

Summary

October 6, 2021

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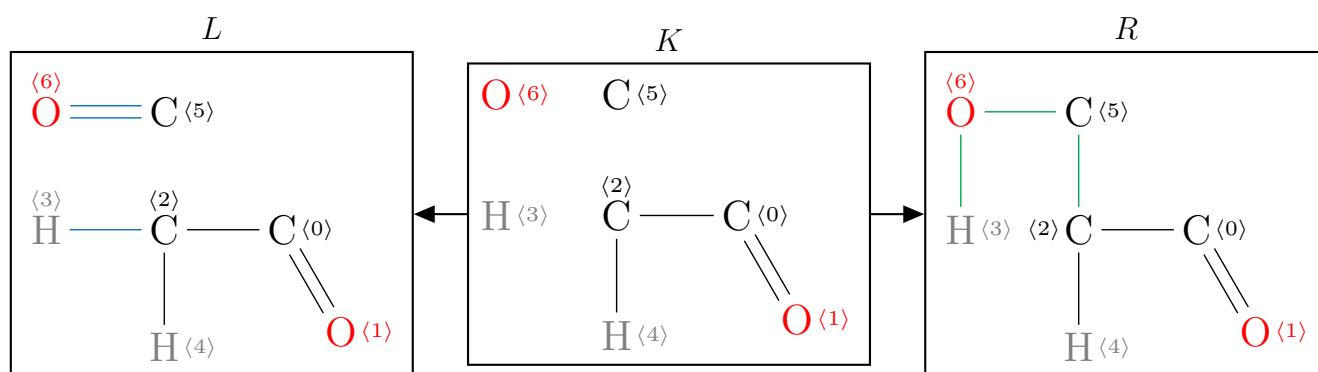
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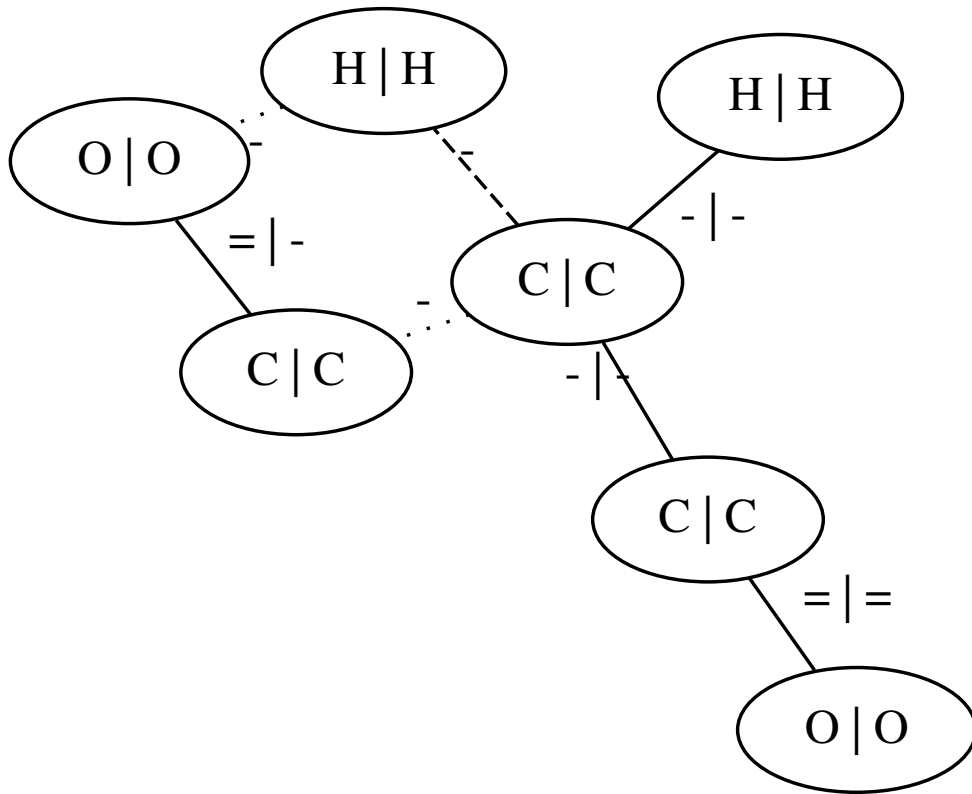
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Chapter 1

