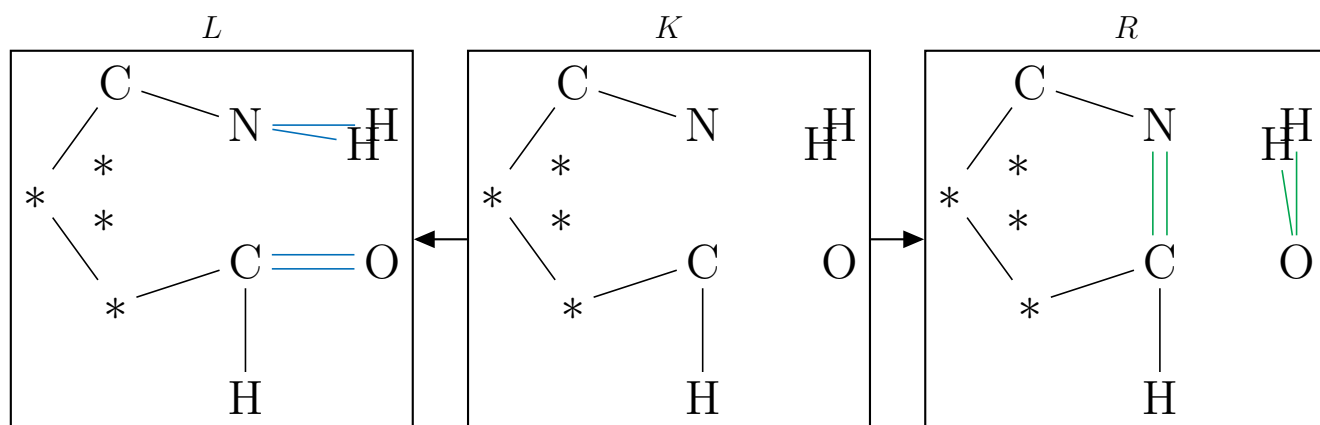
Files: out/915_r_186_10300000_{L, K, R}

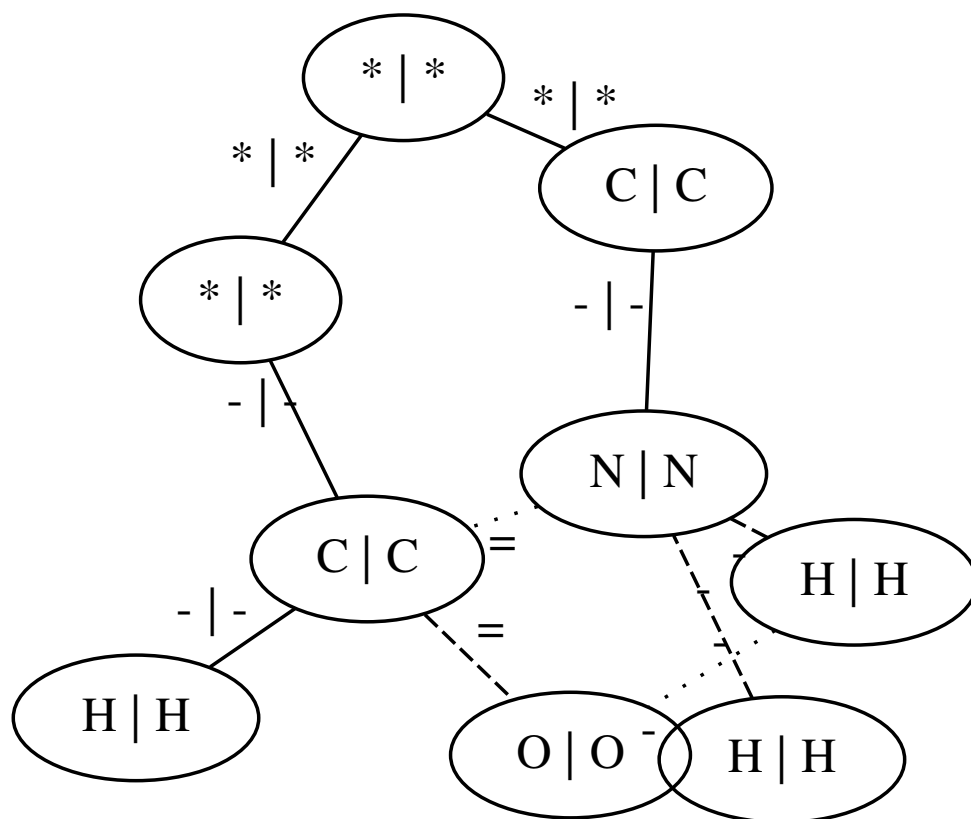




File: out/917_r_186_combined

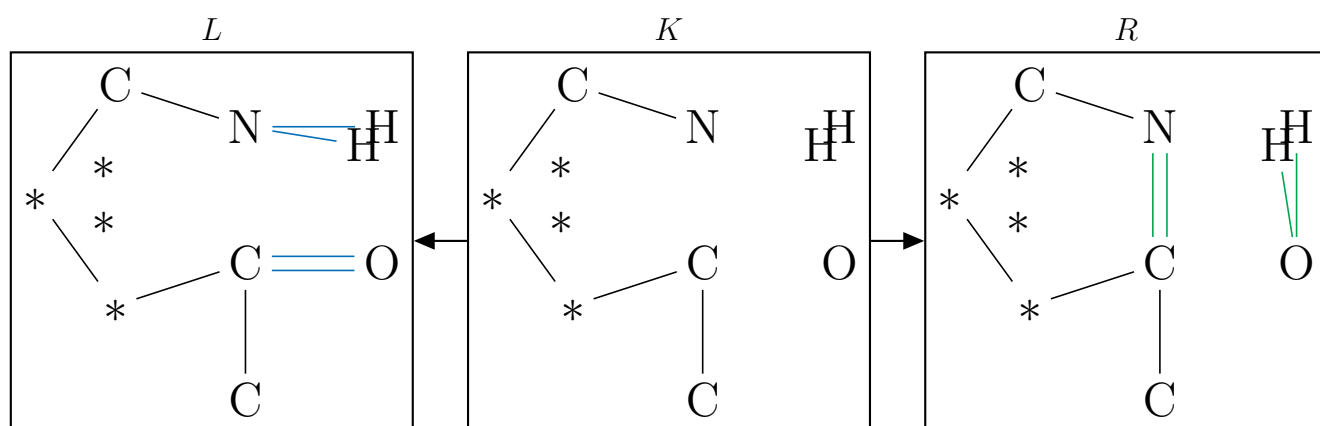
0.0.185 Amine Carbonyl Ring Closure, H, 5



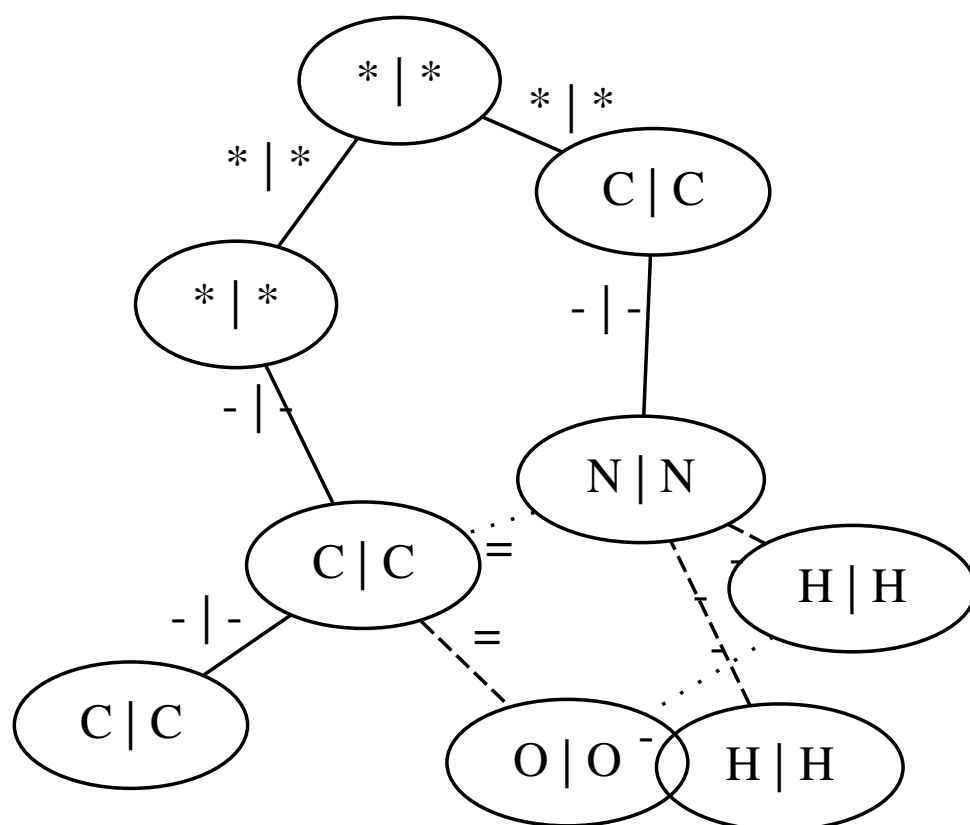
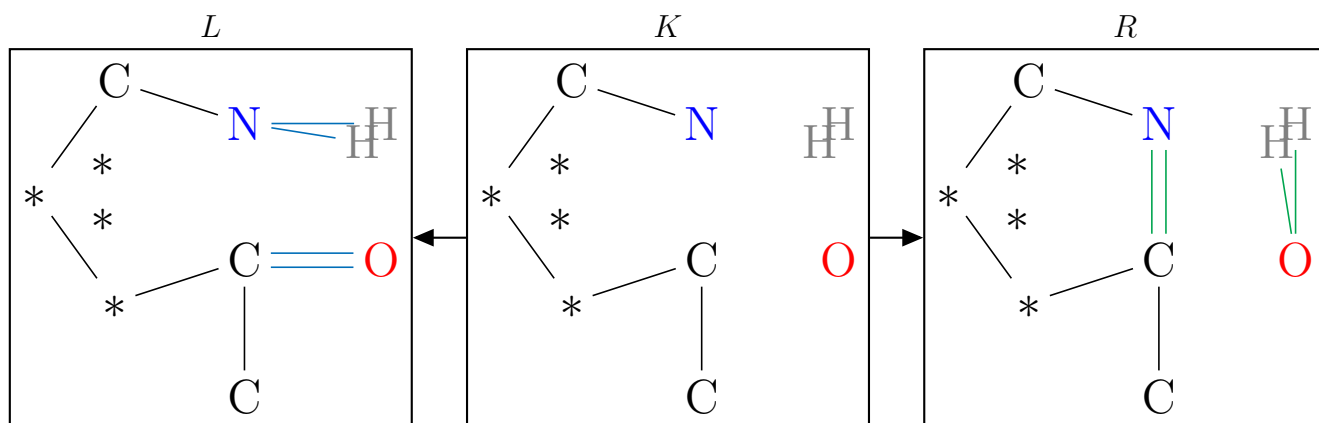


File: out/922_r_187_combined

0.0.186 Amine Carbonyl Ring Closure, C, 5

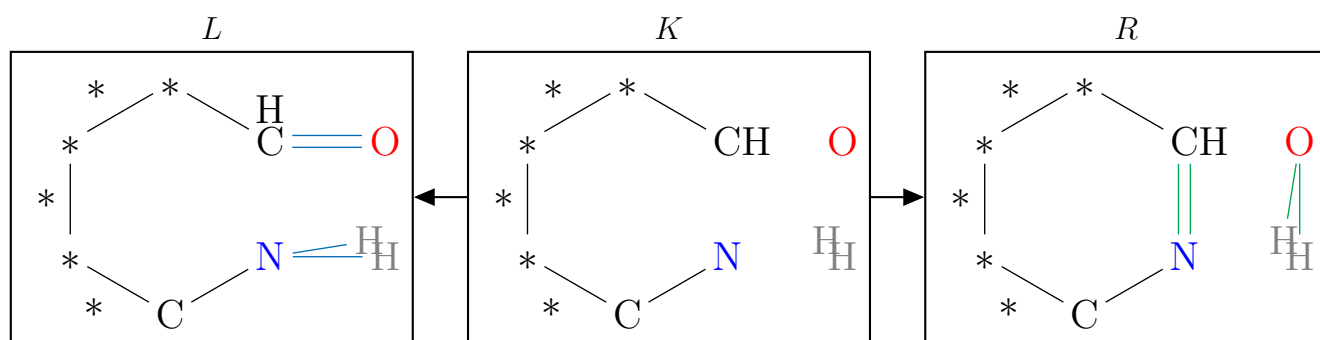
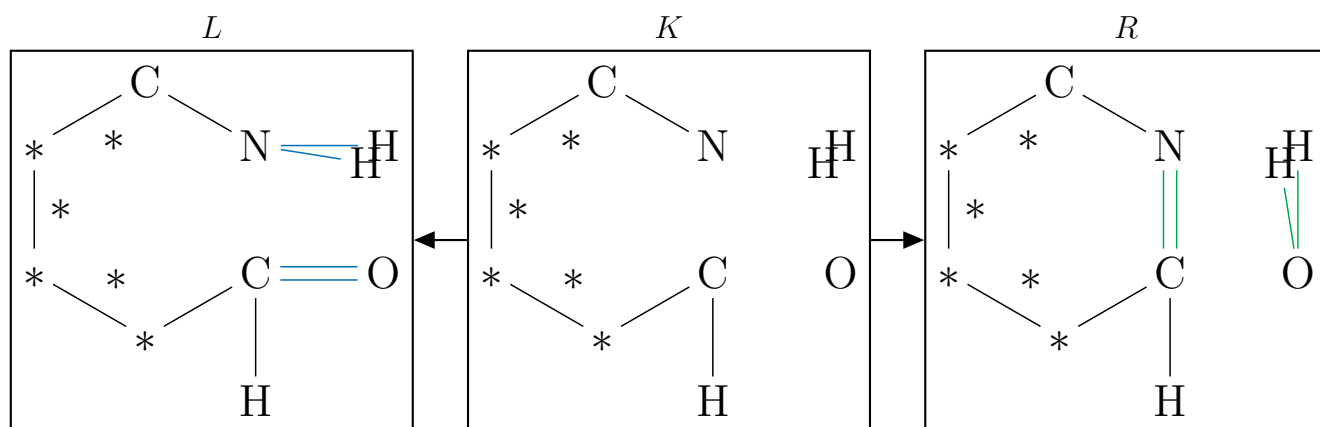


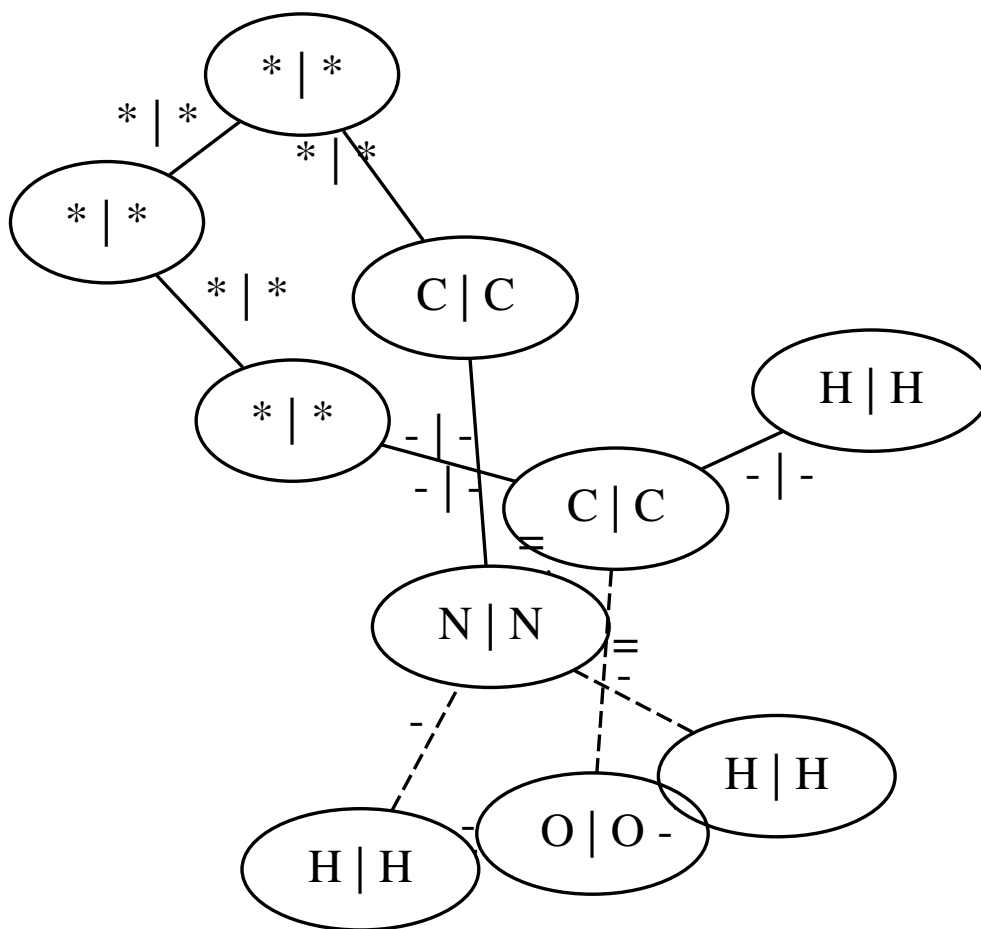
Files: out/925_r_188_10300000_{L, K, R}



File: out/927_r_188_combined

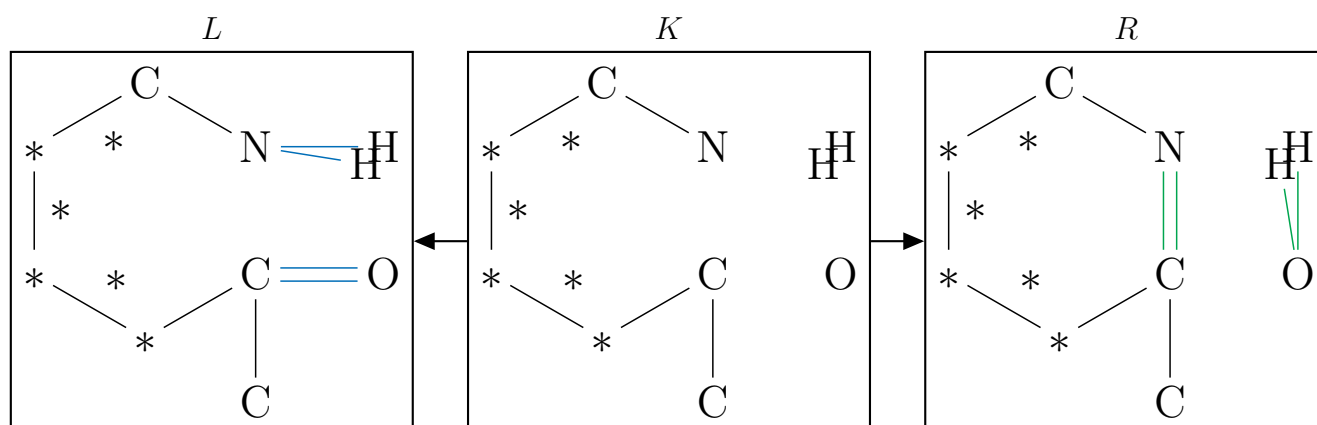
0.0.187 Amine Carbonyl Ring Closure, H, 6



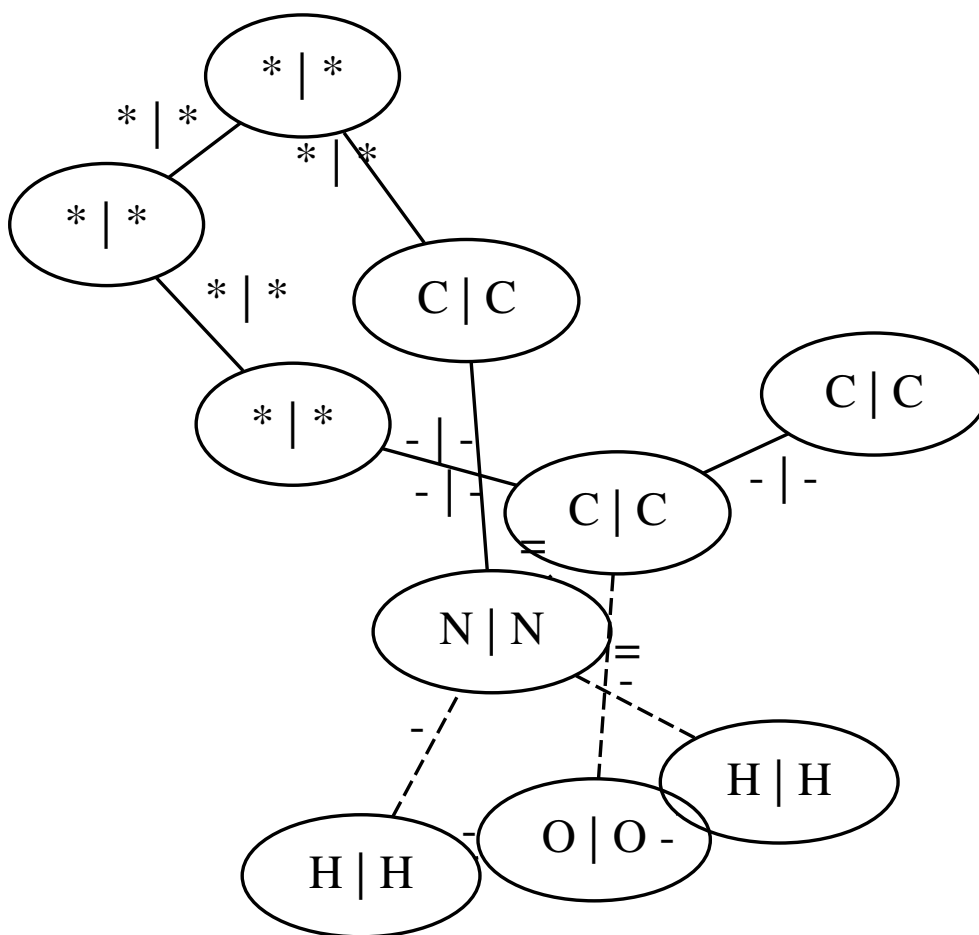
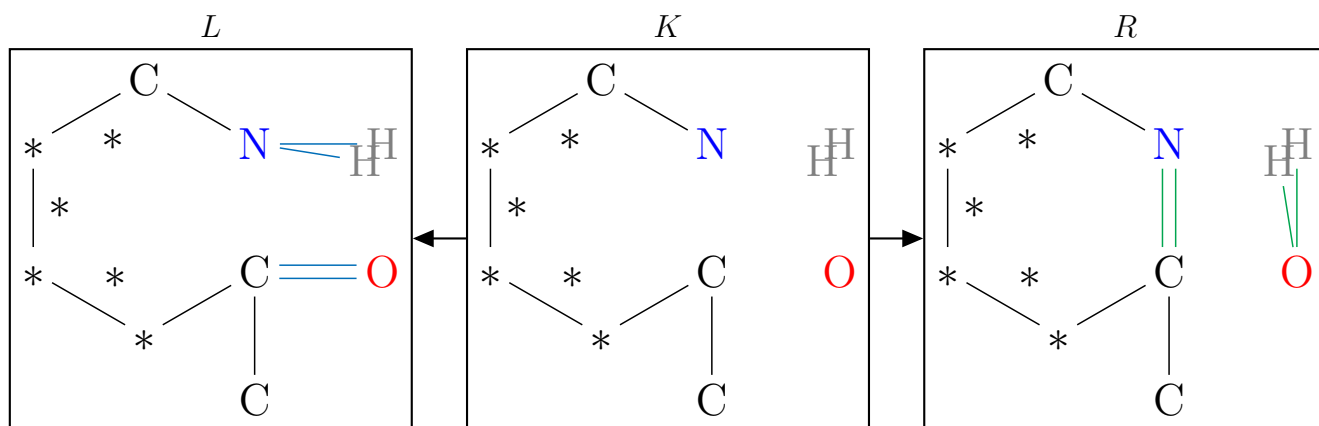


File: out/932_r_189_combined

0.0.188 Amine Carbonyl Ring Closure, C, 6

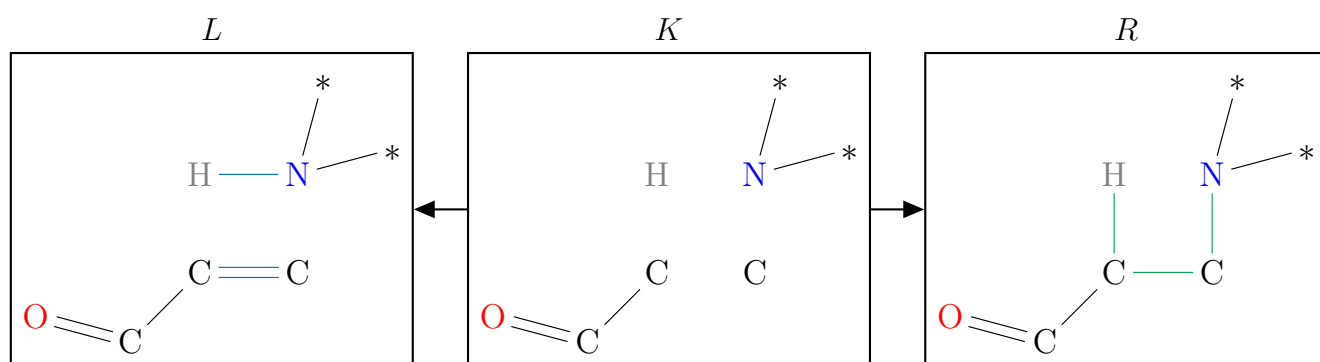
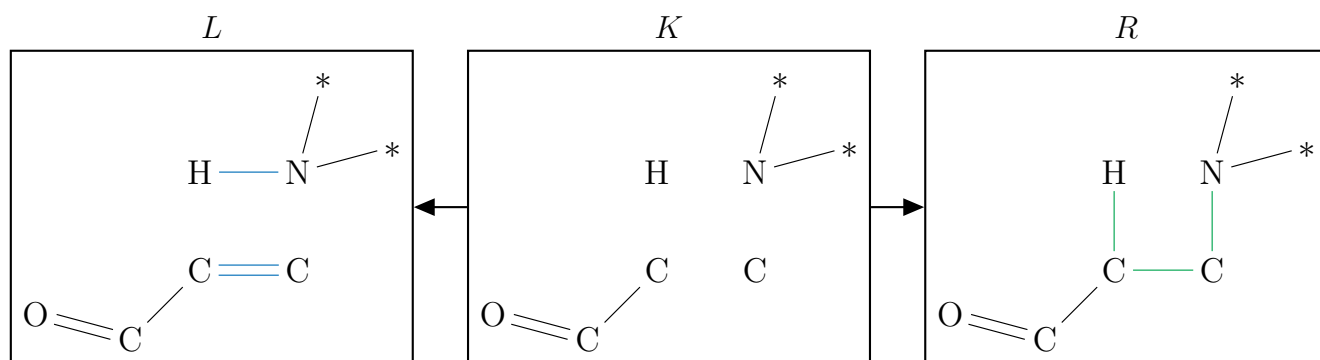


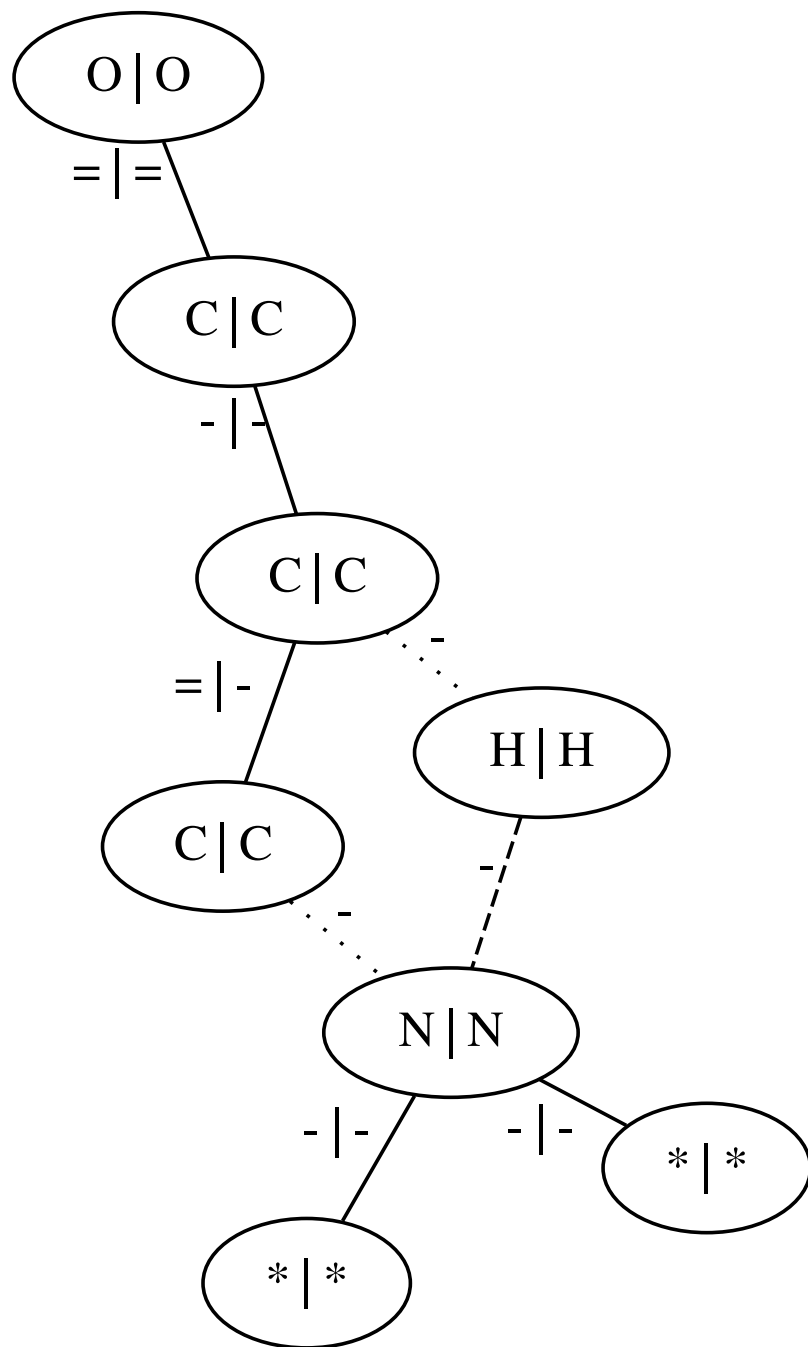
Files: out/935_r_190_10300000_{L, K, R}



File: out/937_r_190_combined

0.0.189 Michael Addition 0,0,





File: out/942_r_191_combined

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

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

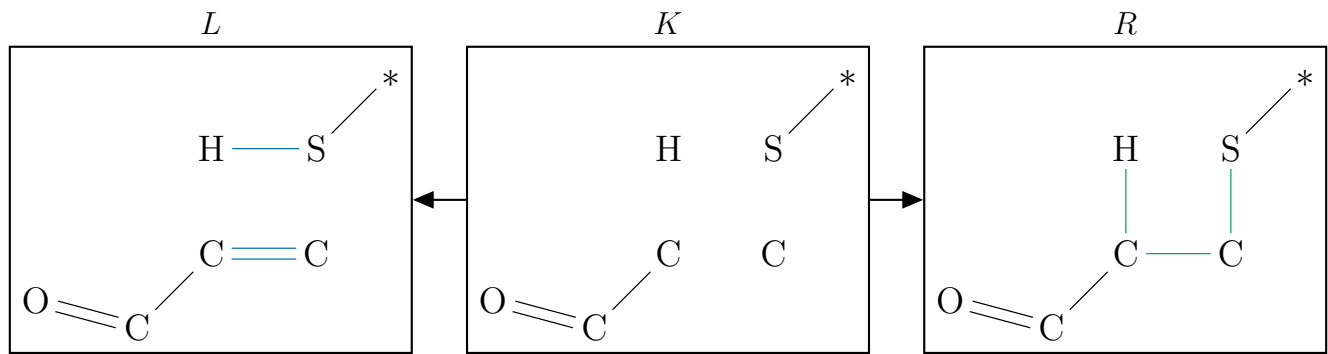
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\mid = 0
\end{aligned}$$

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

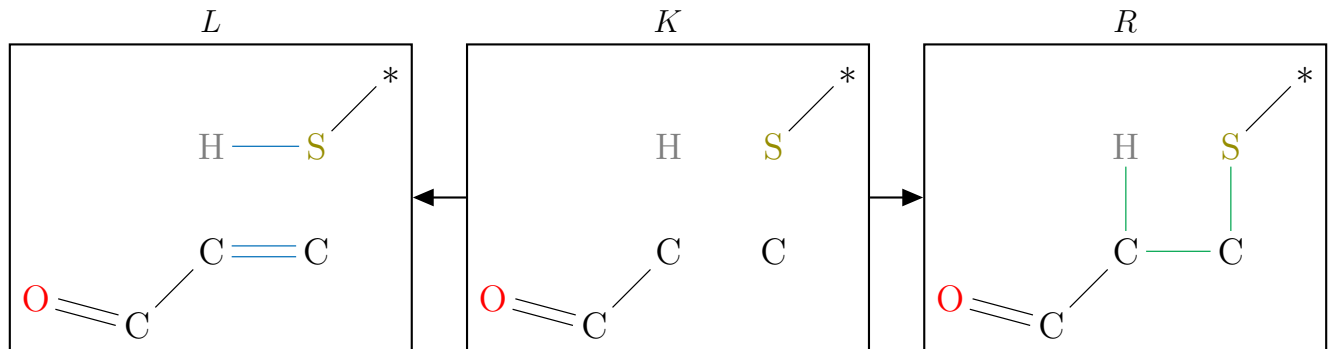
$$\begin{aligned}
& |\{e \in \text{outEdges}(7) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \}\mid = 0
\end{aligned}$$

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

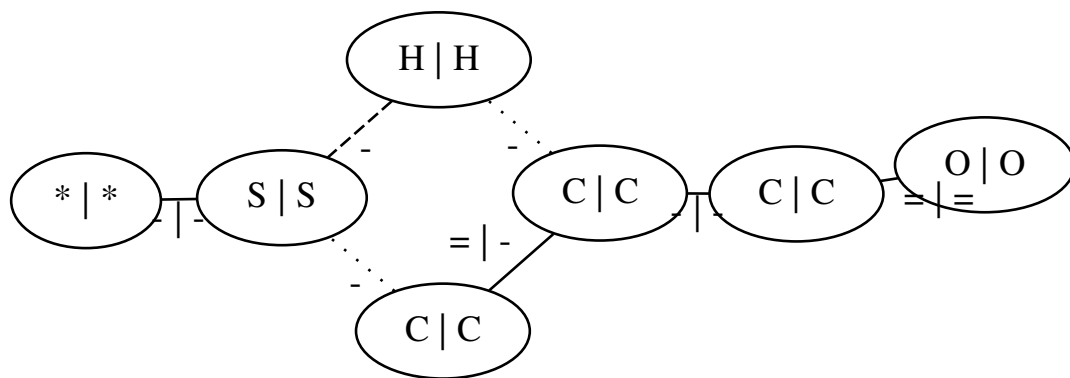
0.0.190 Michael Addition 0,1,



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



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



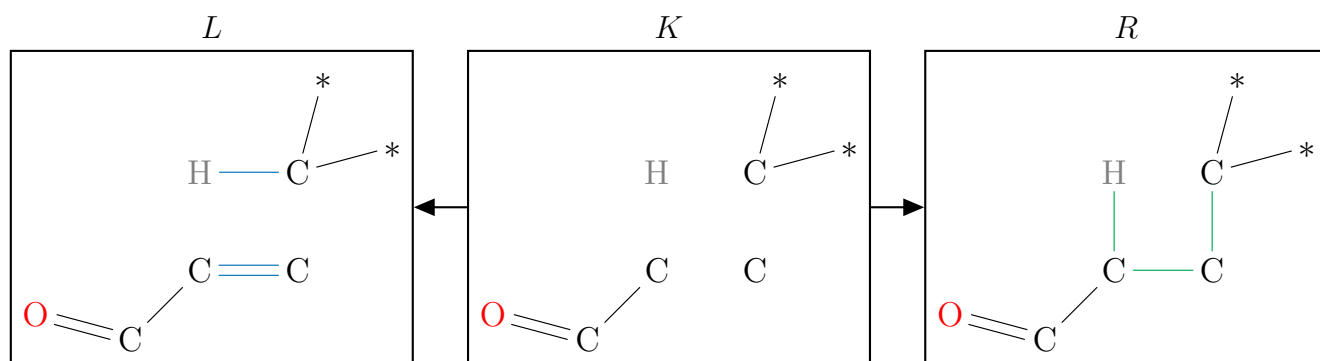
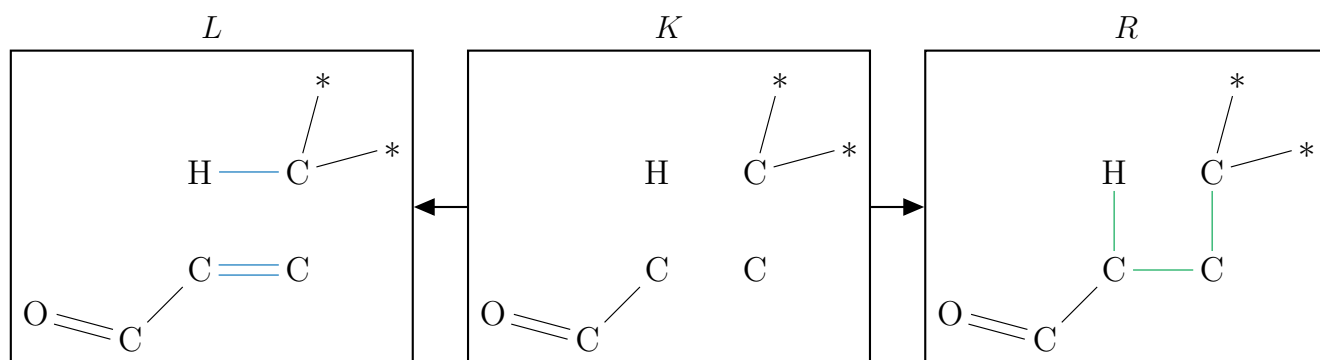
File: out/947_r_192_combined

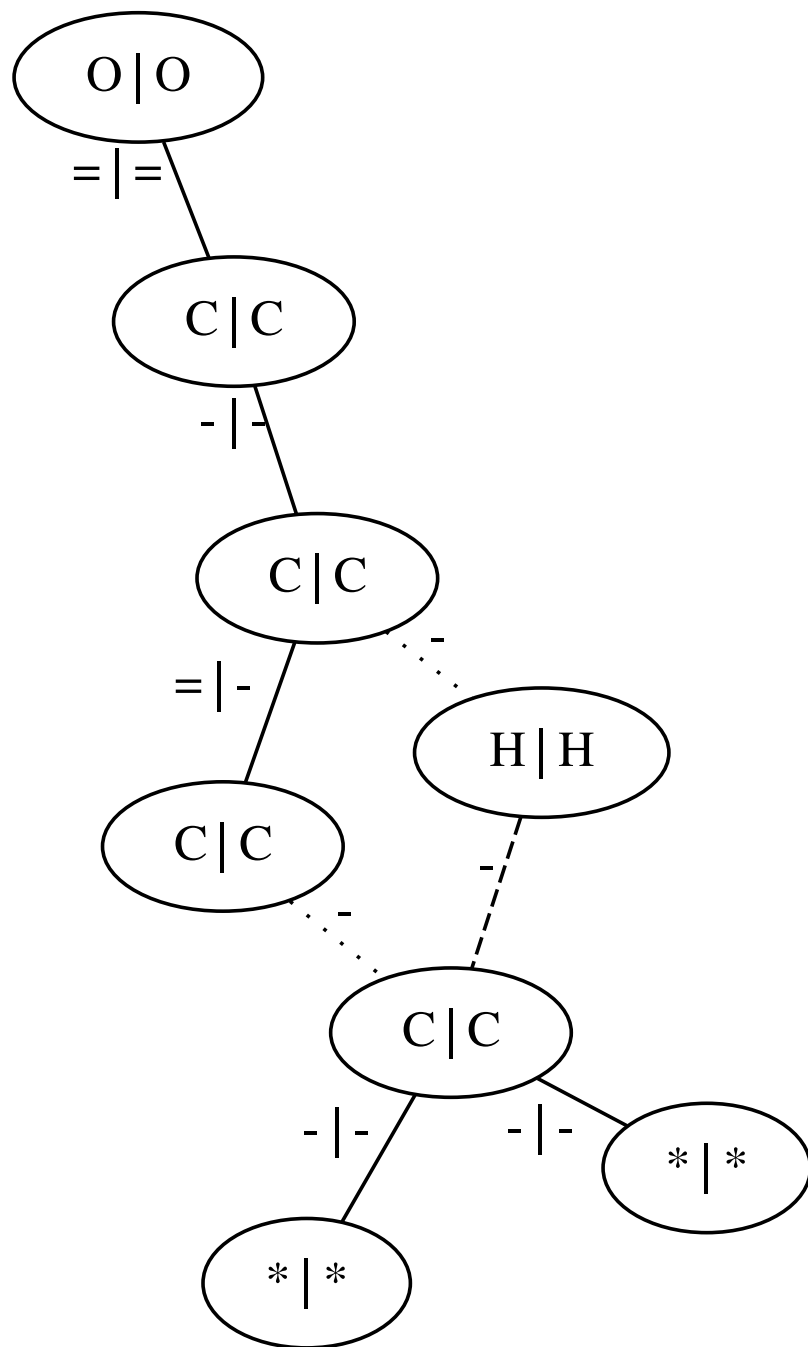
$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{\text{'0'}\} \wedge \text{label}(e) \in \{\text{'-'}\}\}| = 0$$

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

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

0.0.191 Michael Addition 0,2,





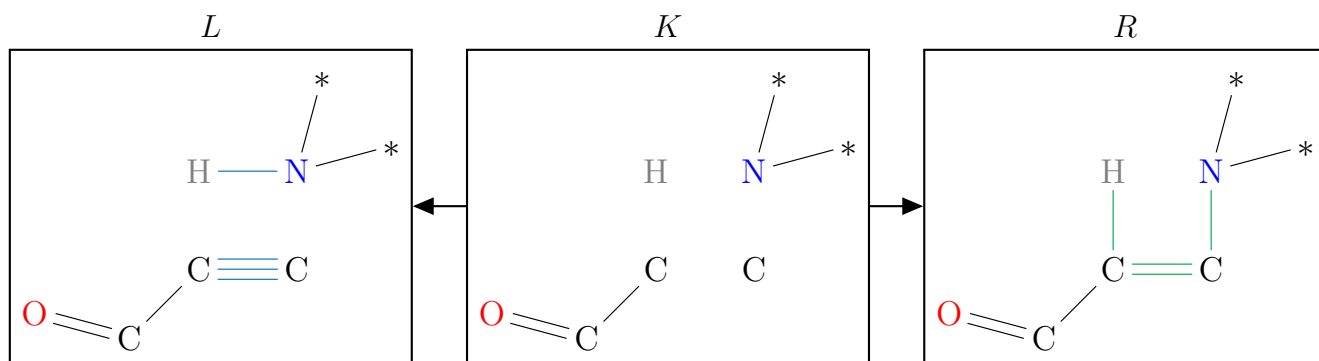
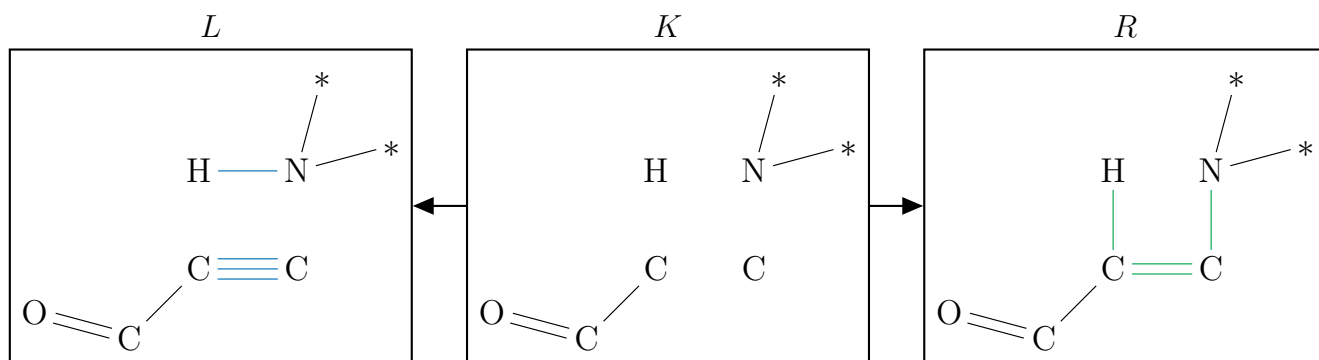
File: out/952_r_193_combined

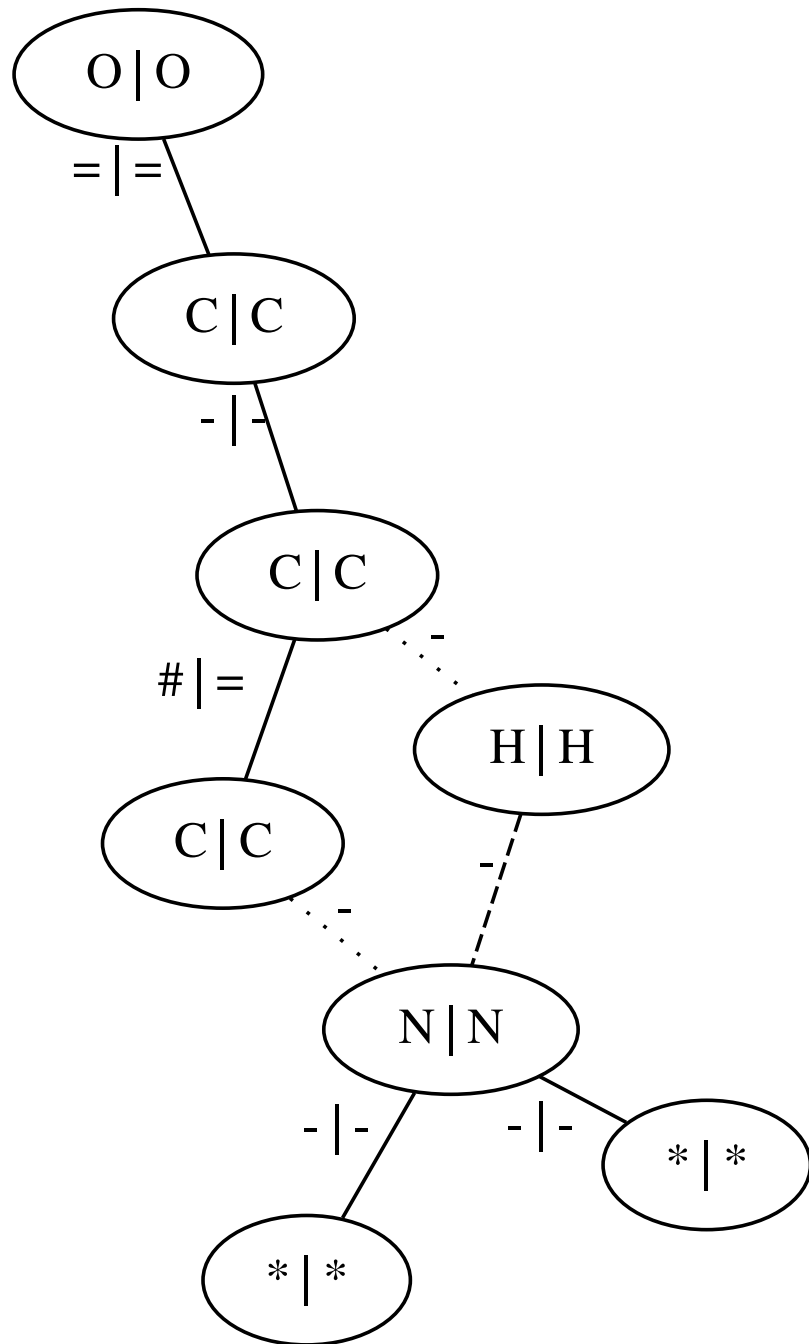
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \mid\} = 0
\end{aligned}$$

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

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

0.0.192 Michael Addition 1,0,





File: out/957_r_194_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(7) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

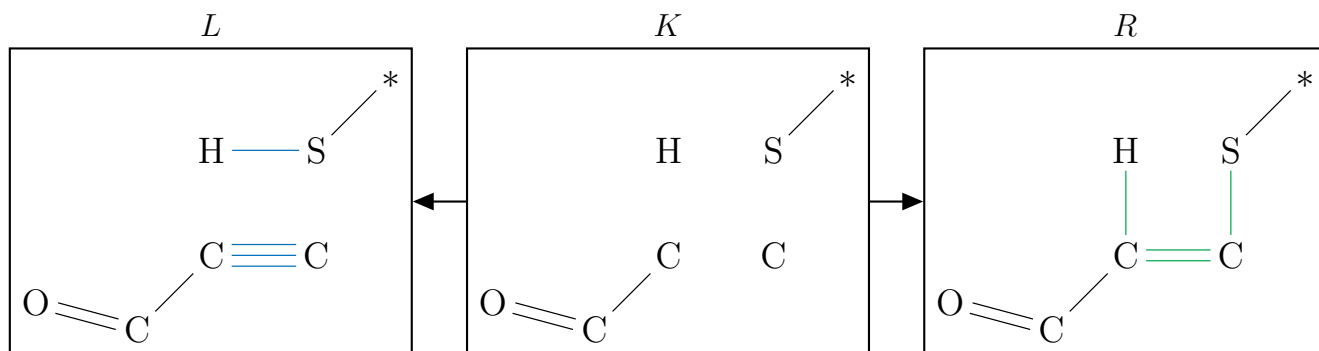
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