Alkaline Glucose Degradation

1.0.1 Aldol Condensation





File: out/002_r_0_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

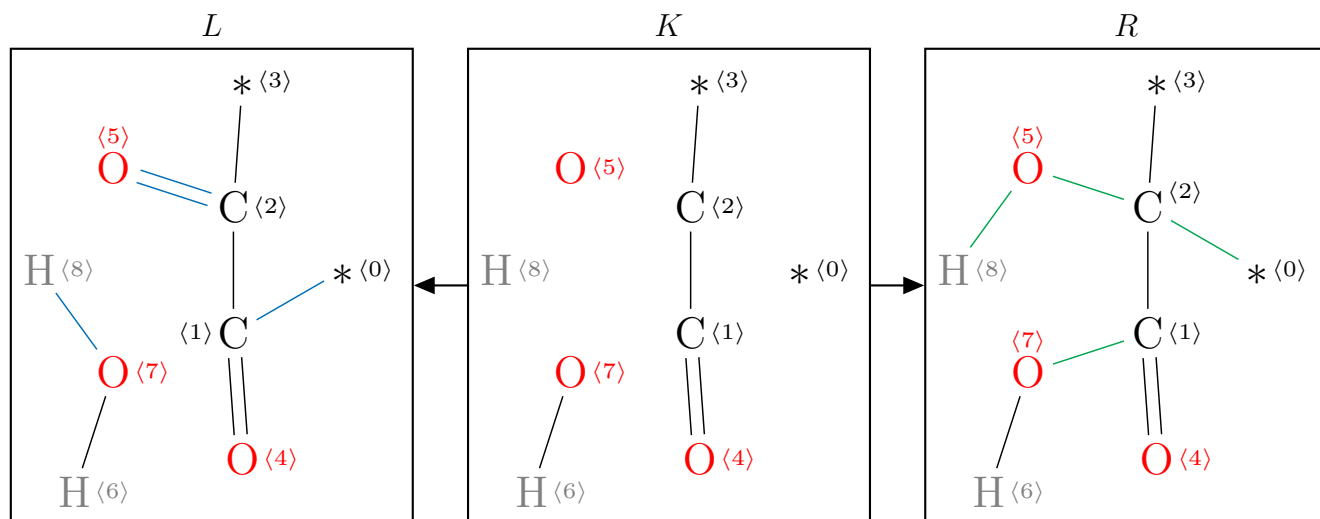
$$\text{label}(\text{target}(e)) \in \{\text{'O'}, \text{'N'}, \text{'S'}\}$$

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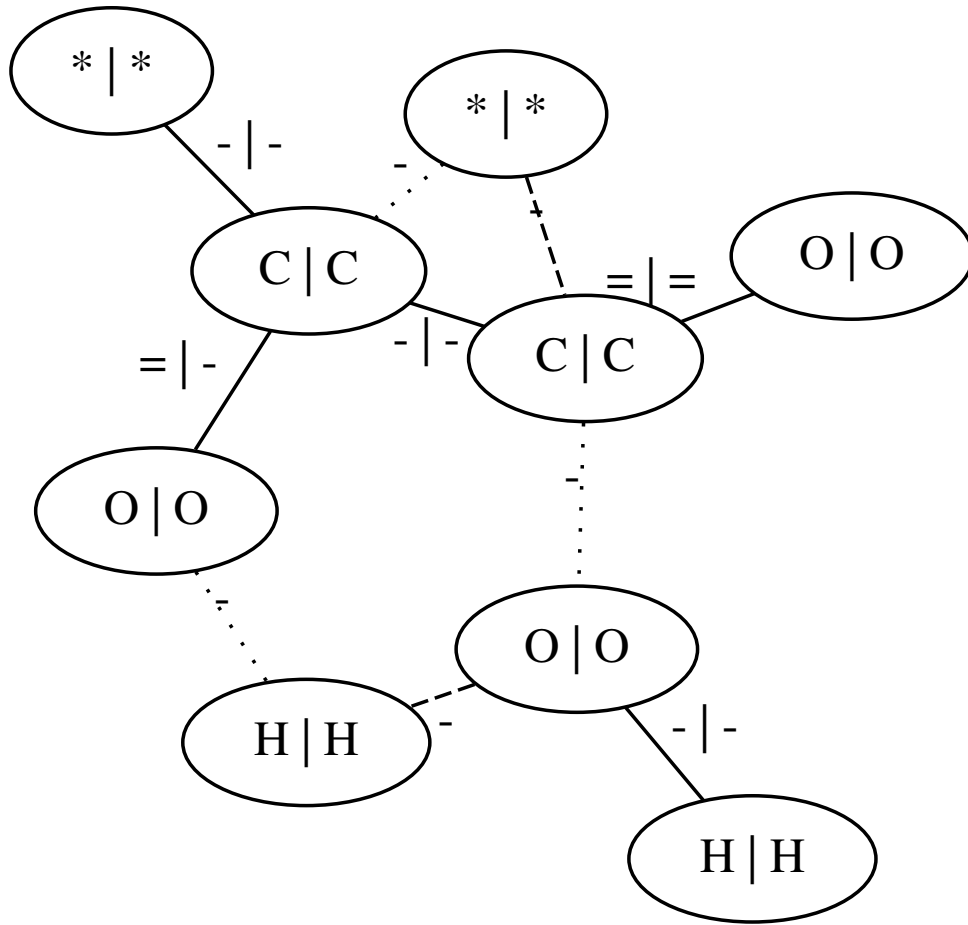
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

1.0.2 Benzilic Acid Rearrangement



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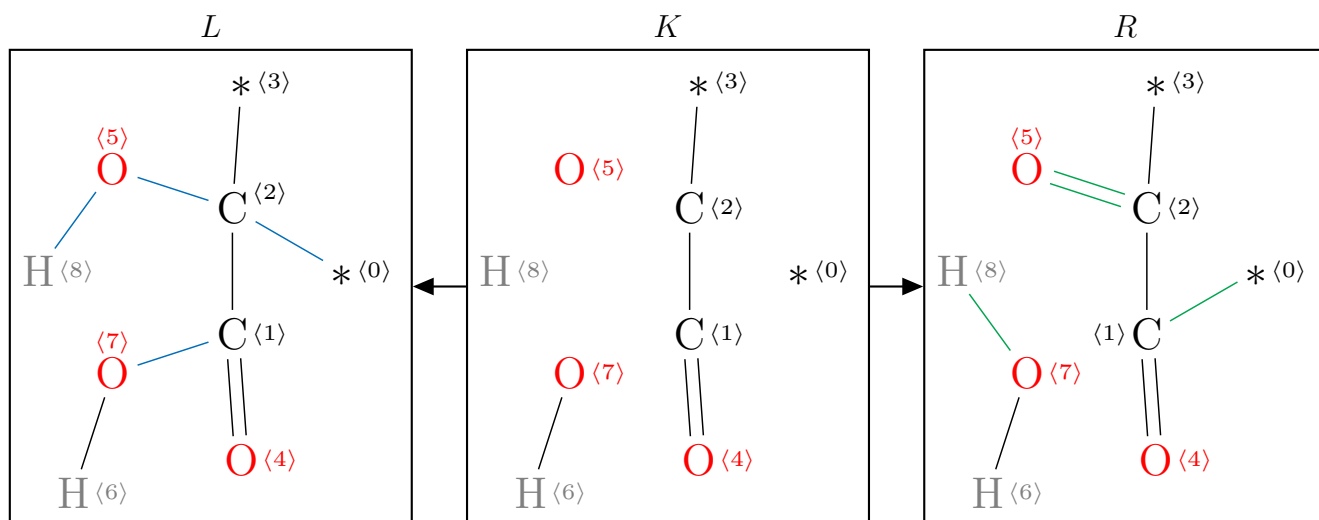
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|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'N', 'O'}
  ∧
  label(e) ∈ {'-'}
}| = 0