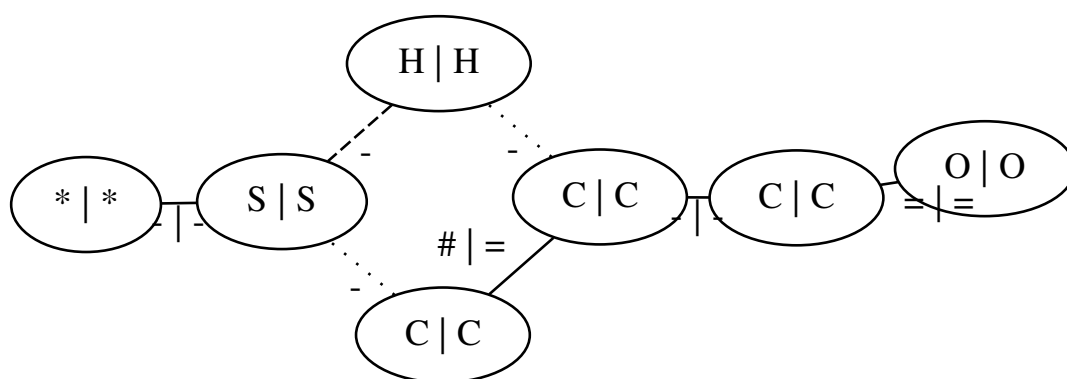
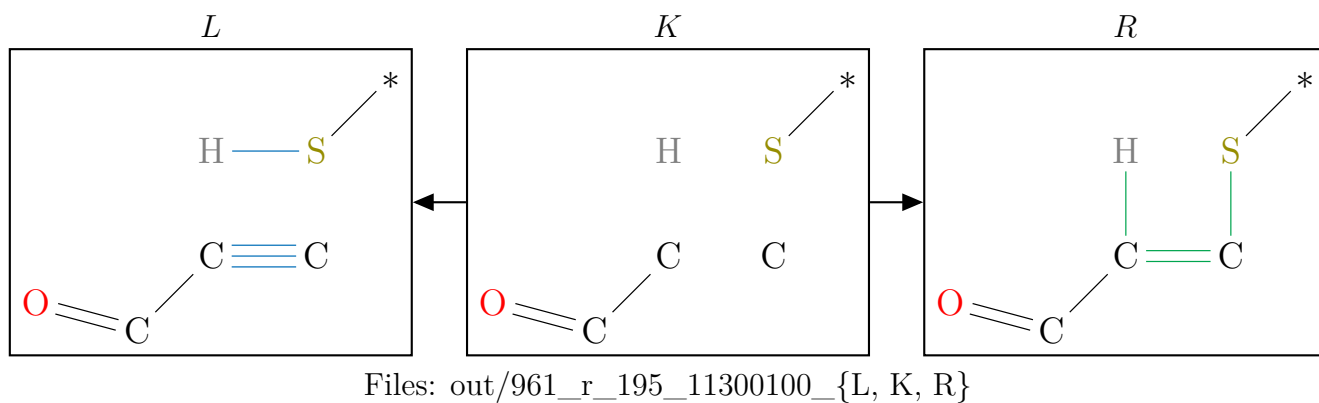
$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

0.0.193 Michael Addition 1,1,

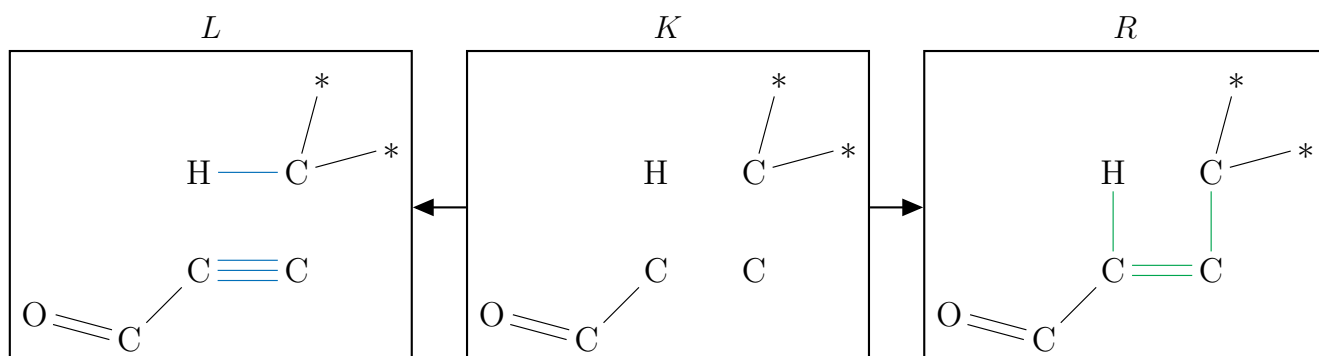




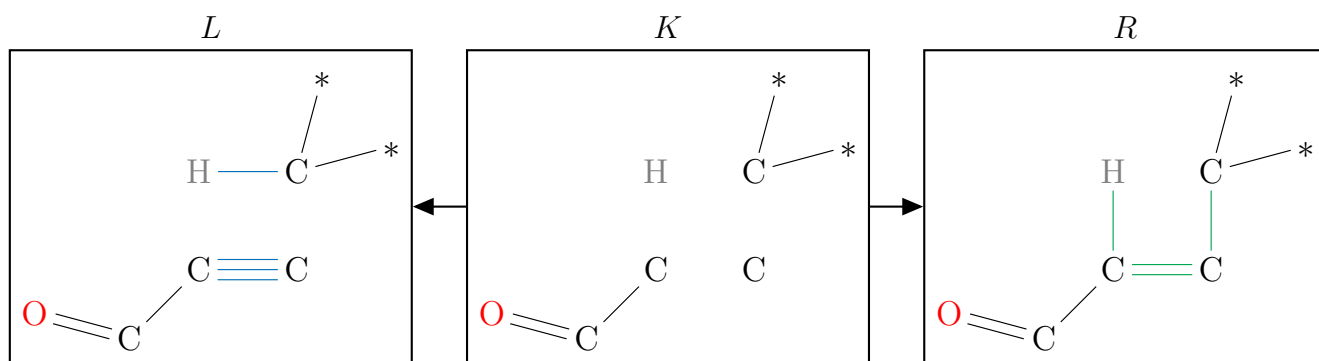
File: out/962_r_195_combined

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

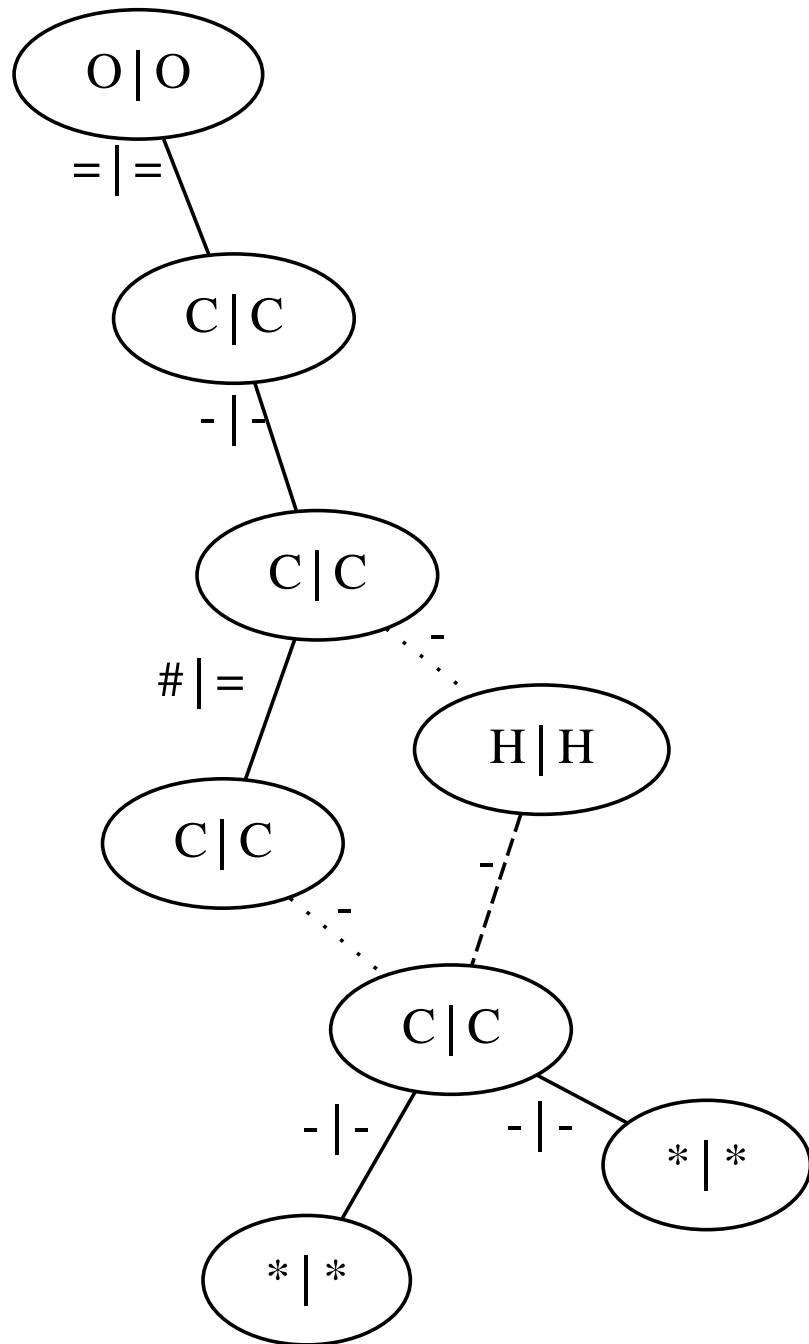
0.0.194 Michael Addition 1,2,



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



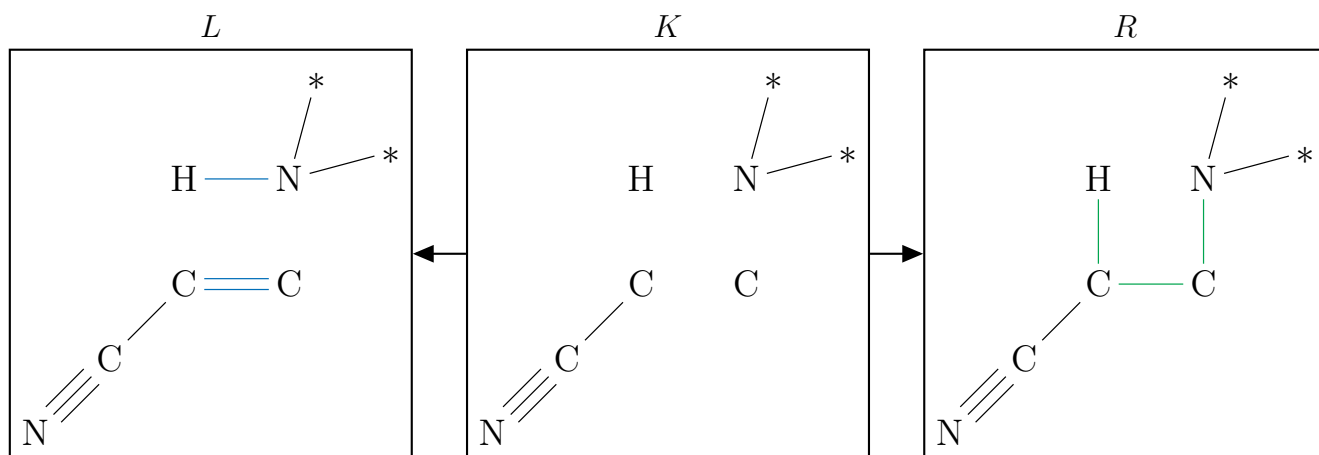
Files: out/966_r_196_11300100_{L, K, R}



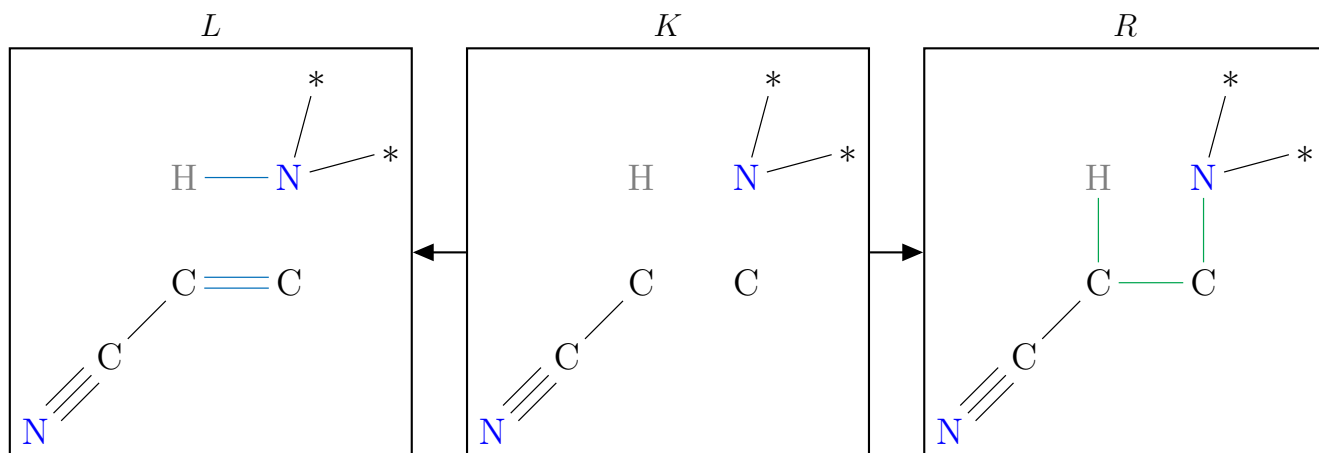
File: out/967_r_196_combined

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

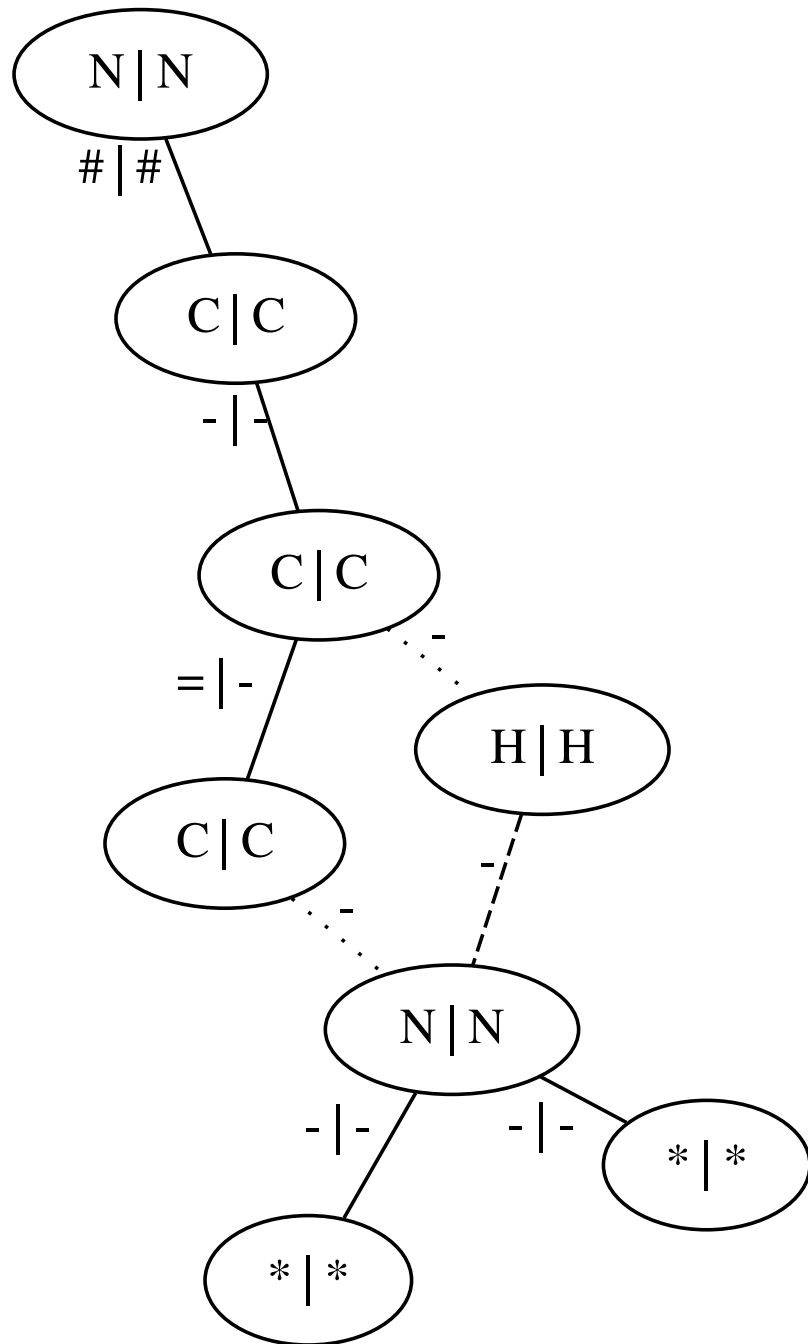
0.0.195 Michael Addition 2,0,



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



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



File: out/972_r_197_combined

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

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

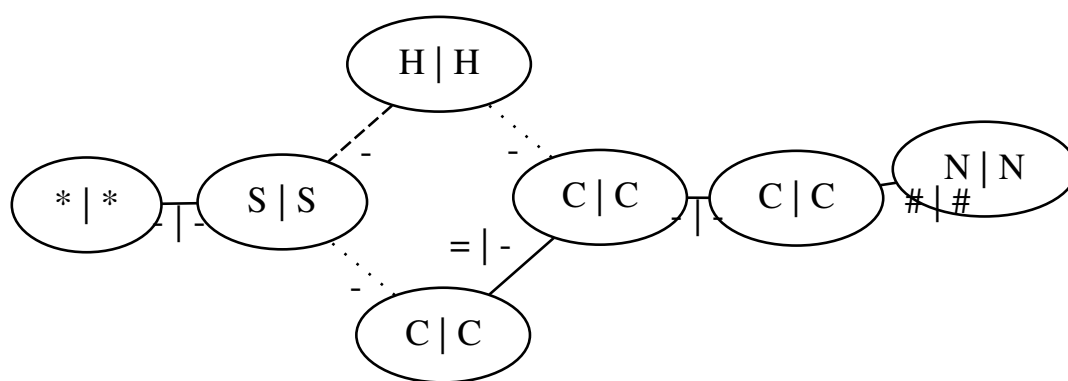
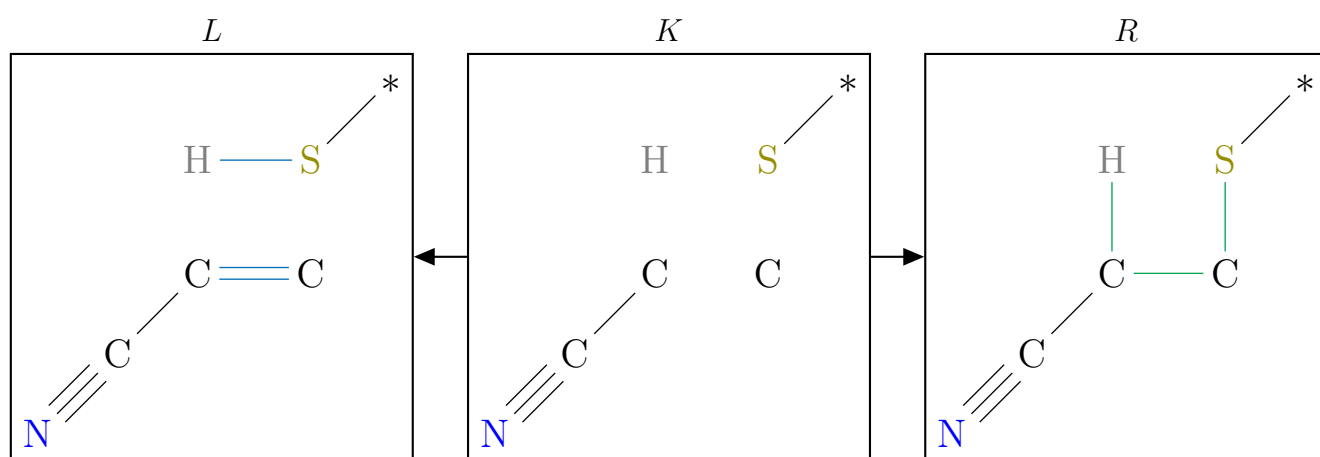
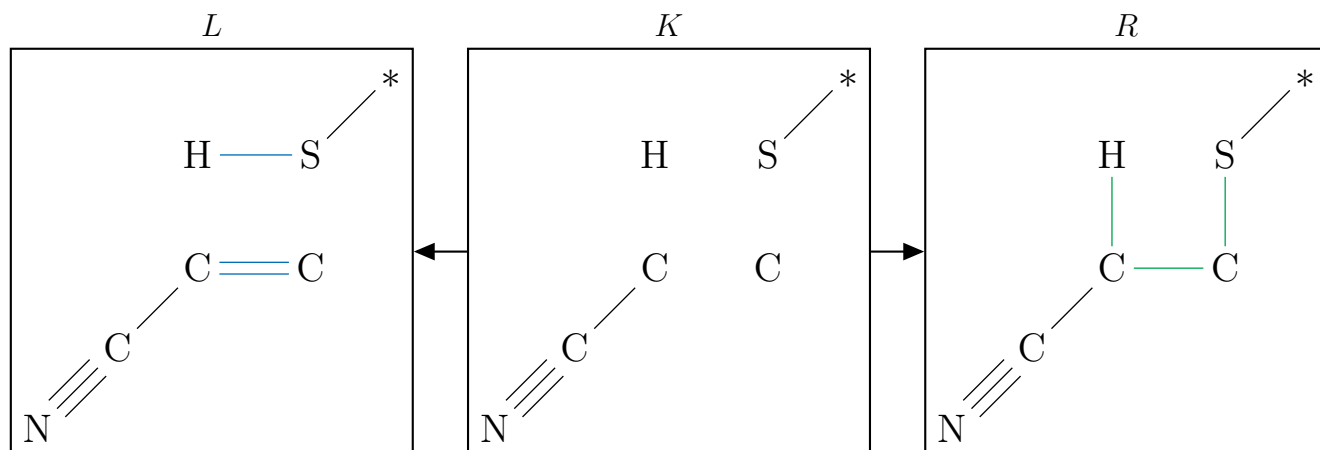
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\} = 0
\end{aligned}$$

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

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

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

0.0.196 Michael Addition 2,1,



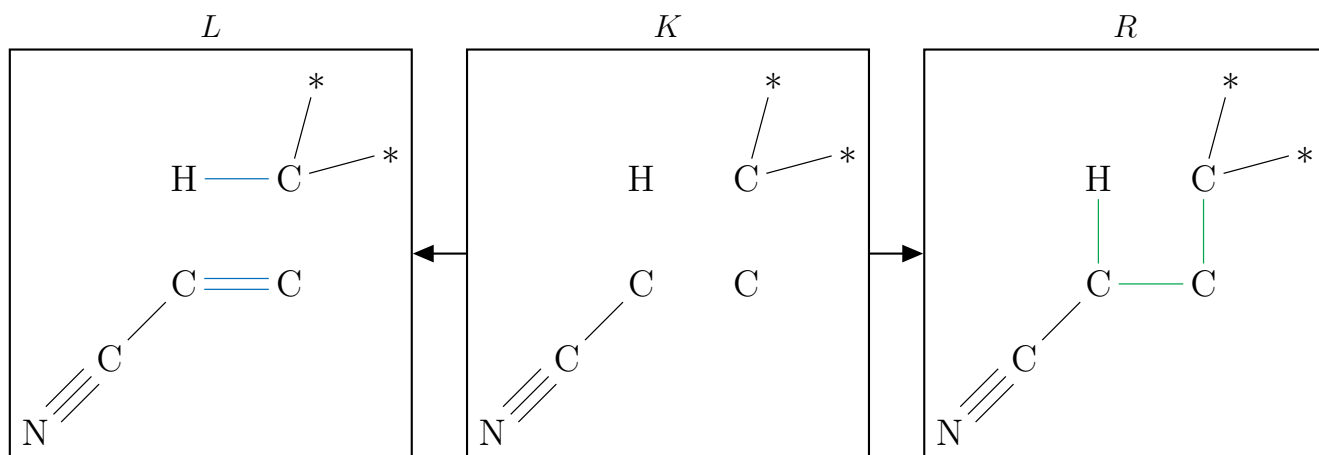
File: out/977_r_198_combined

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

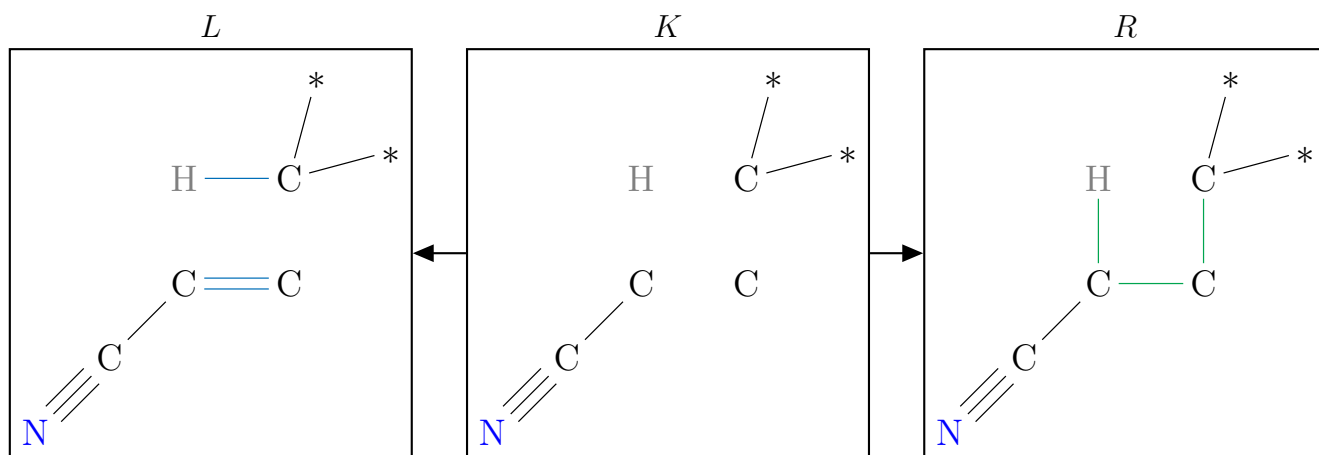
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \mid = 0
\end{aligned}$$

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

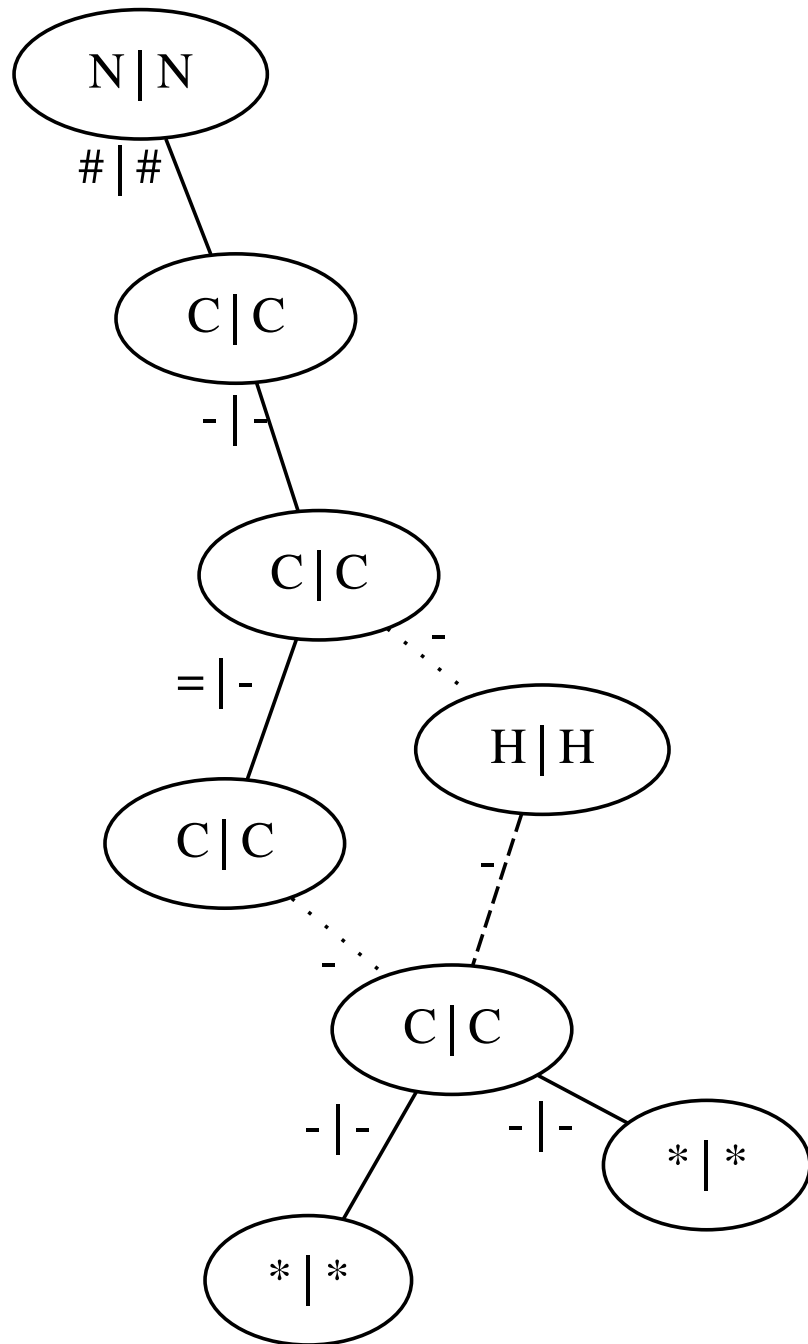
0.0.197 Michael Addition 2,2,



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



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



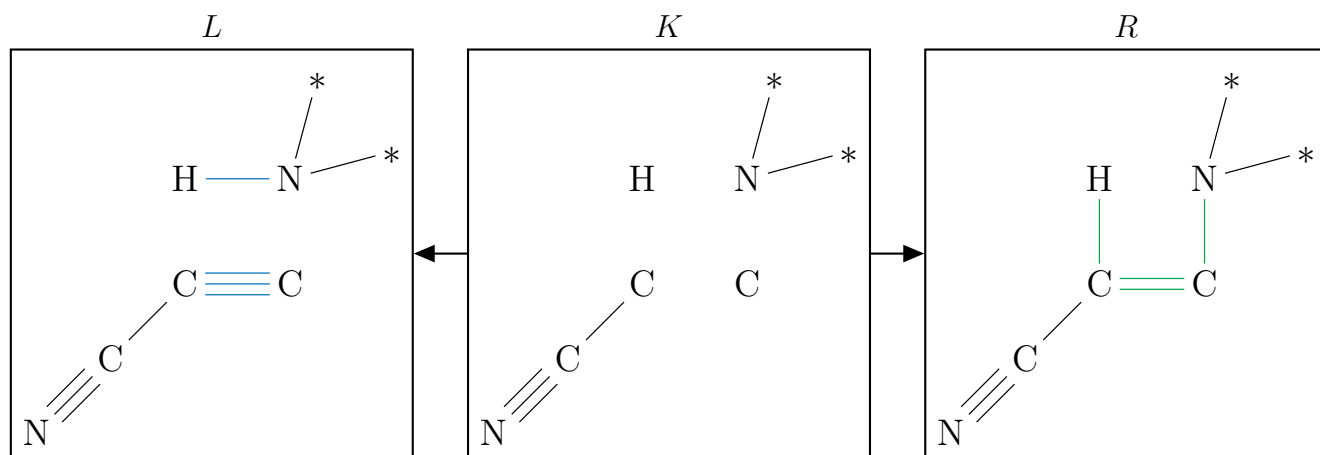
File: out/982_r_199_combined

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

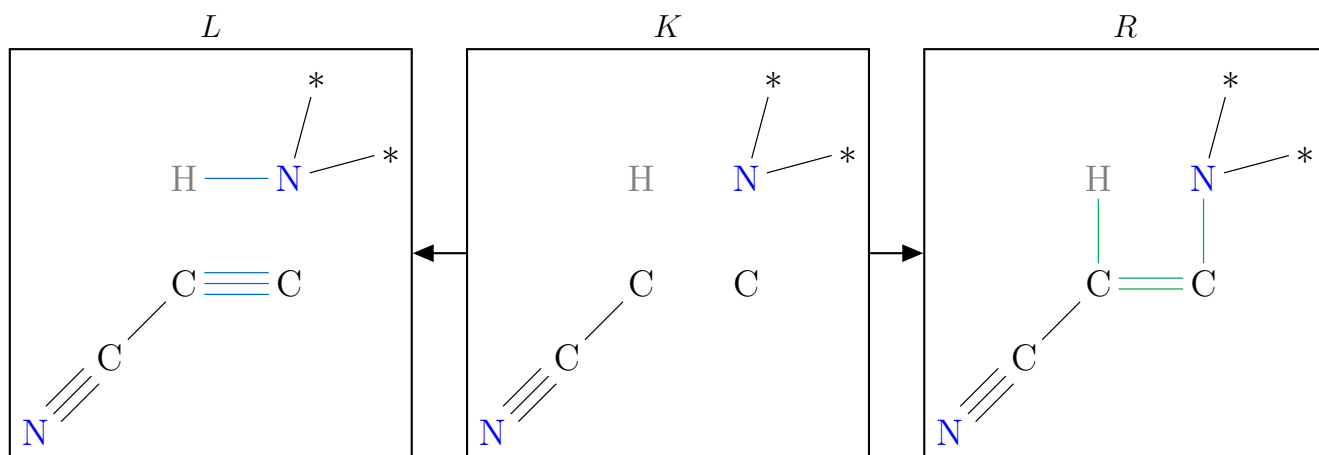
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \mid \mid = 0
\end{aligned}$$

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

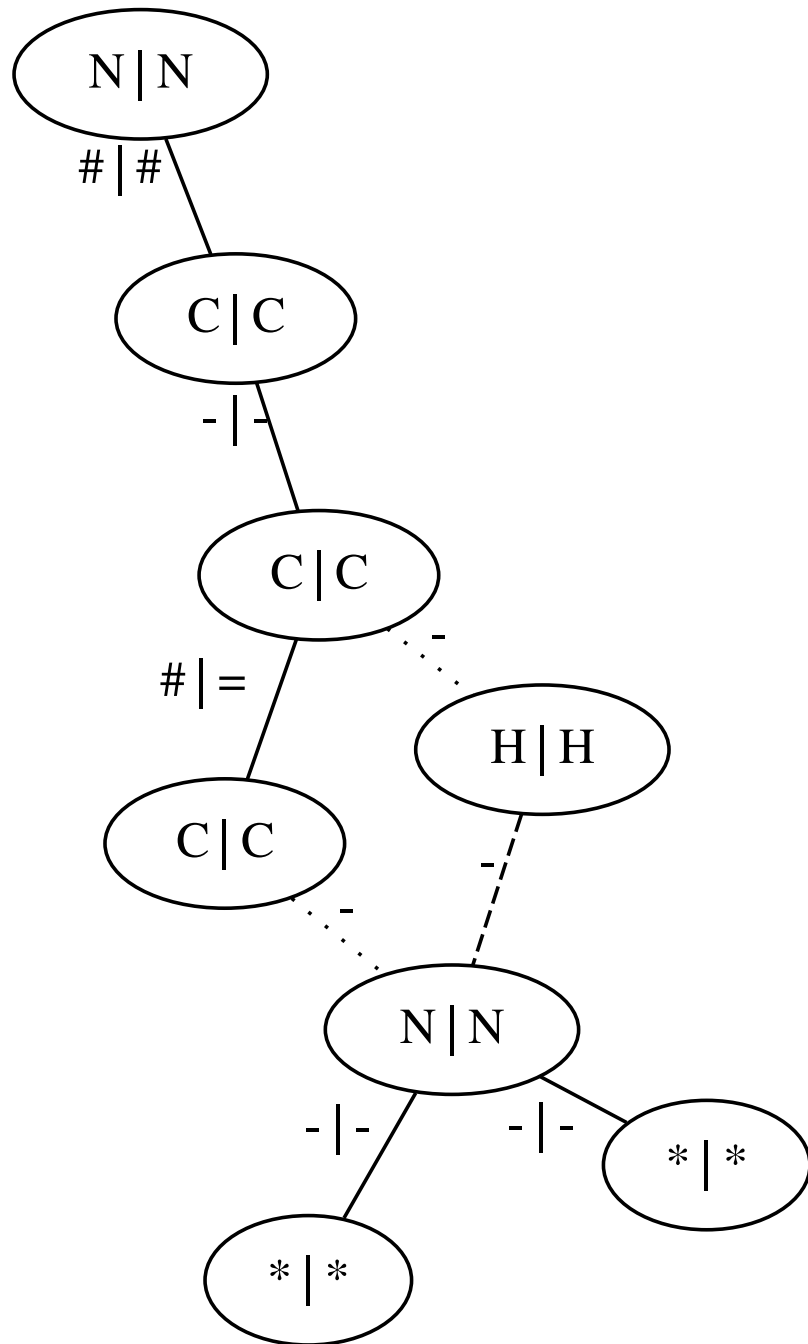
0.0.198 Michael Addition 3,0,



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



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



File: out/987_r_200_combined

$$|\{e \in \text{outEdges}(0) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(6) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(7) \mid$$

$$\text{label}(\text{target}(e)) \in \{\text{'O'}\}$$

$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

$$|\{e \in \text{outEdges}(5) \mid$$

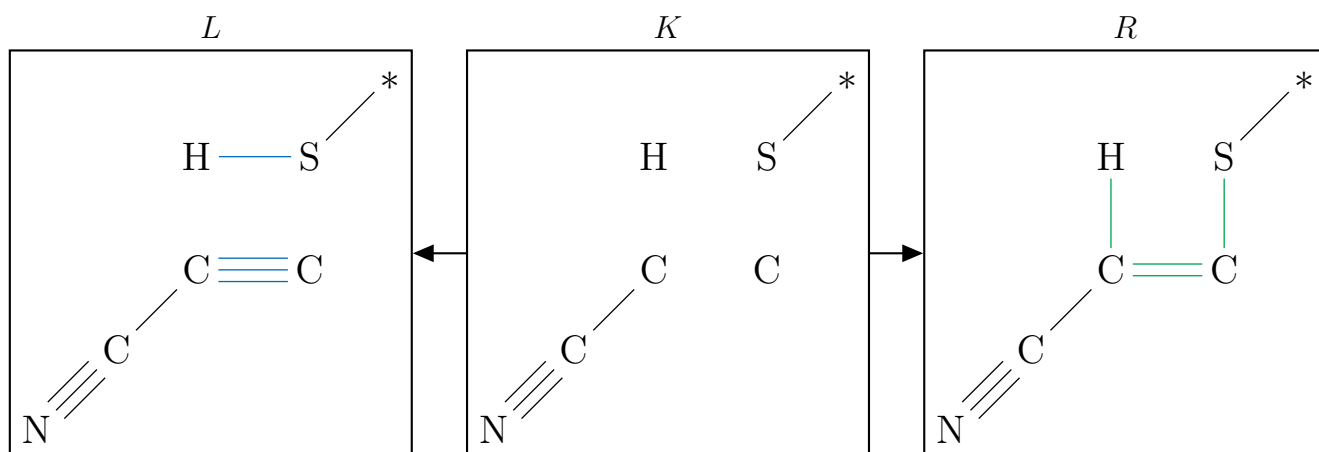
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

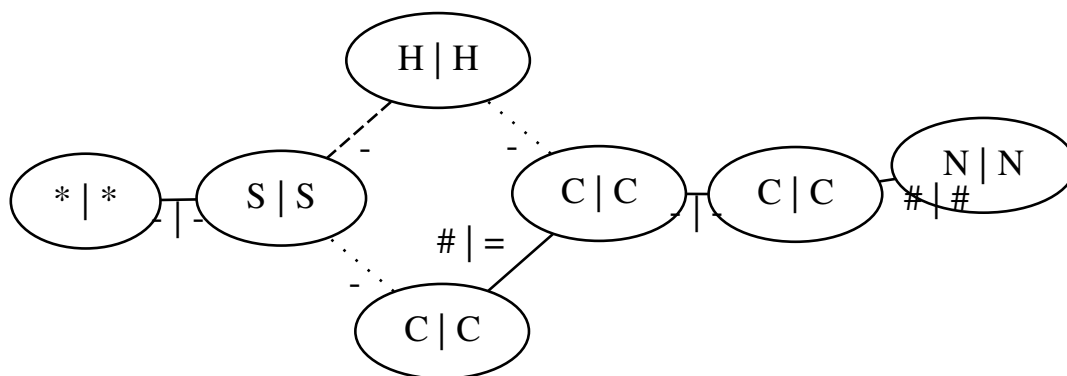
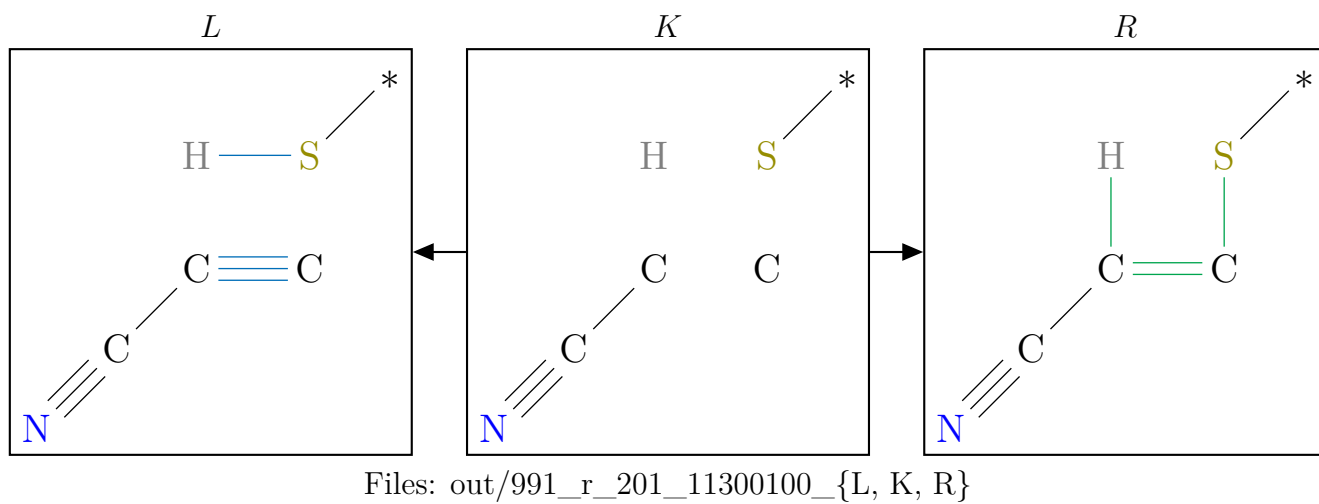
$$\wedge$$

$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

0.0.199 Michael Addition 3,1,

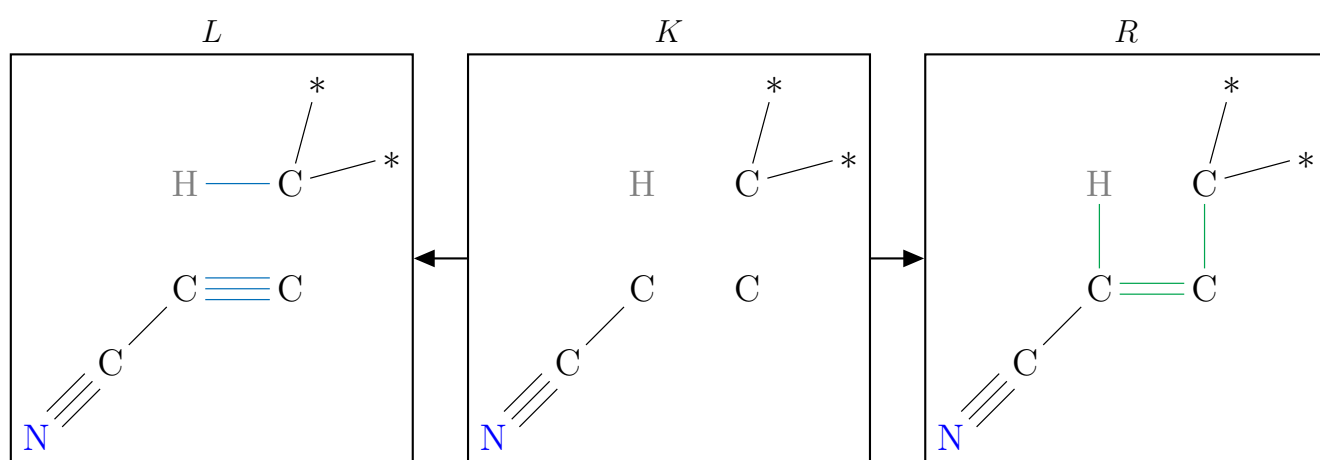
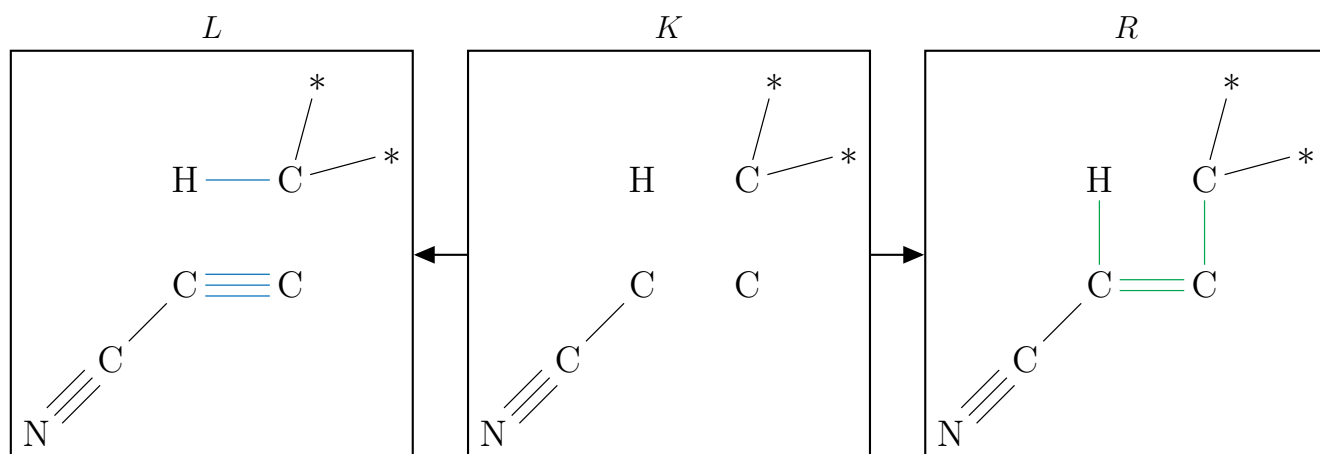


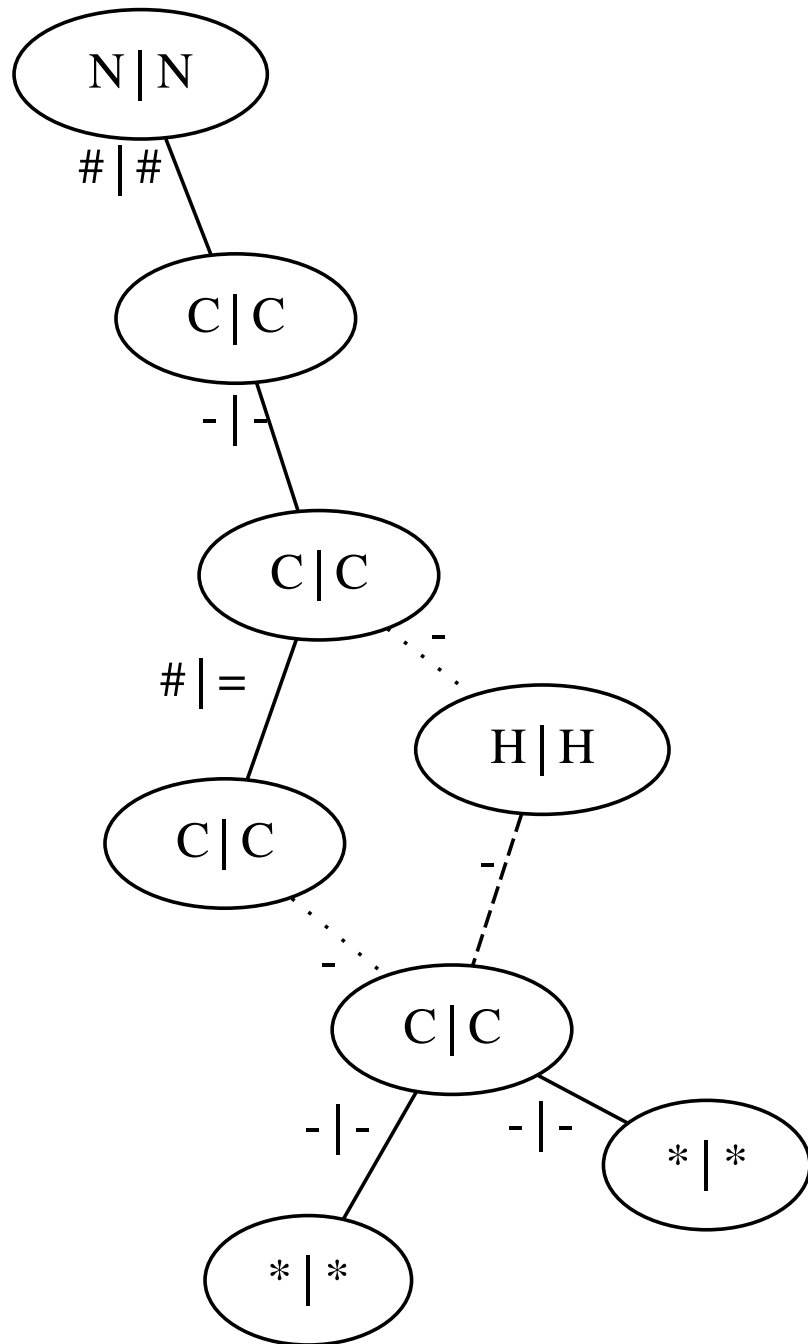


File: out/992_r_201_combined

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

0.0.200 Michael Addition 3,2,

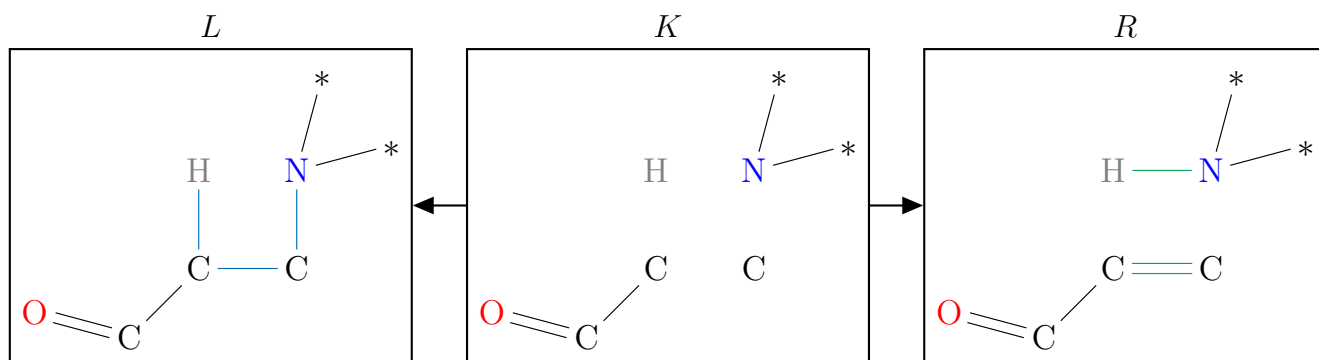
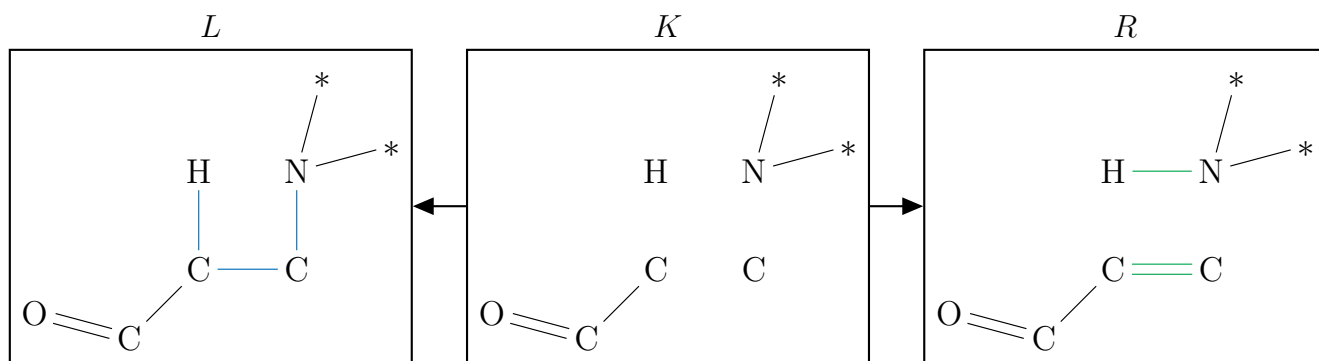