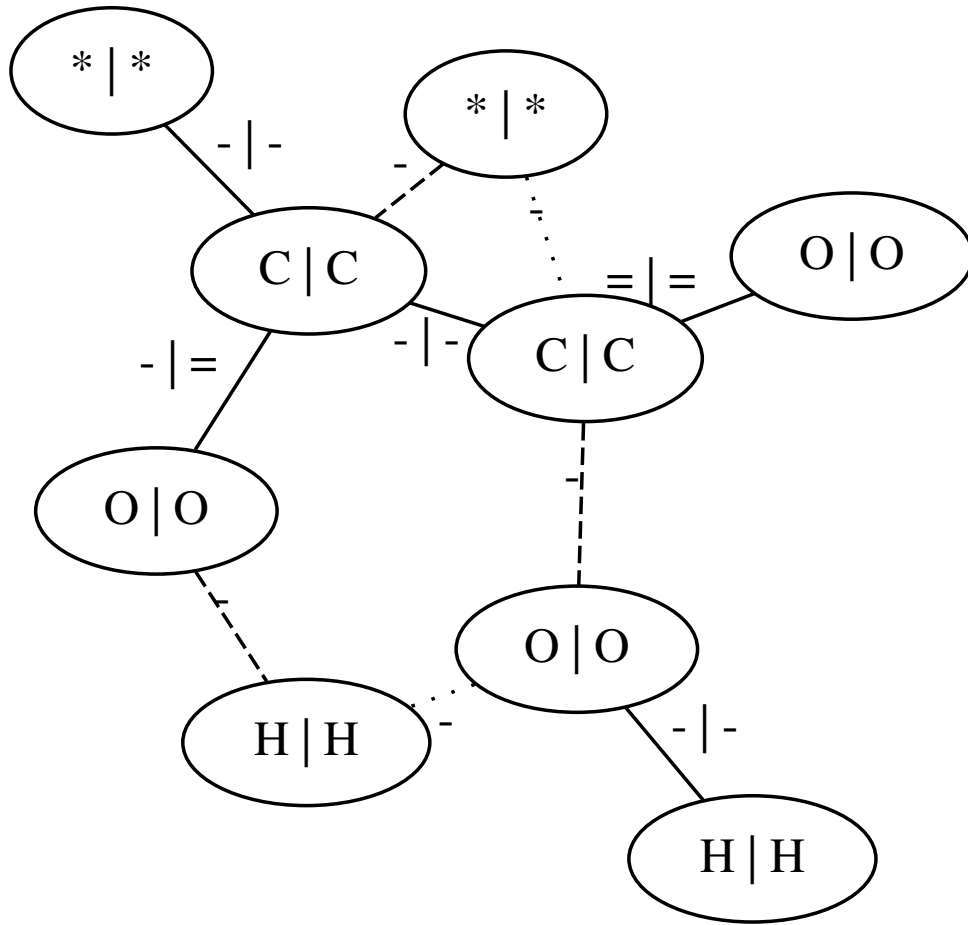
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$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
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& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid = 0
\end{aligned}$$

1.0.3 Benzilic Acid Rearrangement (inverse)



Files: out/009_r_2_10300110_{L, K, R}



File: out/010_r_2_combined

```

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

```

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

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

$$\wedge$$

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

$$\}| = 0$$

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

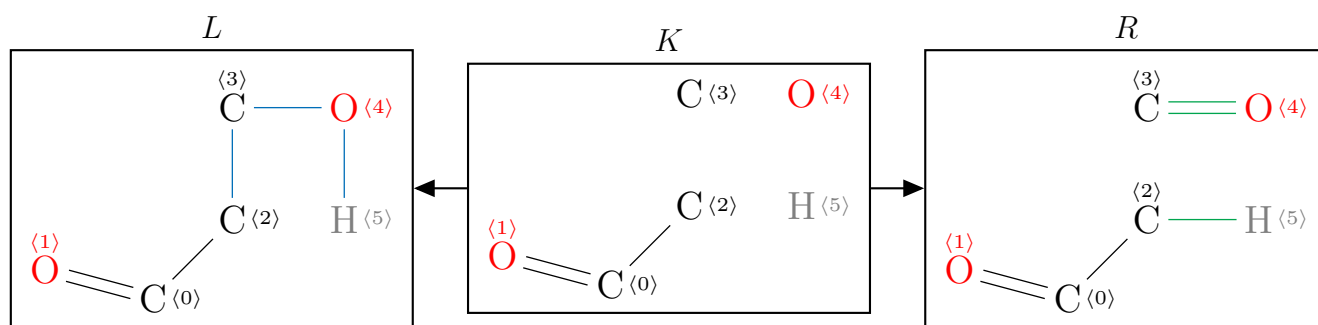
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