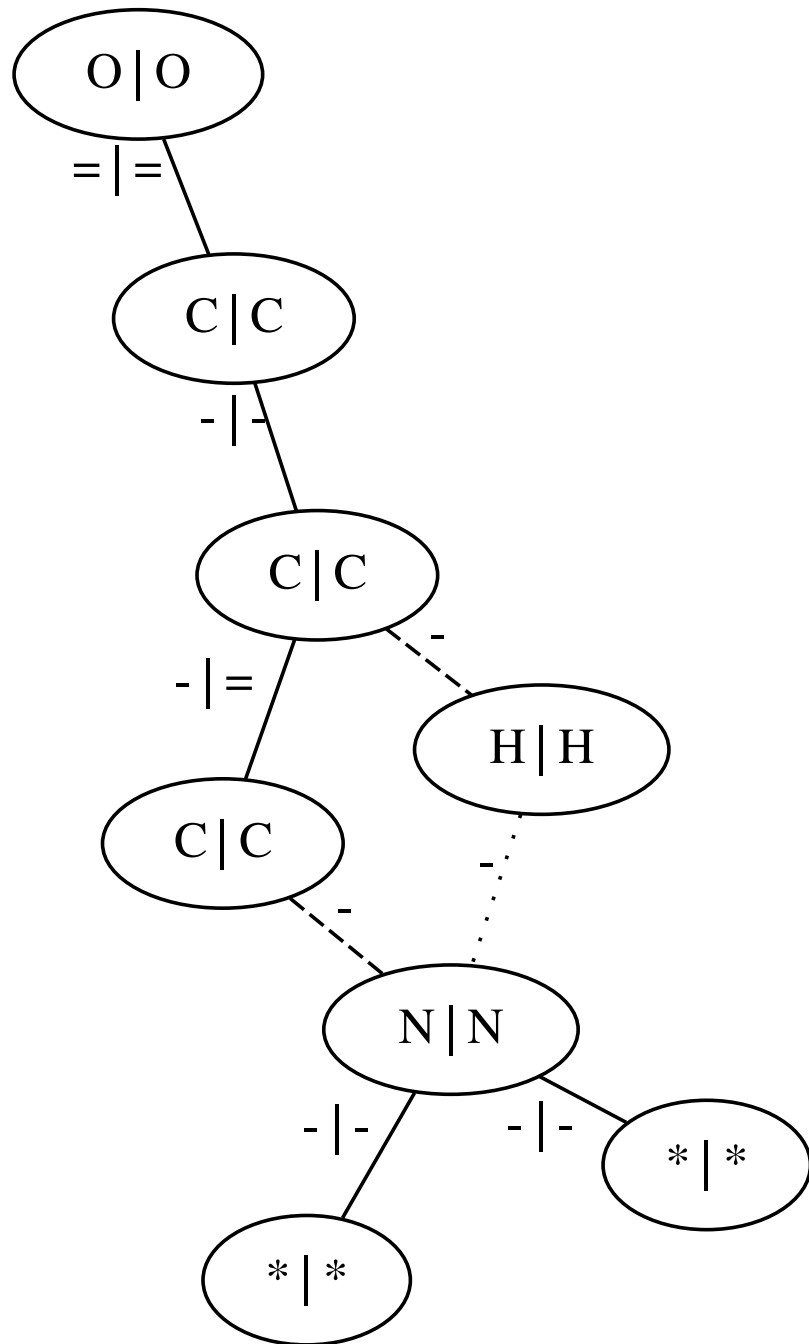


File: out/997_r_202_combined

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

0.0.201 Michael Addition 0,0, (reverse)





File: out/1002_r_203_combined

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

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

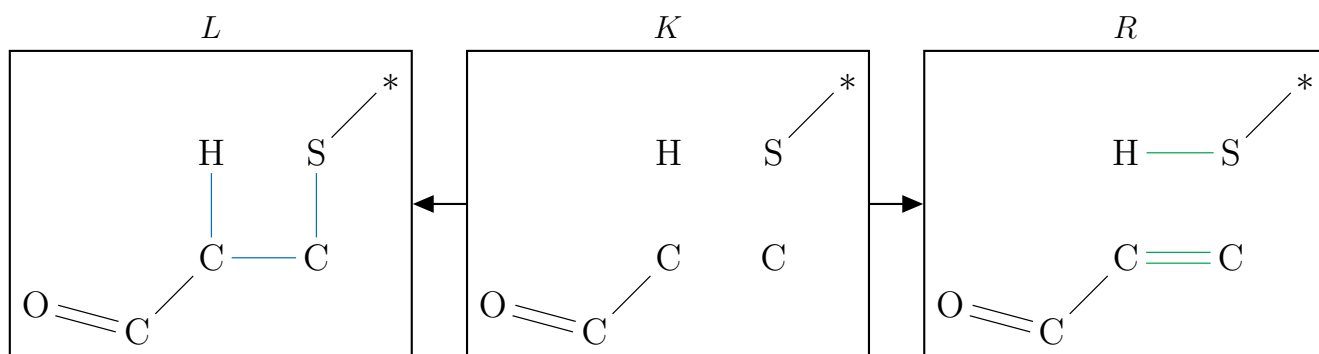
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\mid = 0
\end{aligned}$$

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

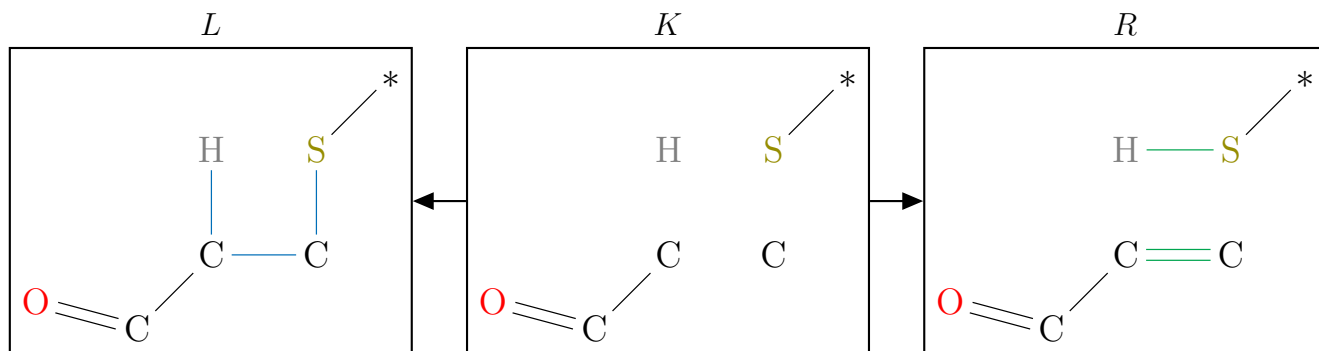
$$\begin{aligned}
& |\{e \in \text{outEdges}(7) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \}\mid = 0
\end{aligned}$$

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

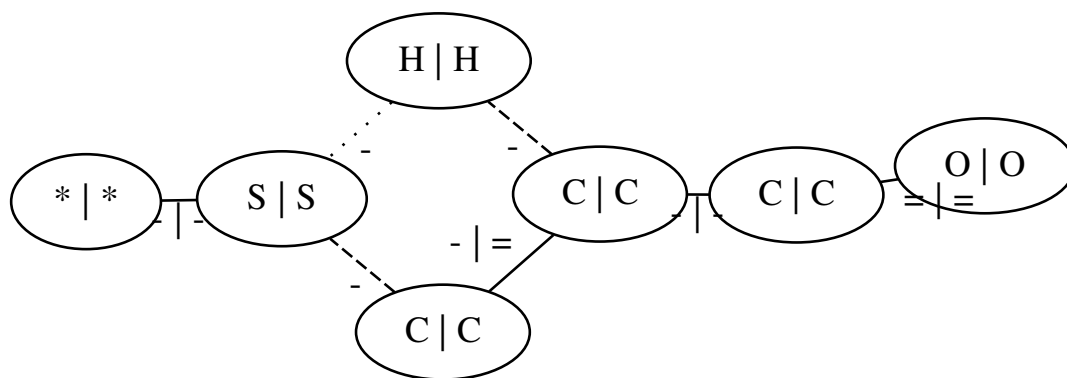
0.0.202 Michael Addition 0,1, (reverse)



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



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



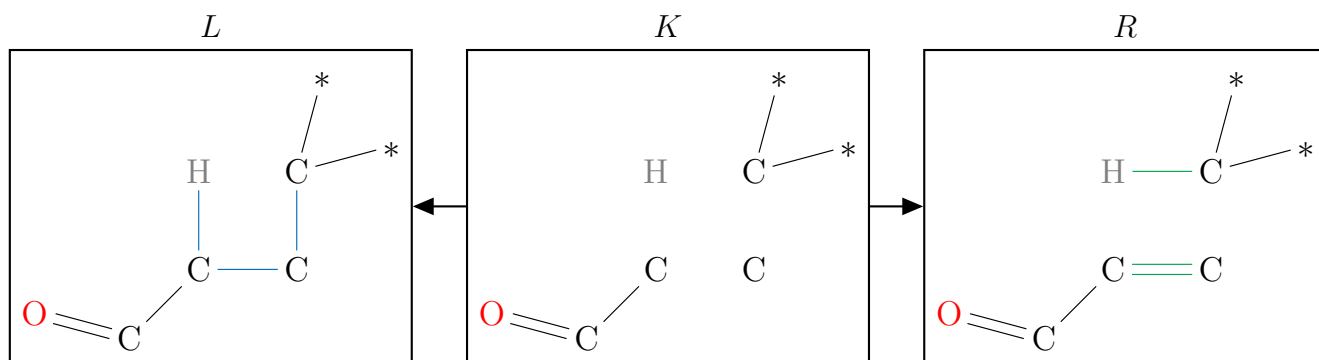
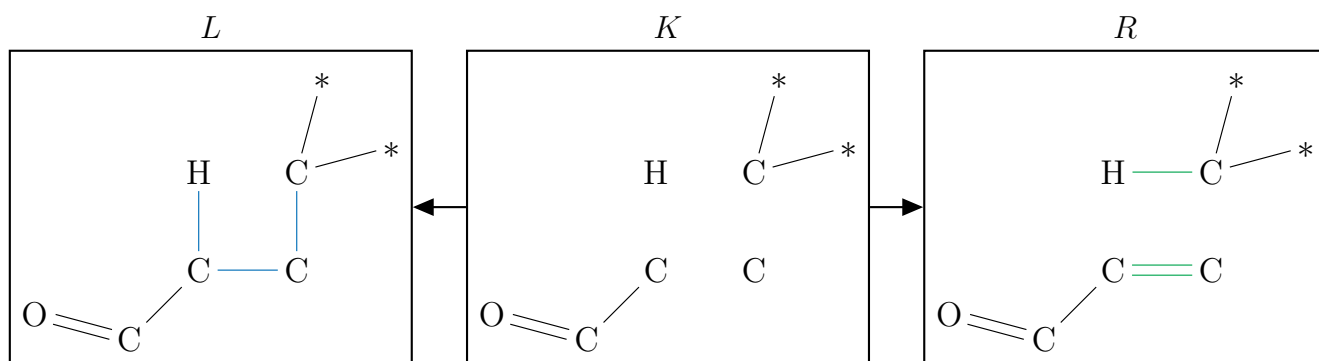
File: out/1007_r_204_combined

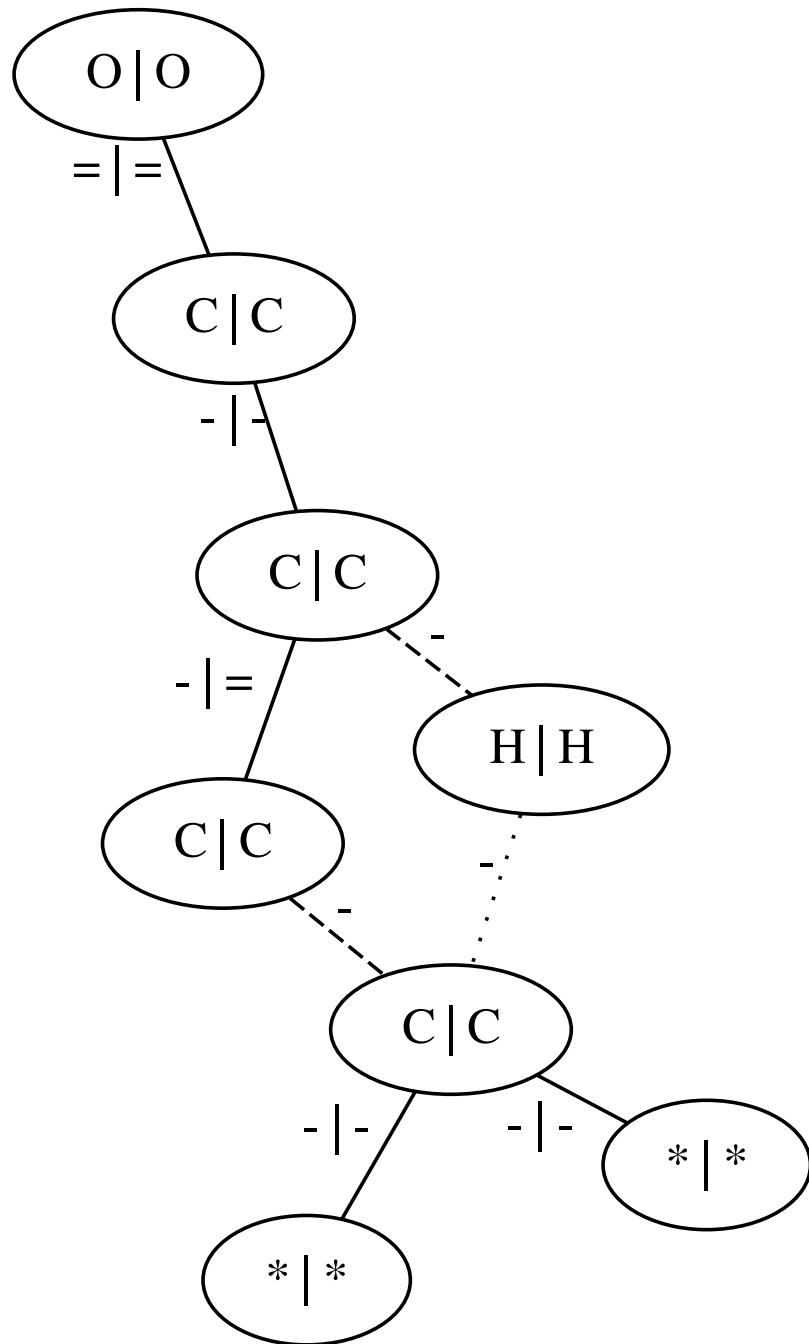
$$|\{e \in \text{outEdges}(0) \mid \text{label}(\text{target}(e)) \in \{ '0' \} \wedge \text{label}(e) \in \{ '-', '=' \} \}| = 0$$

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

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

0.0.203 Michael Addition 0,2, (reverse)



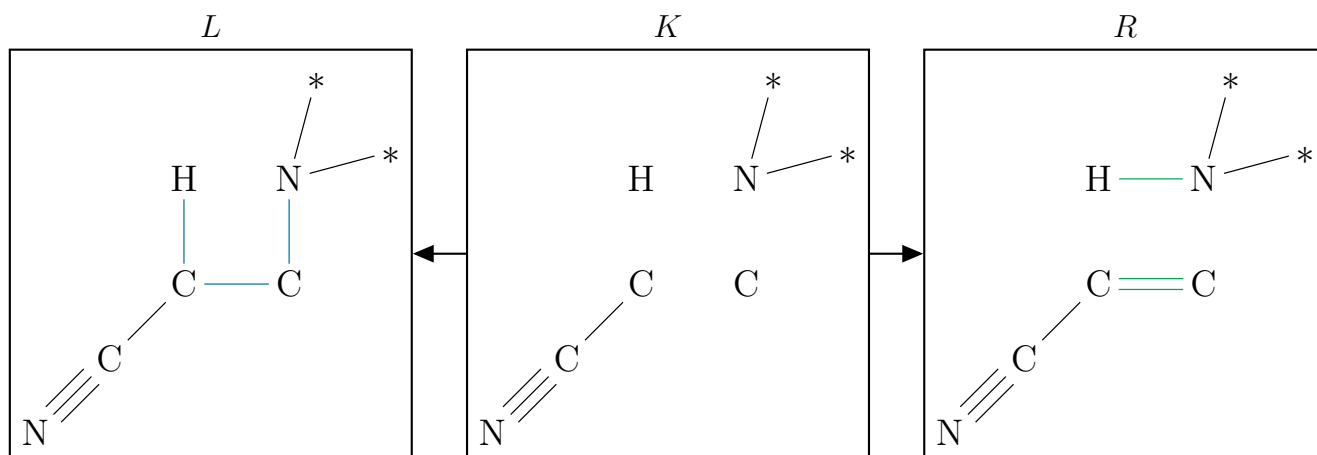


$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

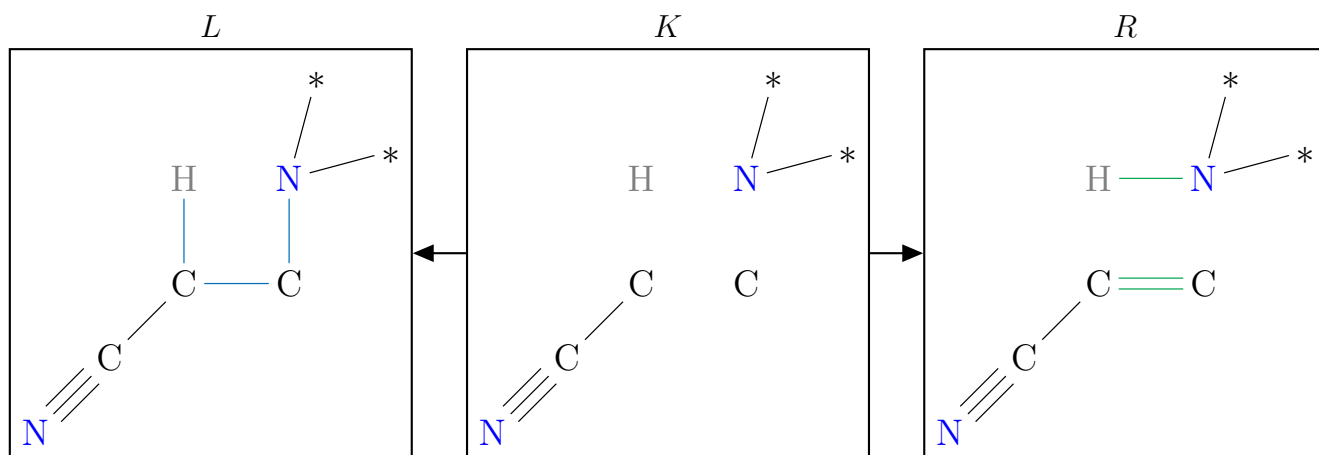
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

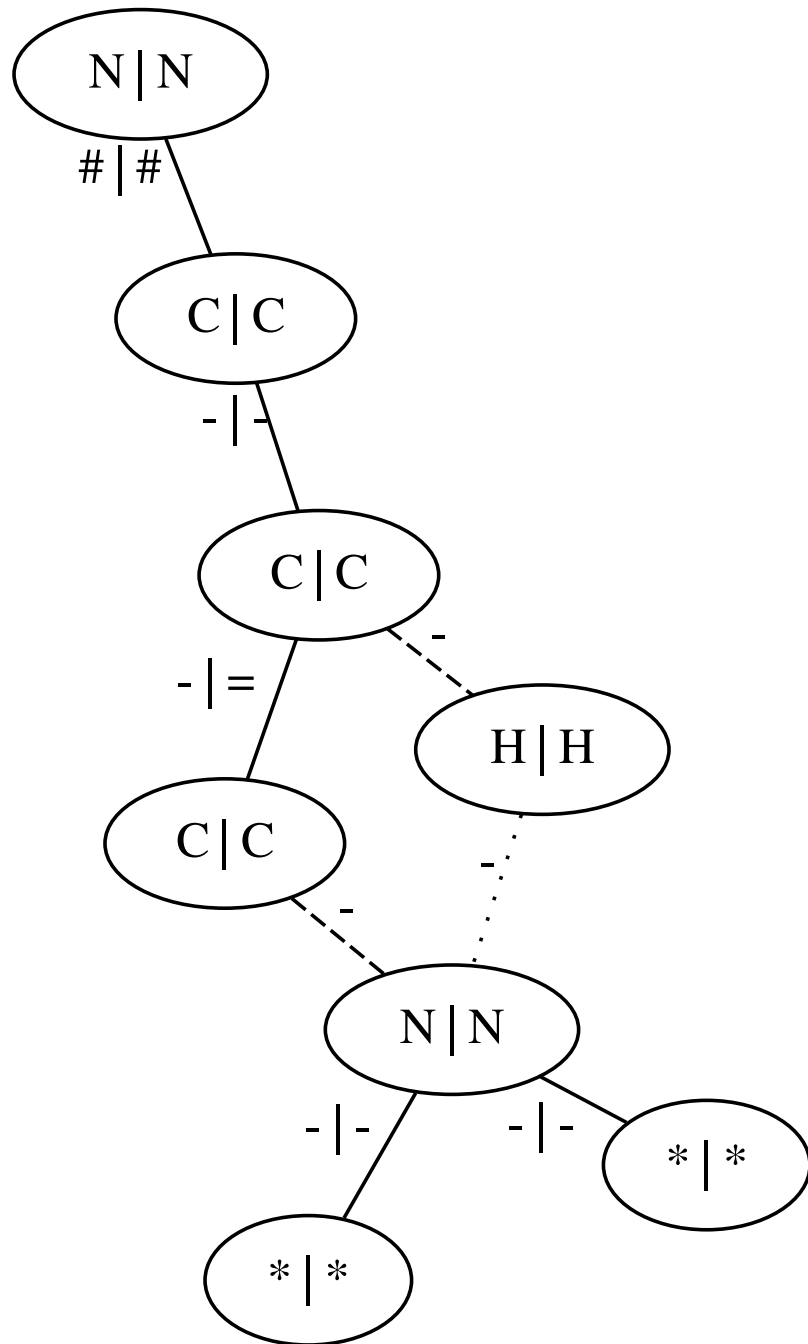
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'#'}, \text{'='}\} \\
& \quad \}| = 0
\end{aligned}$$

0.0.204 Michael Addition 2,0, (reverse)



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





File: out/1017_r_206_combined

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

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

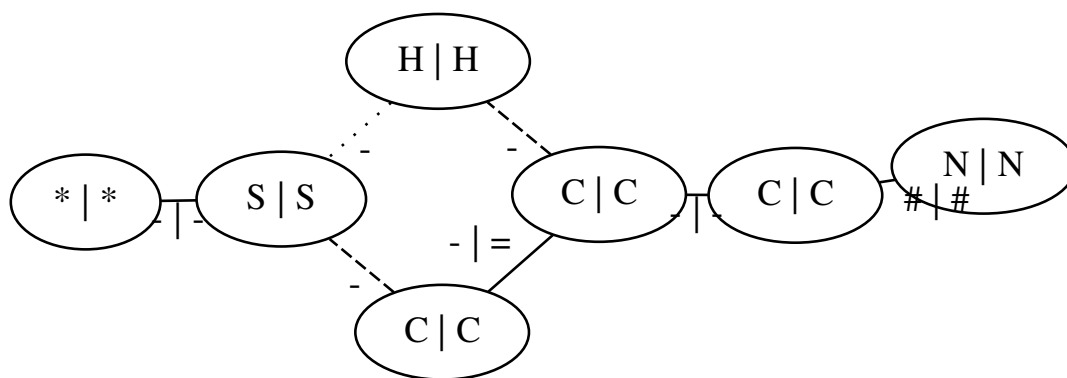
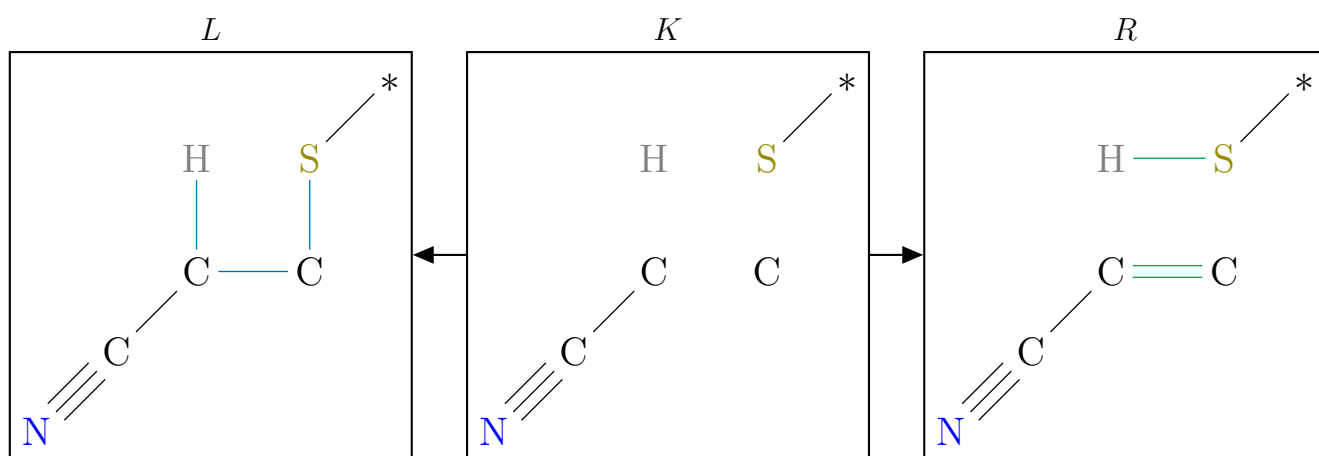
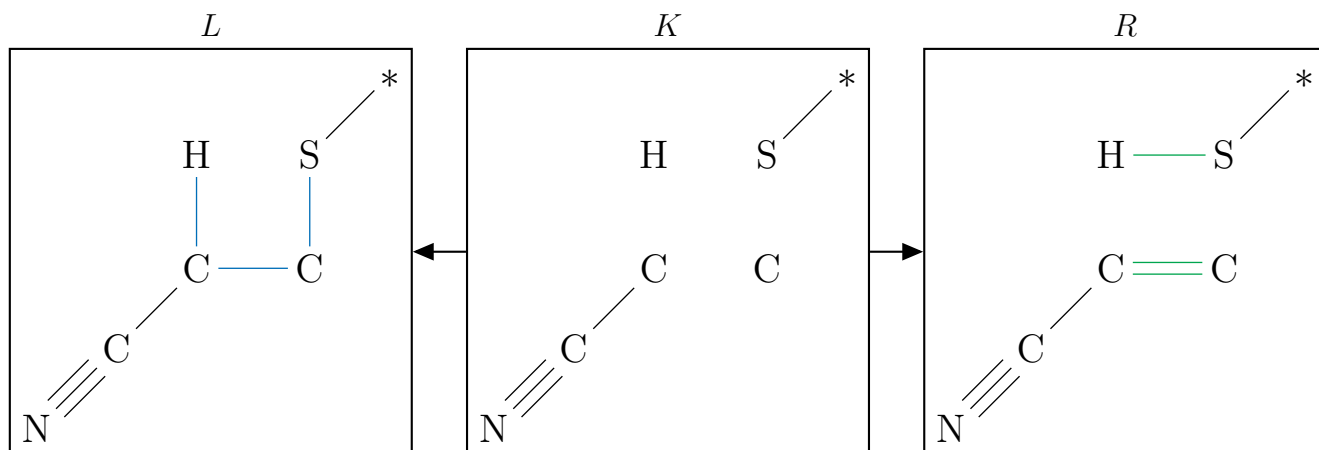
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\} = 0
\end{aligned}$$

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

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

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

0.0.205 Michael Addition 2,1, (reverse)



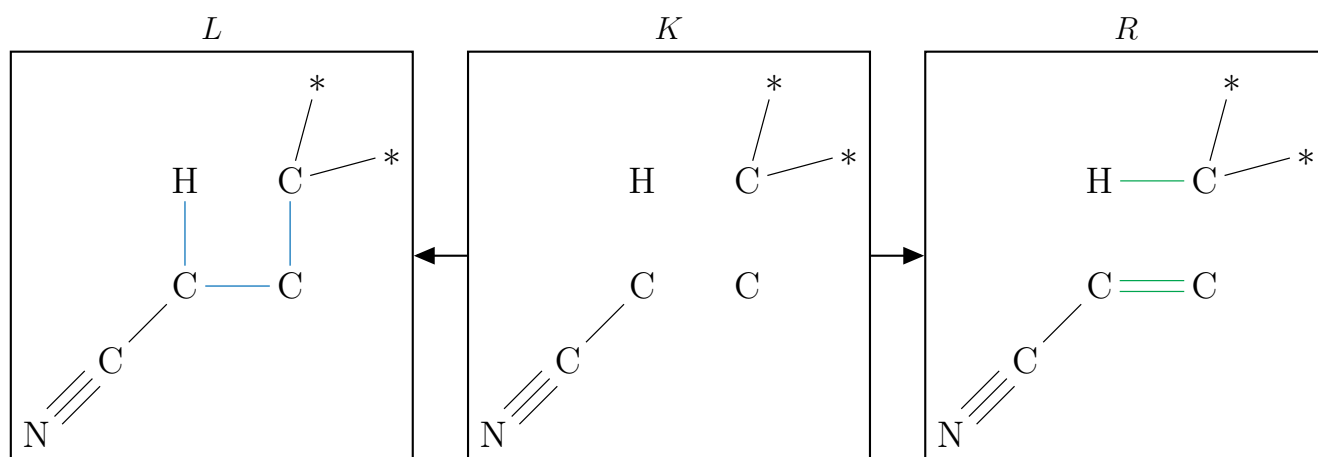
File: out/1022_r_207_combined

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

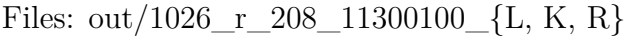
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

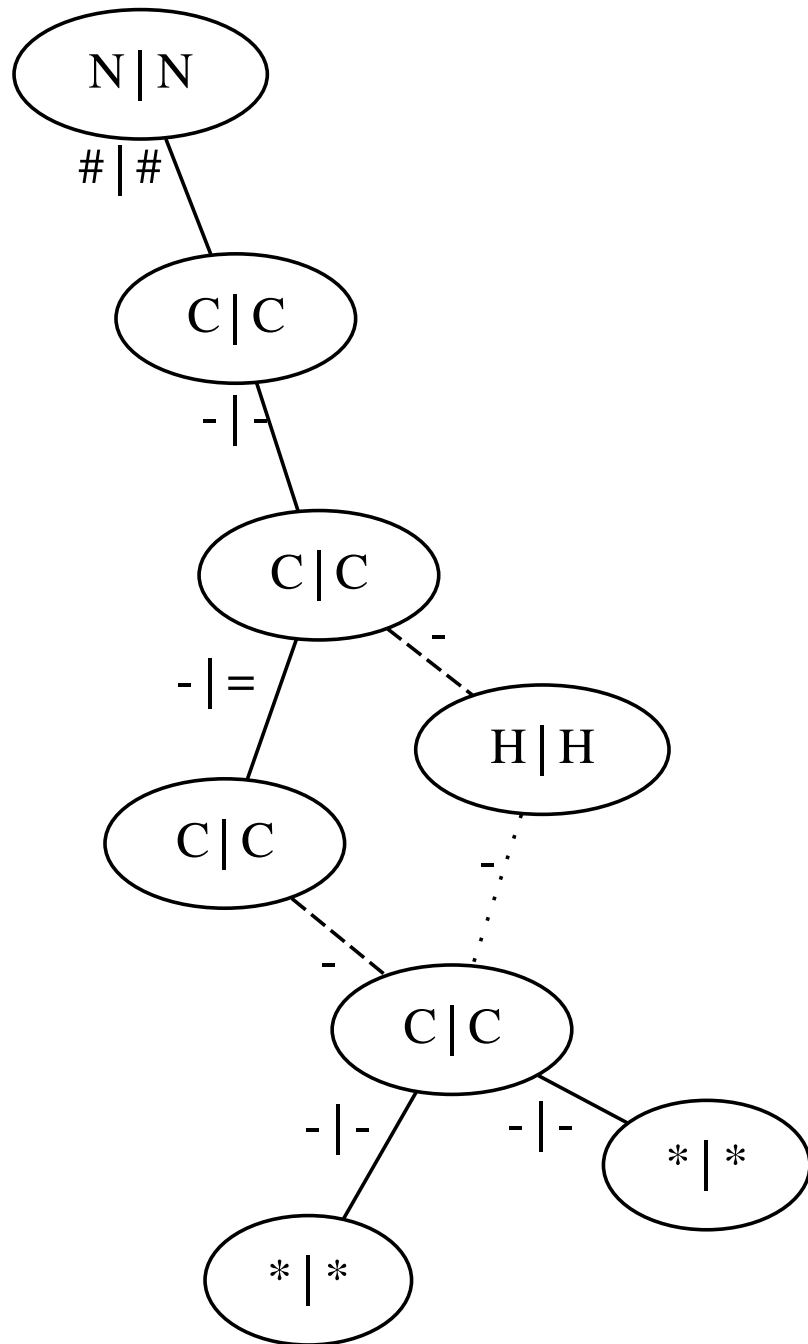
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}| = 0
\end{aligned}$$

0.0.206 Michael Addition 2,2, (reverse)



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





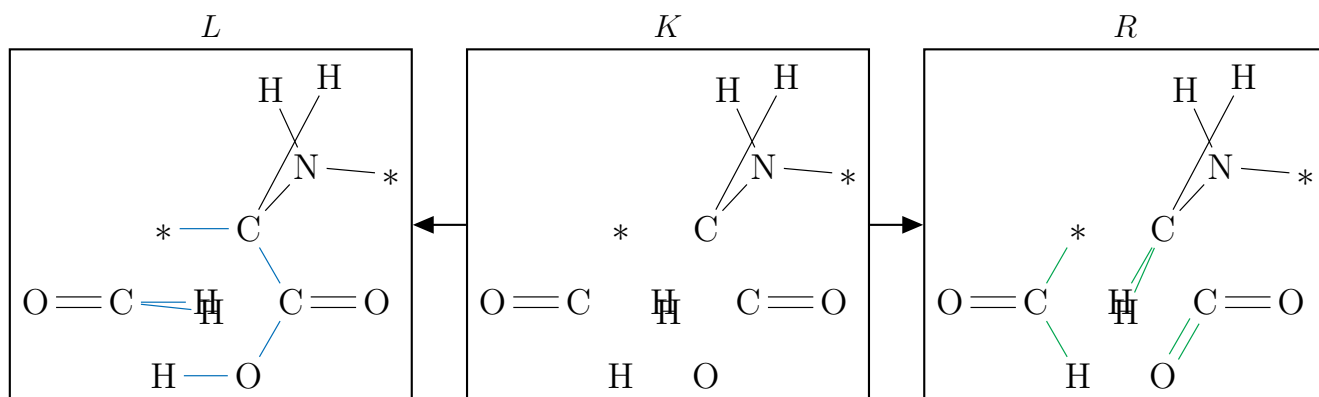
File: out/1027_r_208_combined

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

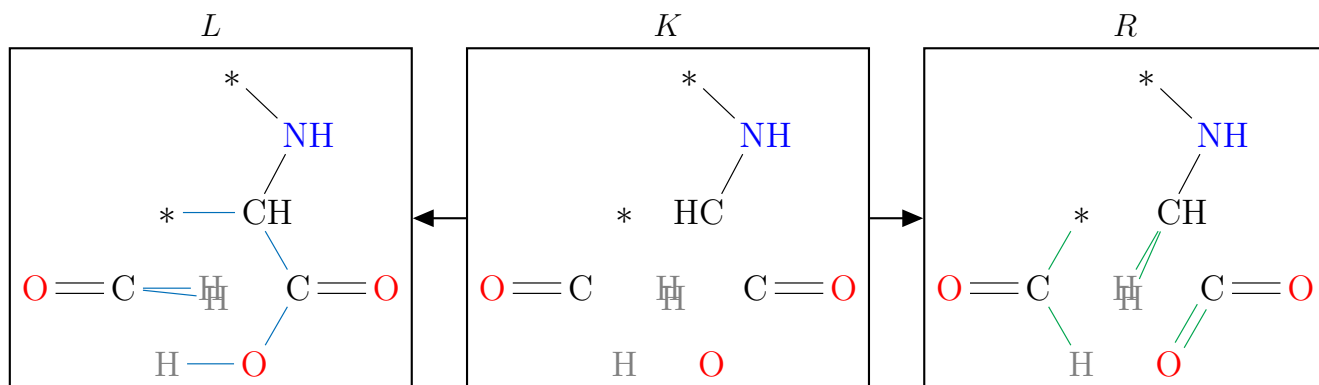
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{'-\'} \\
& \quad \}| = 0
\end{aligned}$$

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

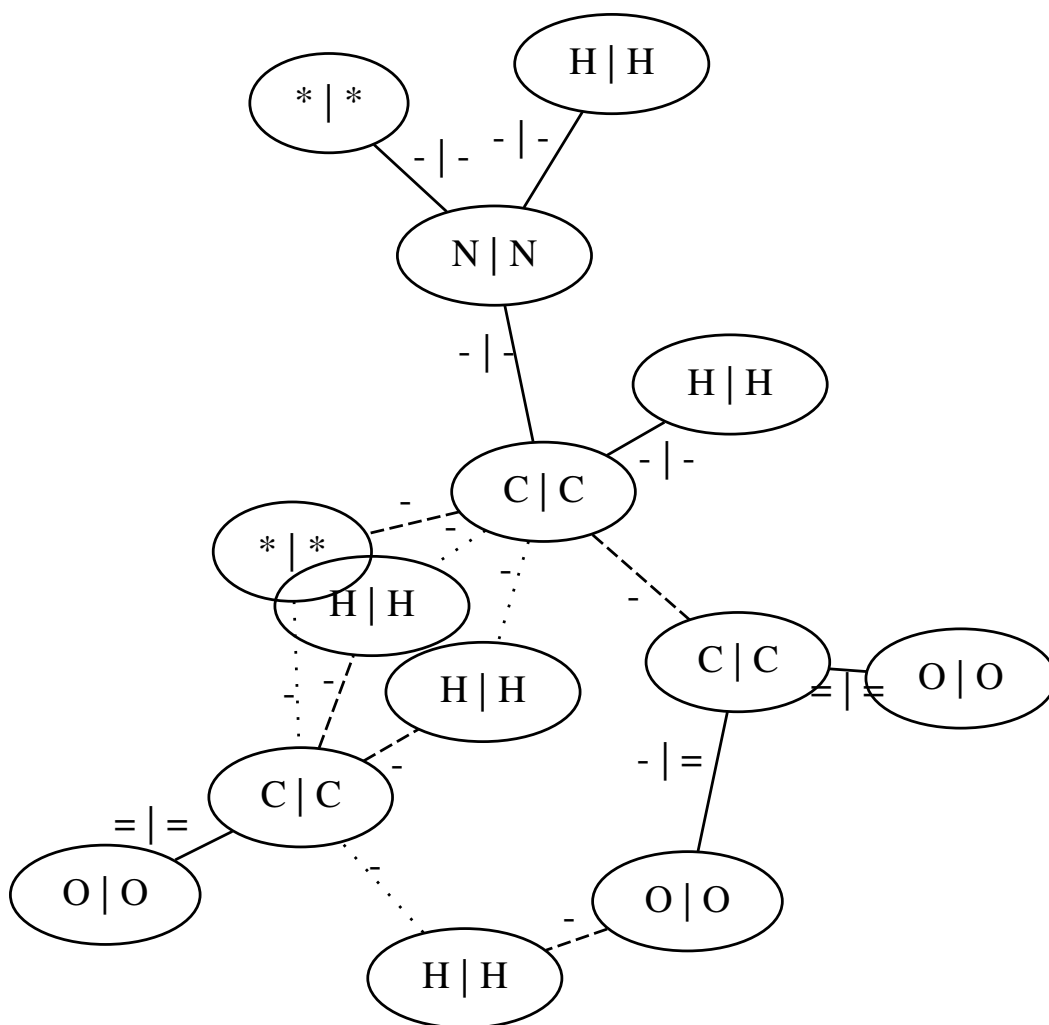
0.0.207 Strecker Degradation, HH



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

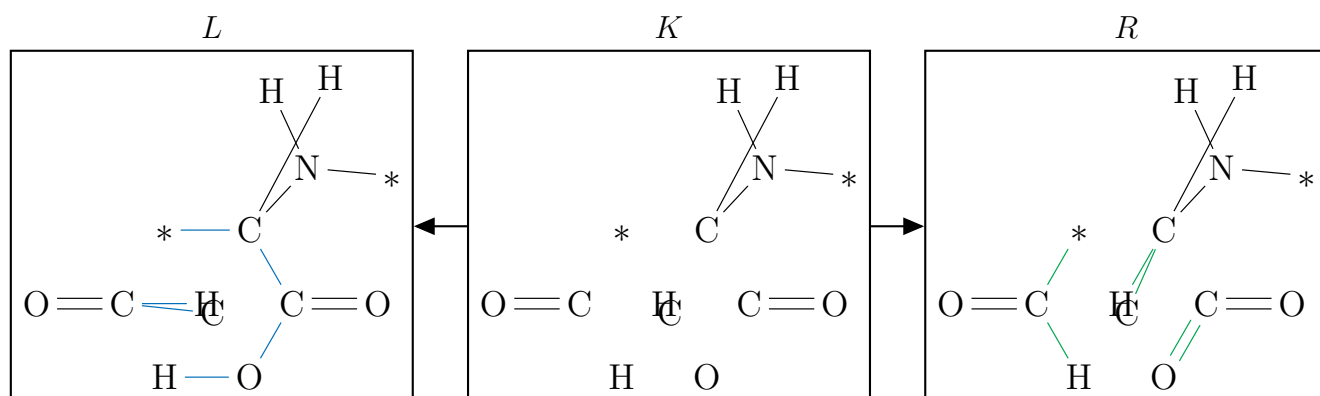


Files: out/1031_r_209_11300100_{L, K, R}

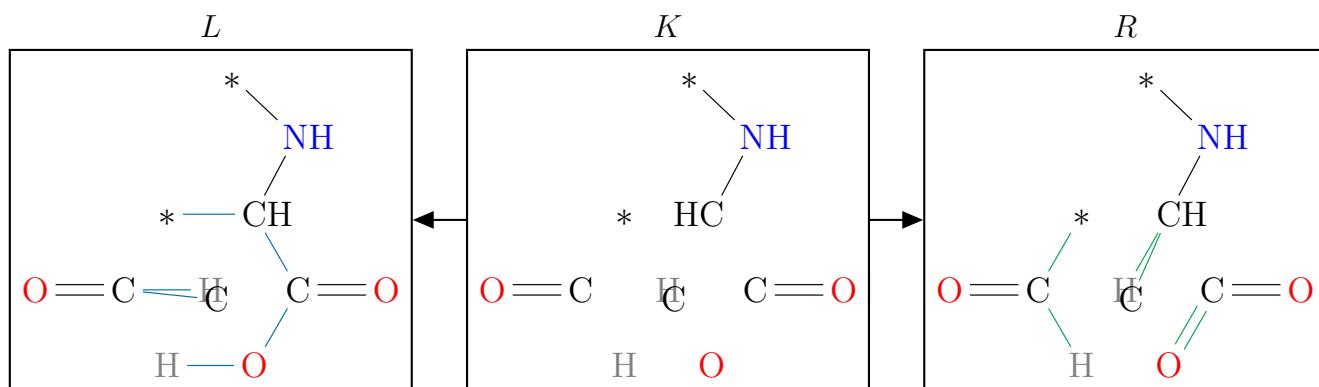


File: out/1032_r_209_combined

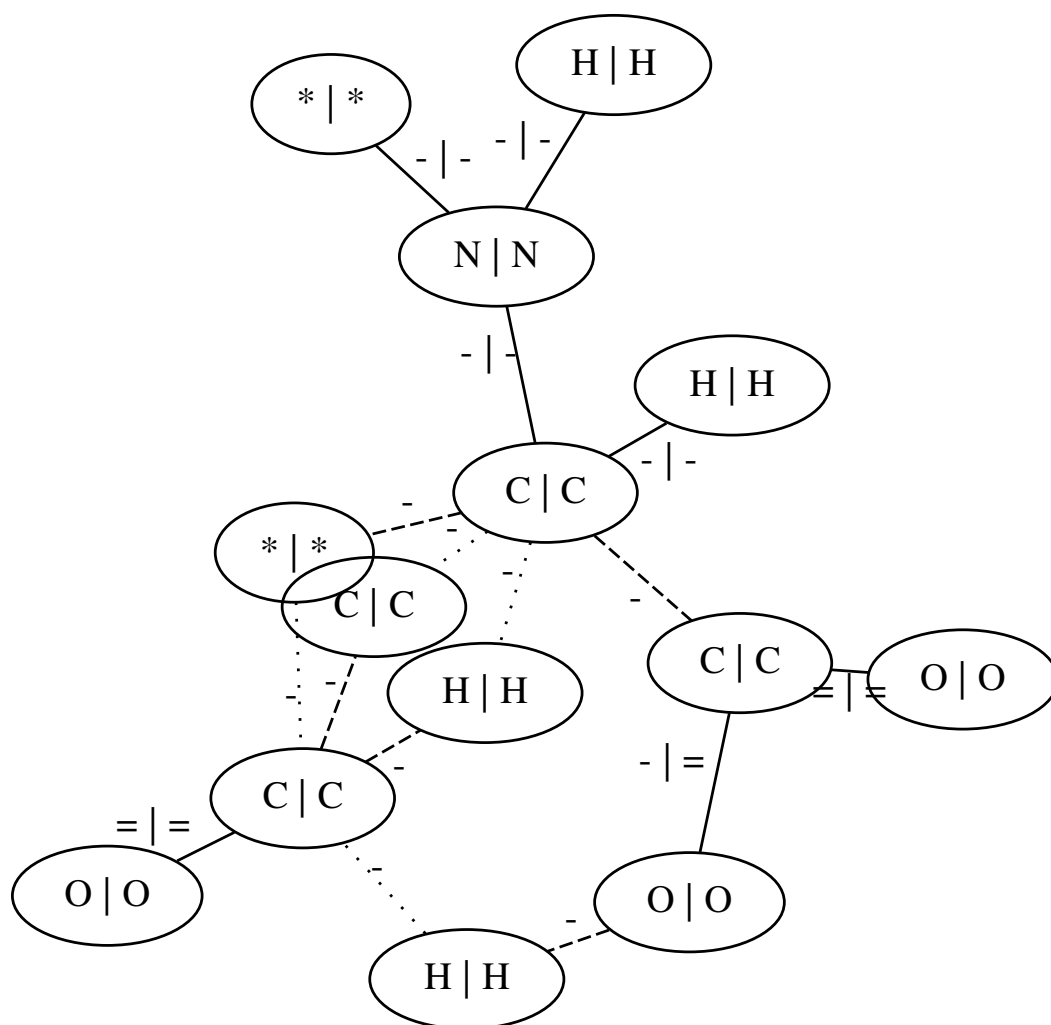
0.0.208 Strecker Degradation, HC



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



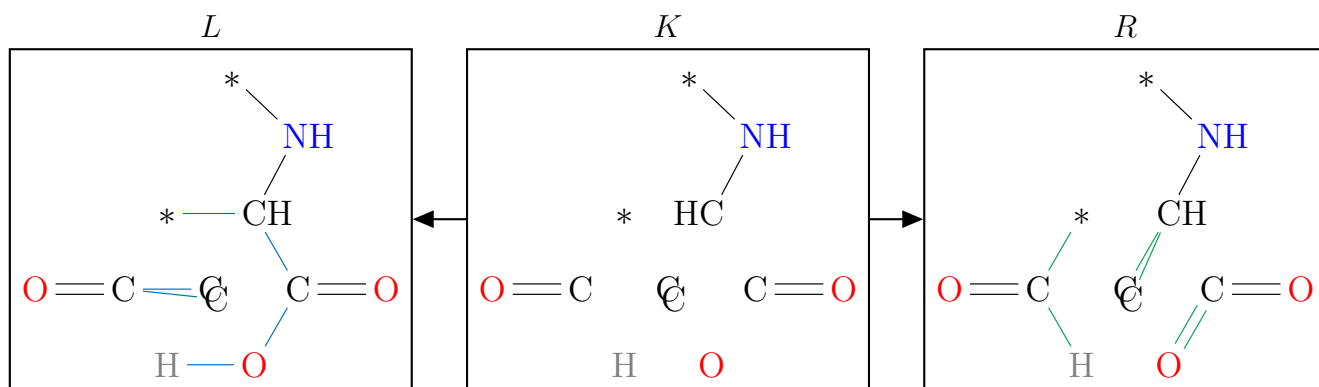
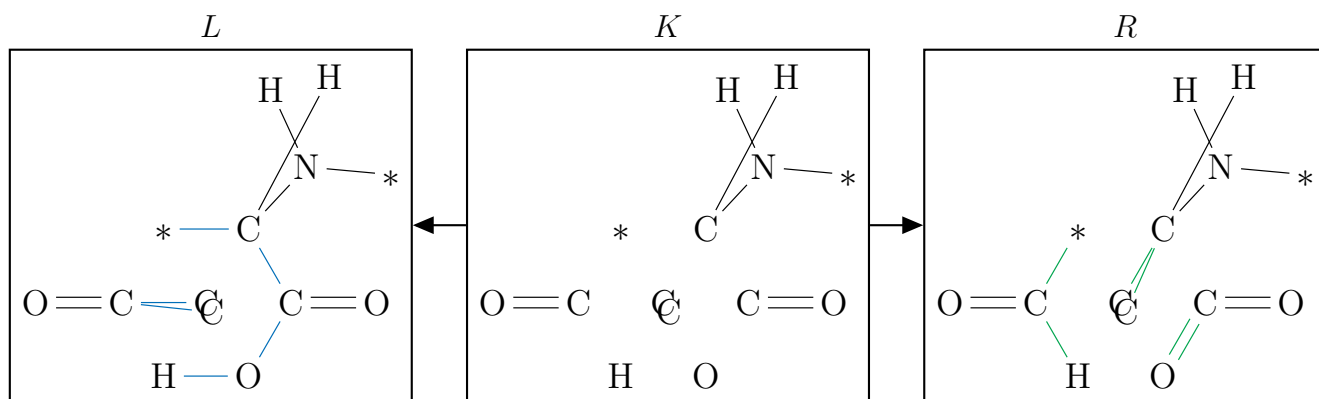
Files: out/1036_r_210_11300100_{L, K, R}

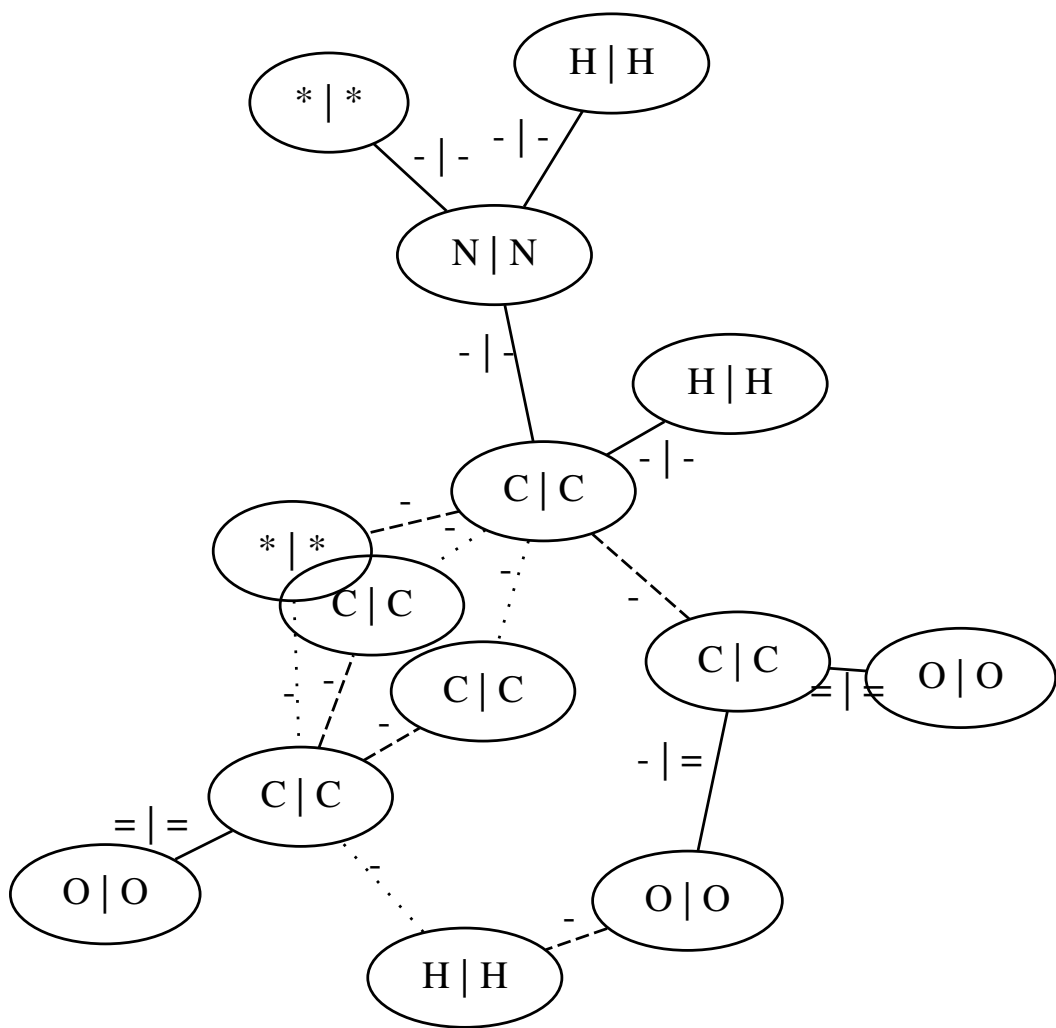


File: out/1037_r_210_combined

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

0.0.209 Strecker Degradation, CC





File: out/1042_r_211_combined

$$|\{e \in \text{outEdges}(12) \mid$$

$$\text{label}(\text{target}(e)) \in \{'0'\}$$

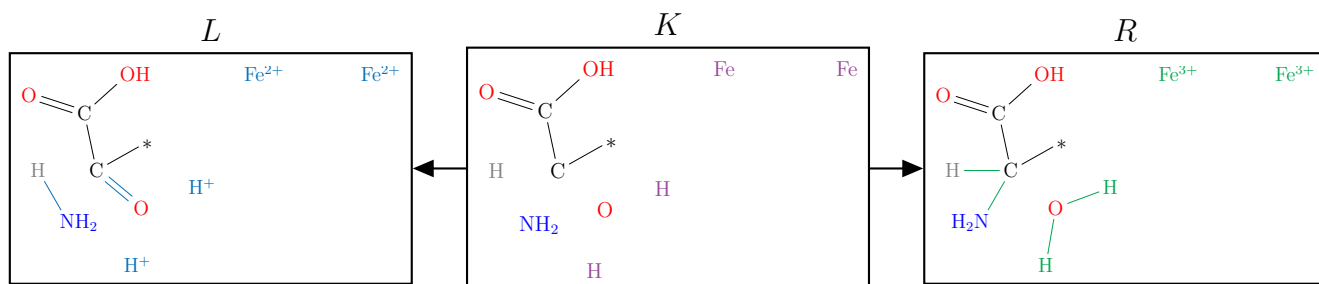
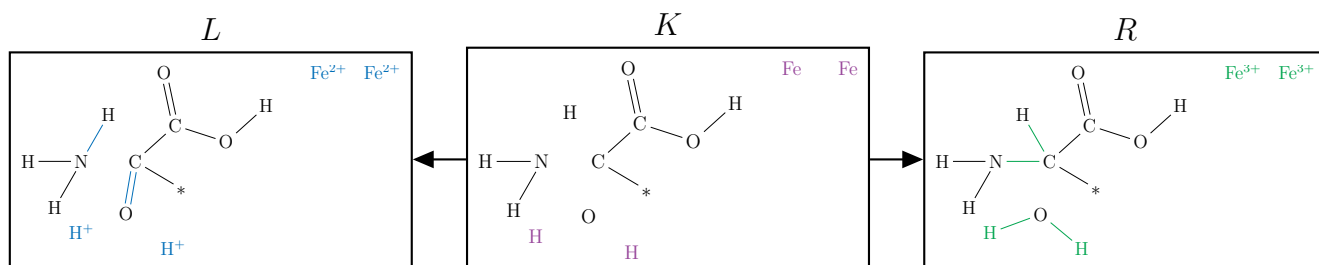
$$\wedge$$

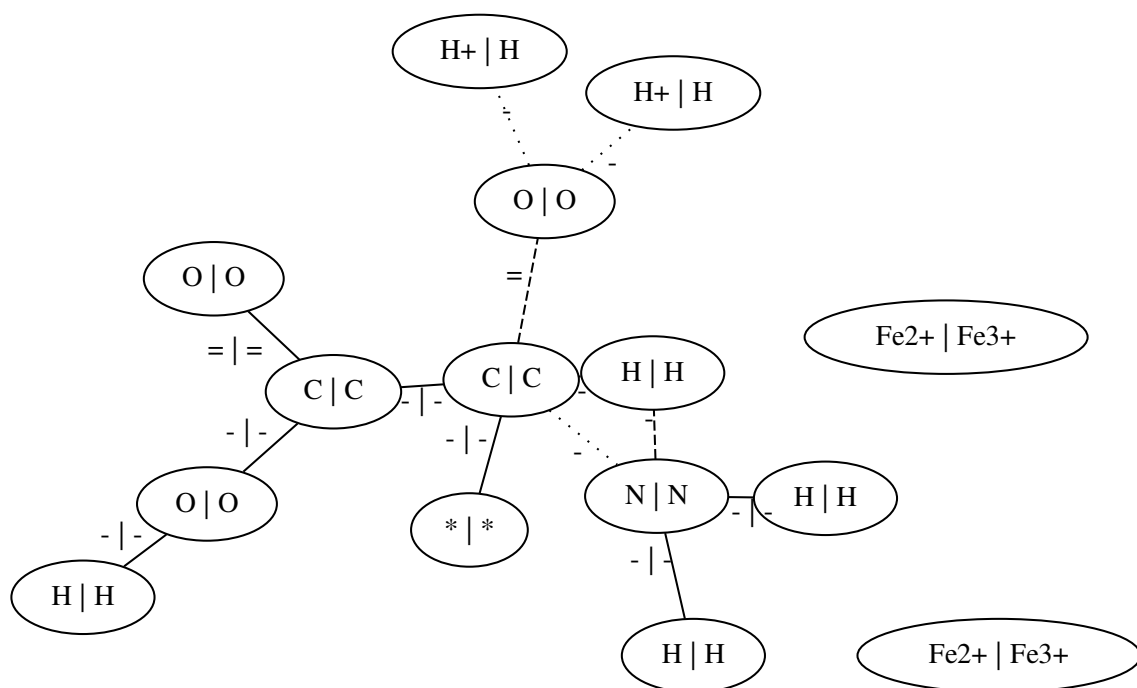
$$\text{label}(e) \in \{'=\'}\}$$

$$| = 0$$

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

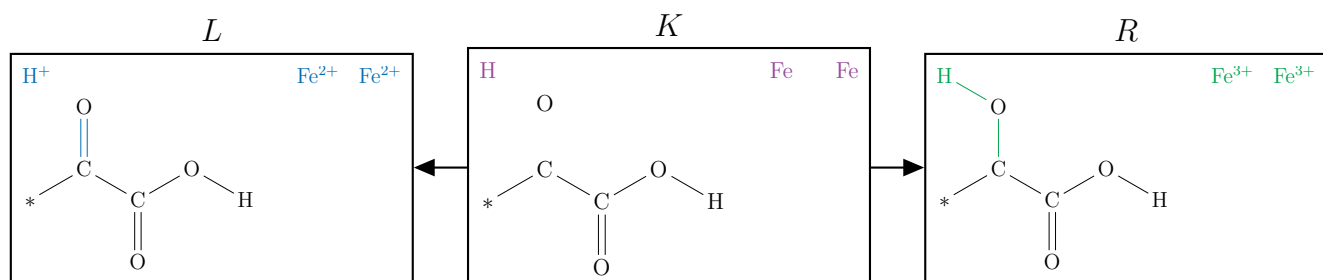
0.0.210 Fe2 \longrightarrow Fe3 Alpha Keto Reduction, conversion to amino acid



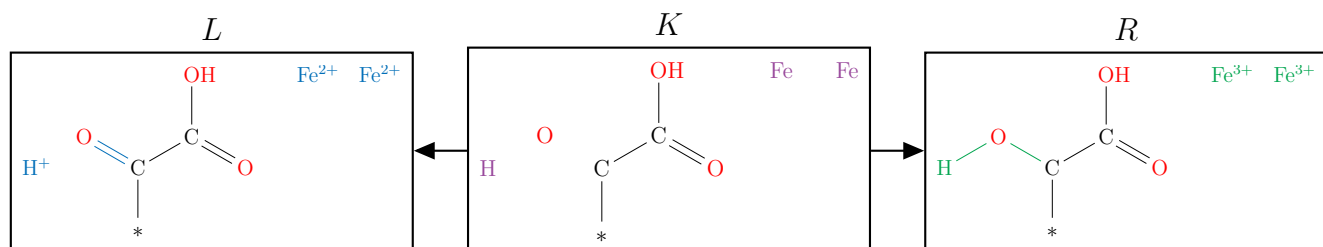


File: out/1047_r_212_combined

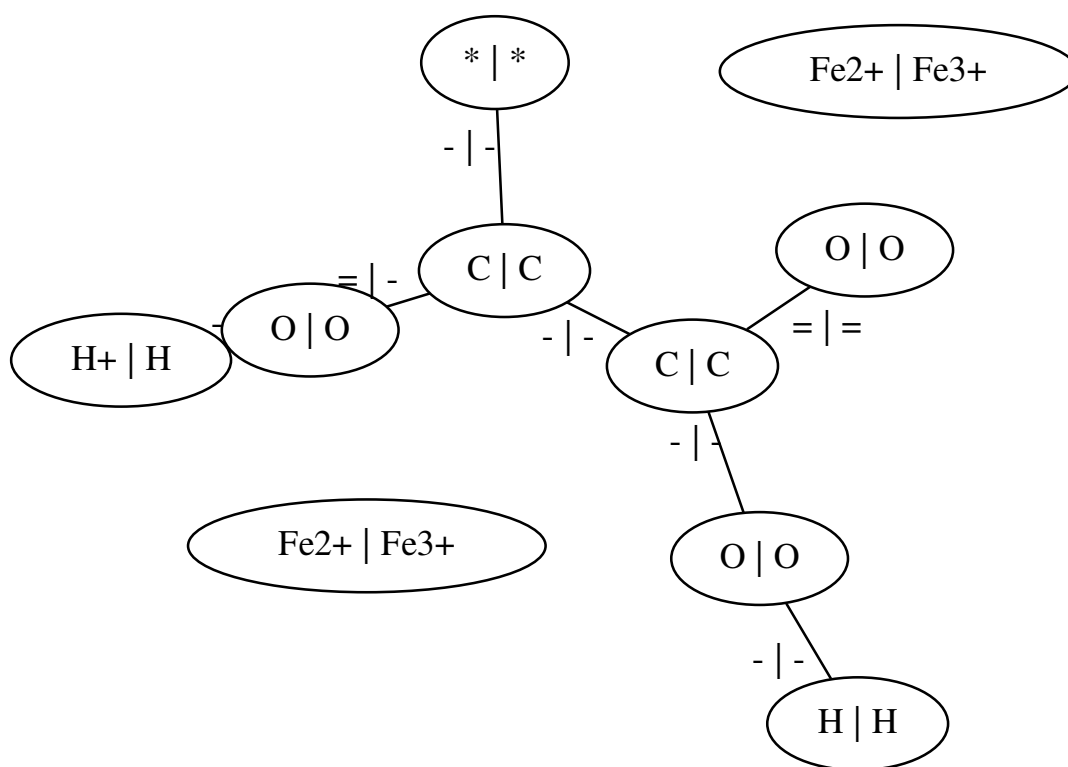
0.0.211 Fe2 \rightarrow Fe3 Alpha Keto Reduction of a Carboxylic Acid (Fe2+ to Fe3+)



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

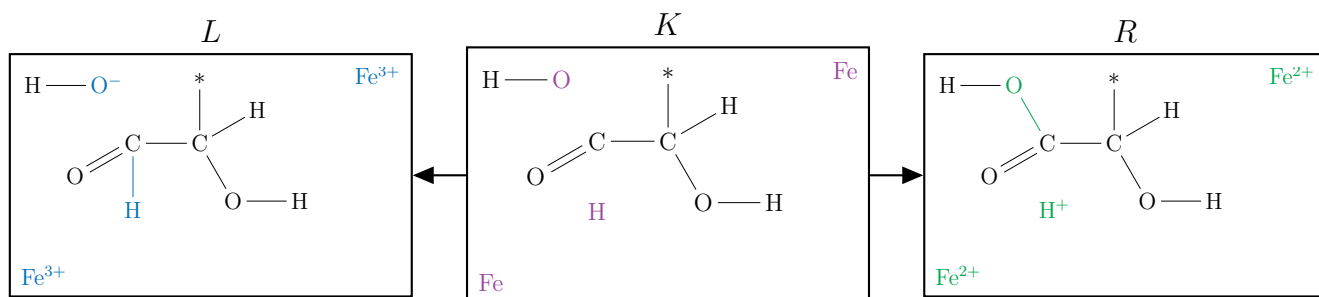


Files: out/1051_r_213_11300100_{L, K, R}

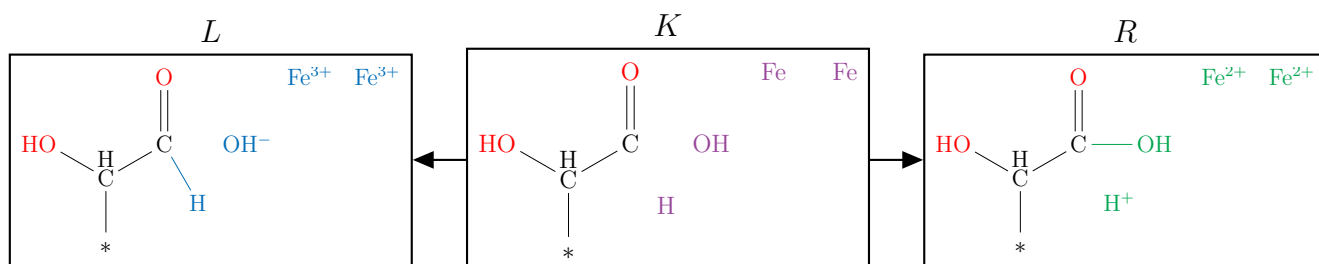


File: out/1052_r_213_combined

0.0.212 Fe3 \longrightarrow Fe2 Aldehyde to acid

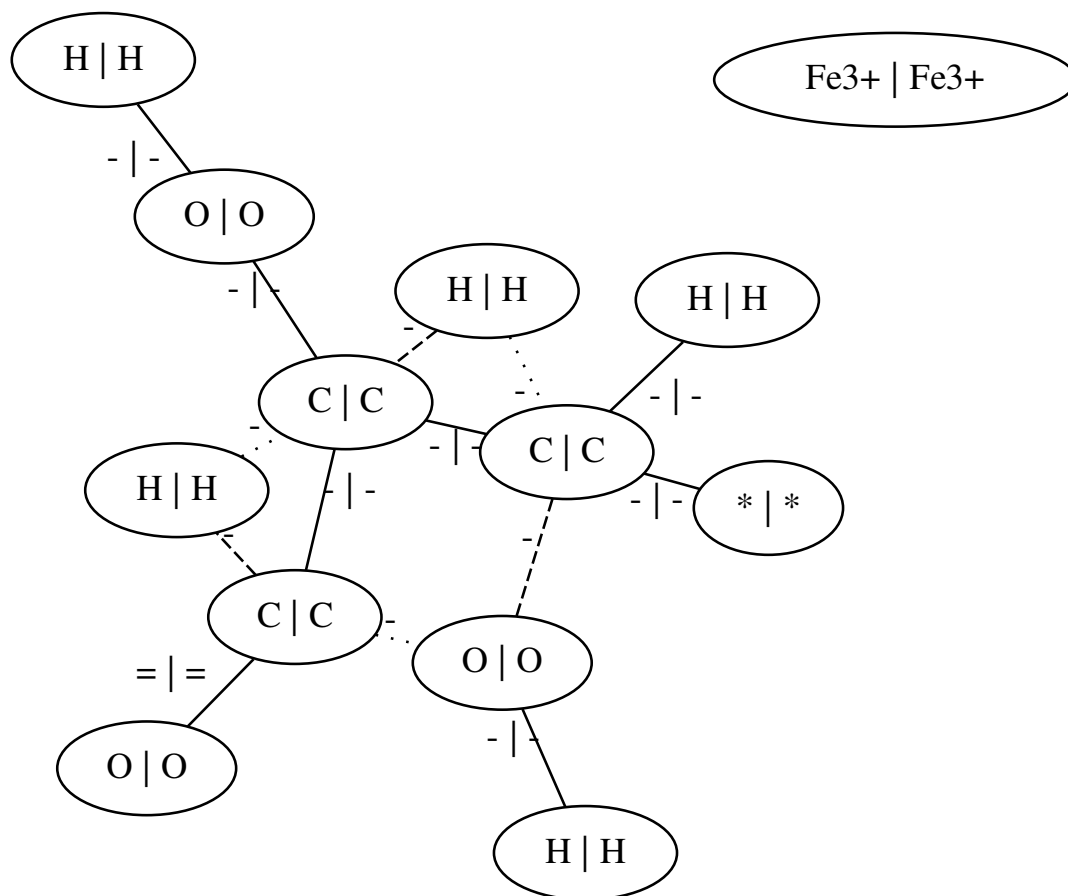
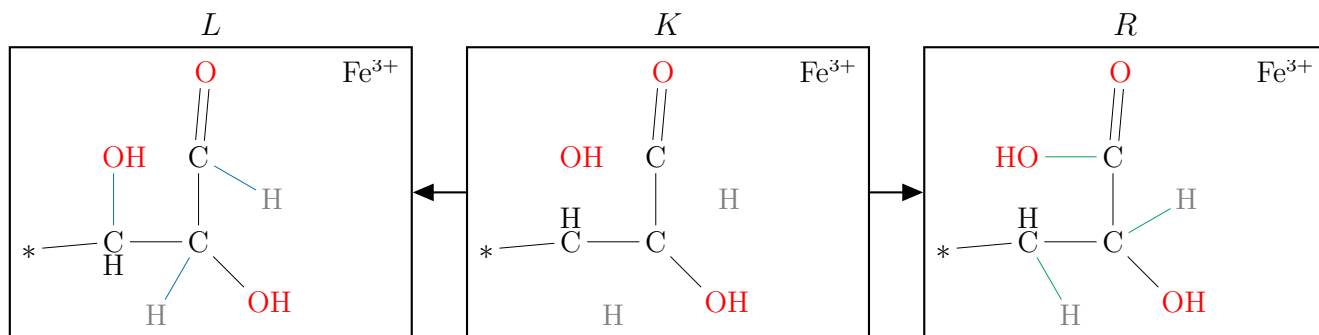


Files: out/1055_r_214_10300000_{L, K, R}



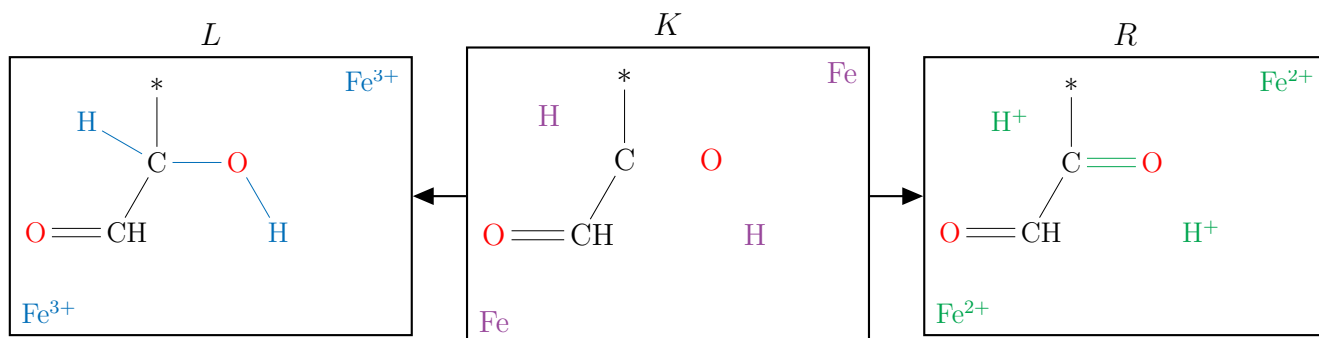
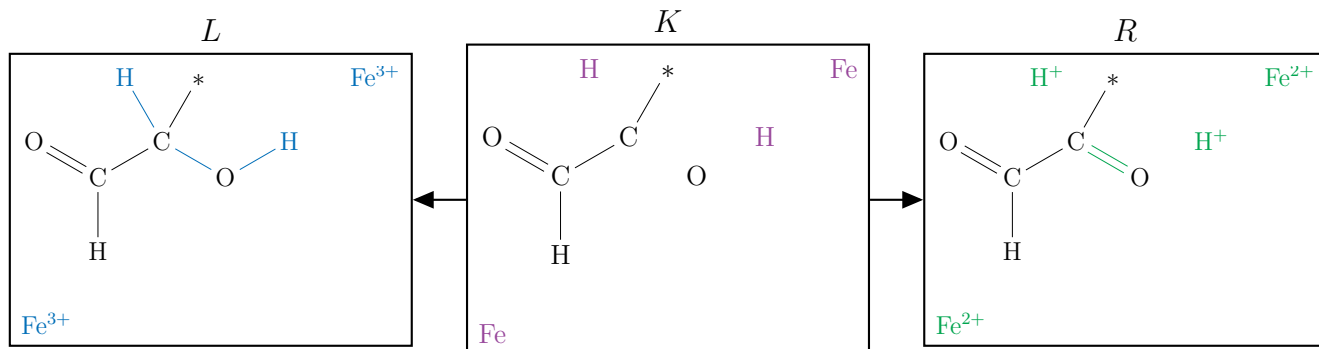
Files: out/1056_r_214_11300100_{L, K, R}

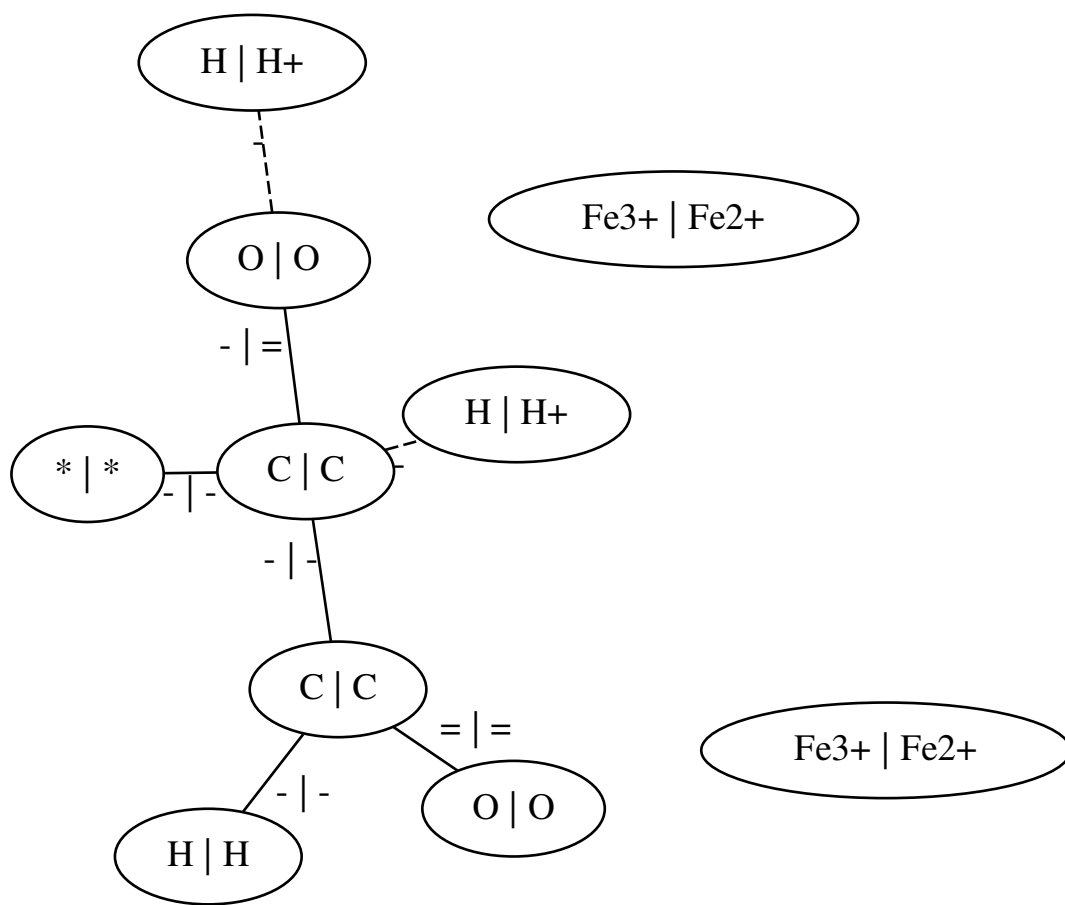
Files: out/1060_r_215_10300000_{L, K, R}



File: out/1062_r_215_combined

0.0.214 Fe3 \longrightarrow Fe2 Conversion of Alpha Hydroxy Group of an aldehyde to Alpha Keto group

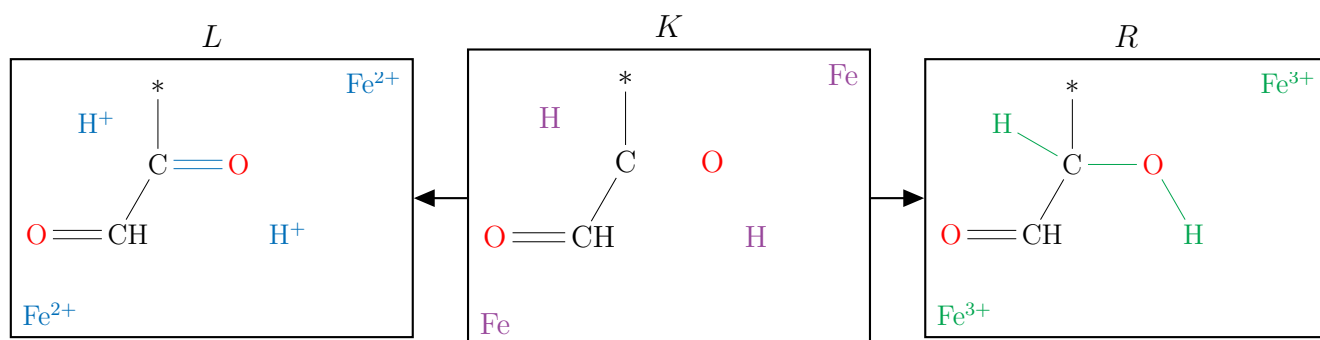
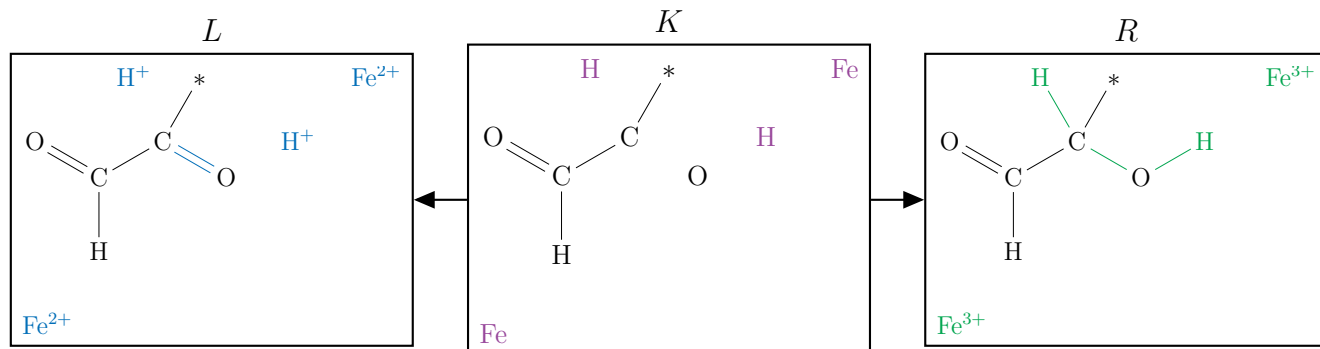


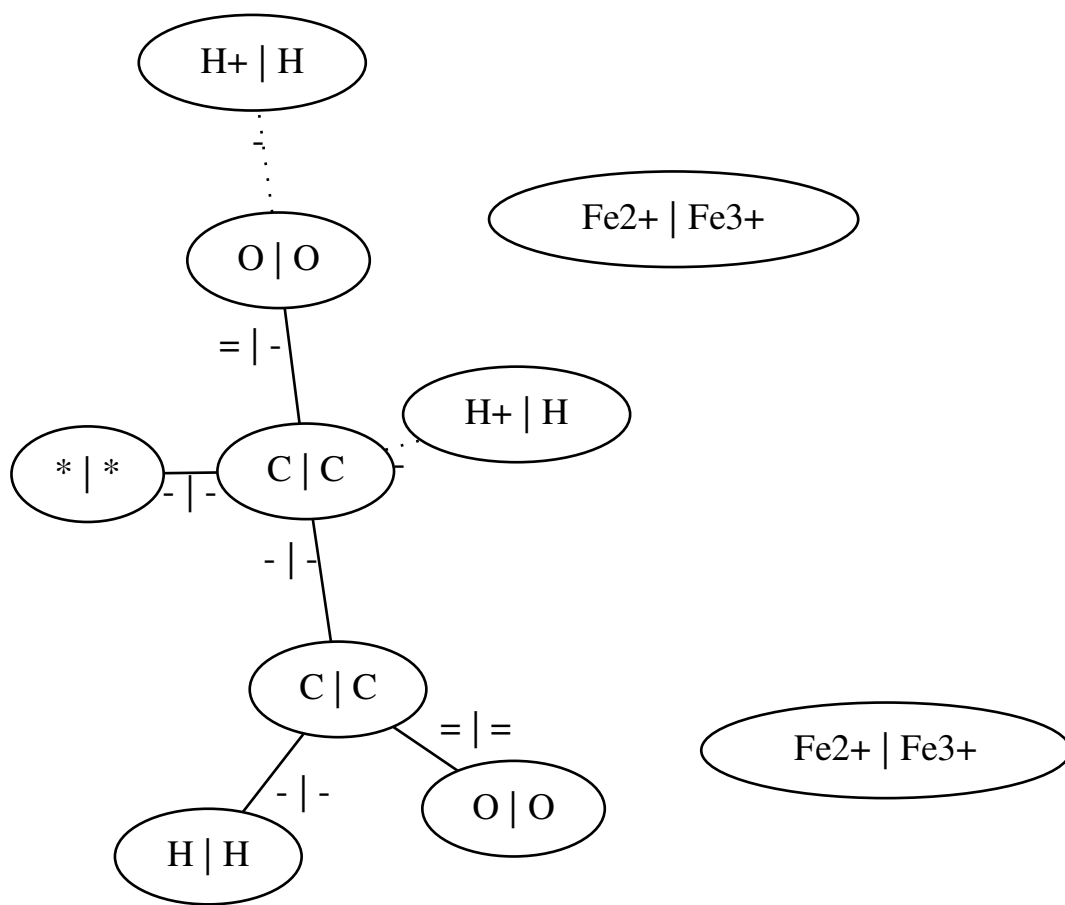


File: out/1067_r_216_combined

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

0.0.215 Fe2 \rightarrow Fe3 Conversion of Alpha Hydroxy Group of an aldehyde to Alpha Keto group, inverse





File: out/1072_r_217_combined

$$|\{e \in \text{outEdges}(6) \mid$$

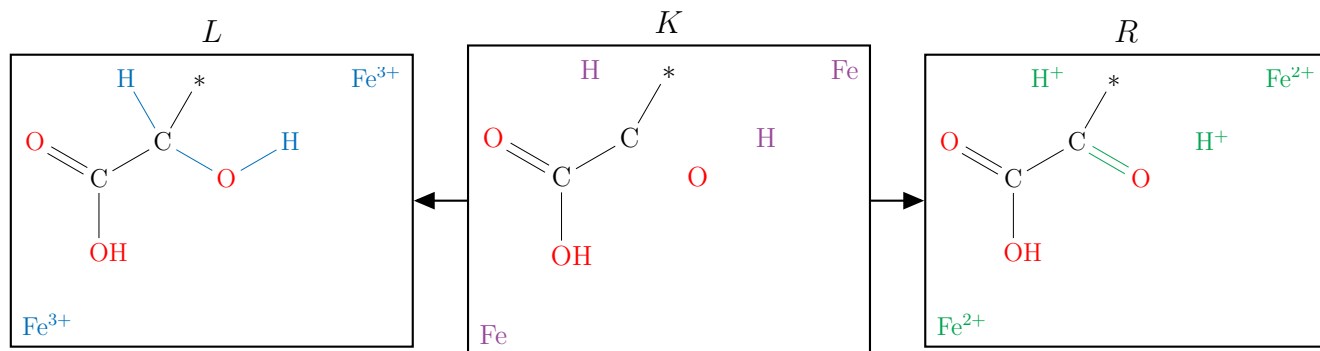
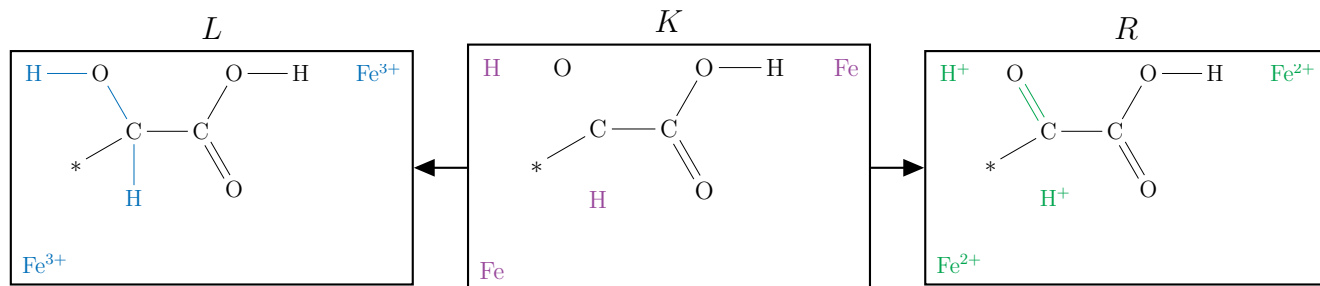
$$\text{label}(\text{target}(e)) \in \{\text{'O'}, \text{'N'}, \text{'S'}\}$$

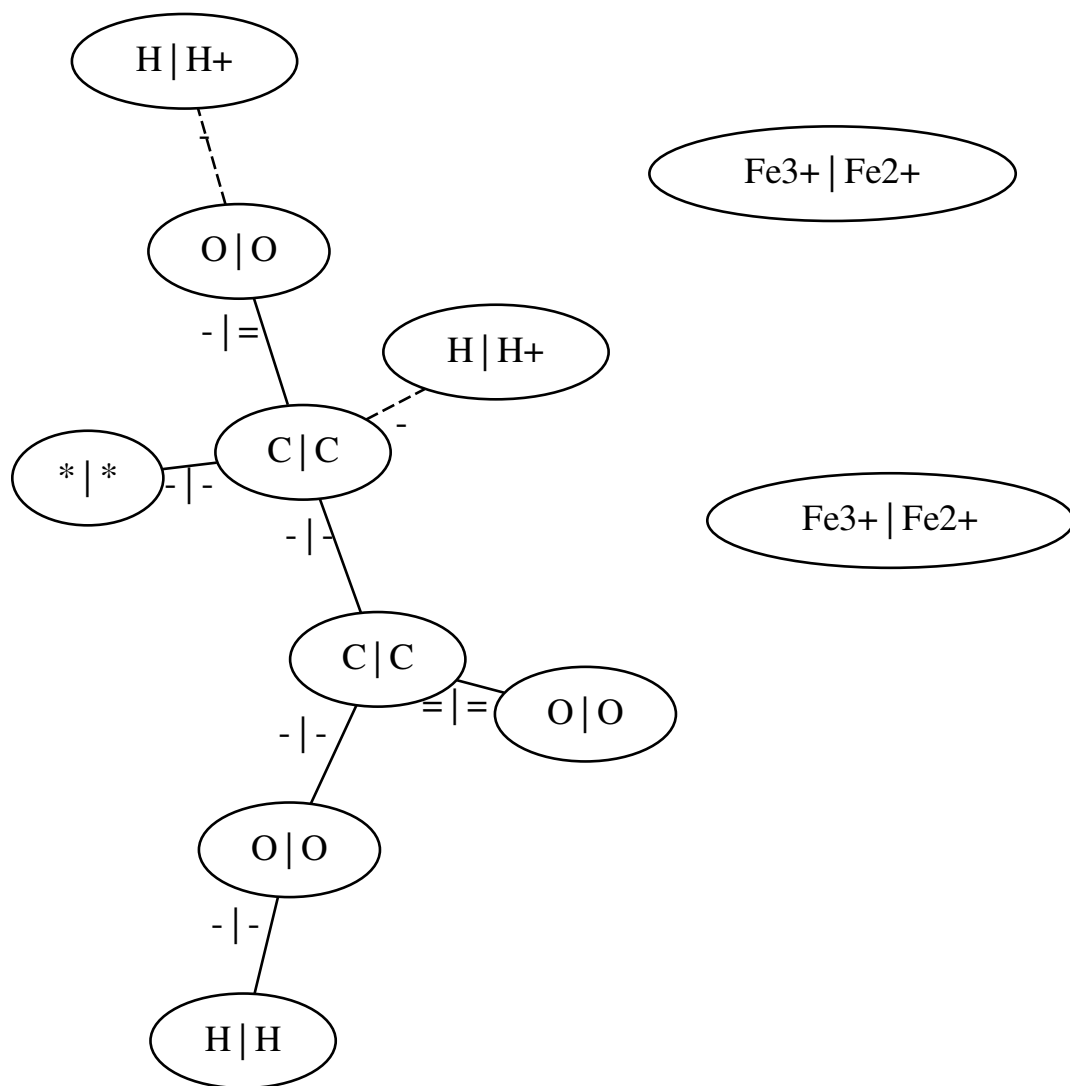
$$\wedge$$

$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

0.0.216 Fe3 \longrightarrow Fe2 Conversion of Alpha Hydro Group of an ACID to Alpha Keto group

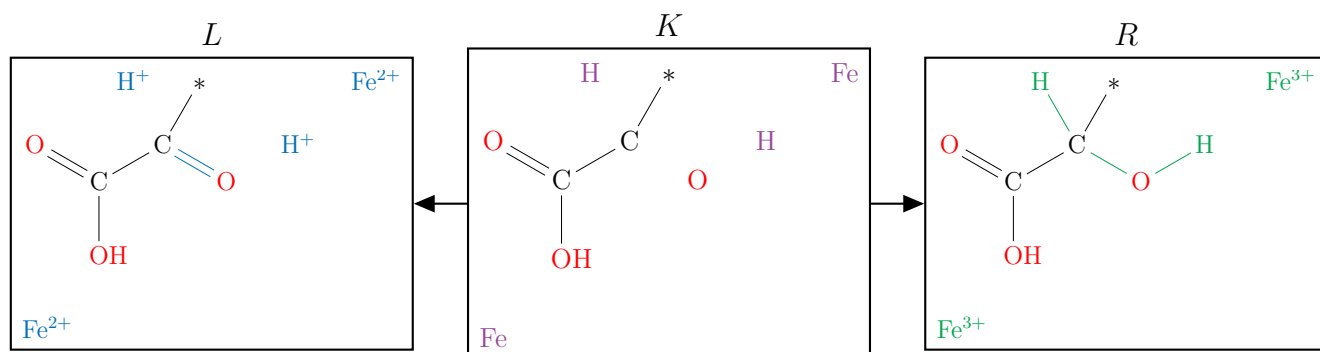
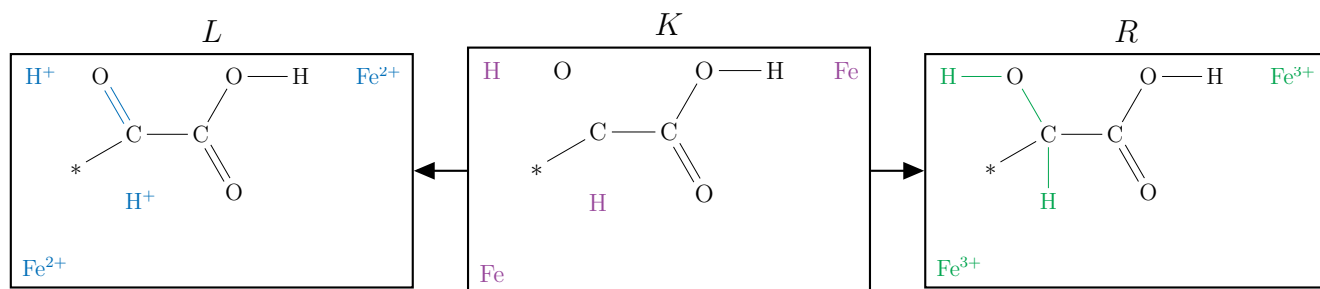


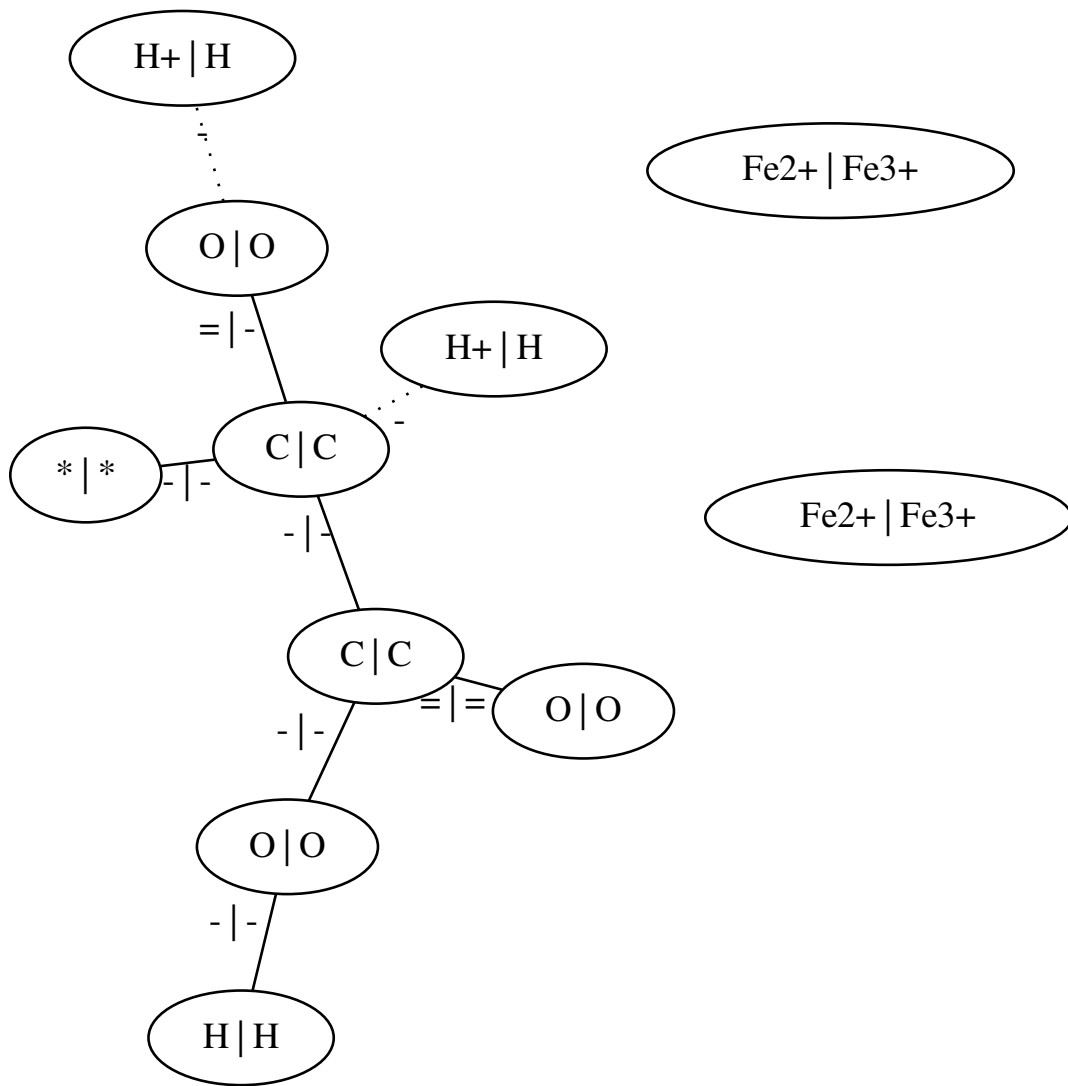


File: out/1077_r_218_combined

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

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





File: out/1082_r_219_combined

```

|{e ∈ outEdges(6) |
  label(target(e)) ∈ {'O', 'N', 'S'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

Chapter 1

Formose Reaction