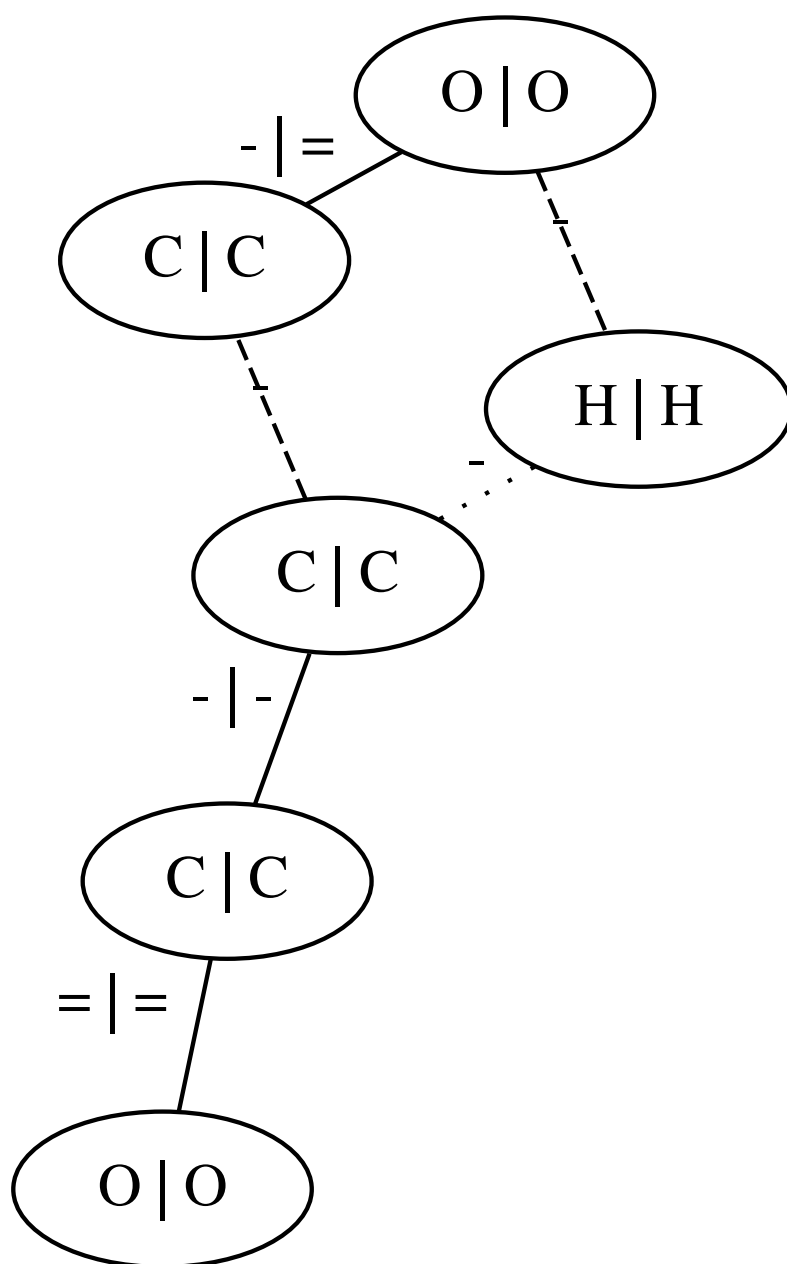
$$\text{label}(e) \in \{\text{'='}\}$$

$$\}| = 0$$

1.0.4 Retro Aldol



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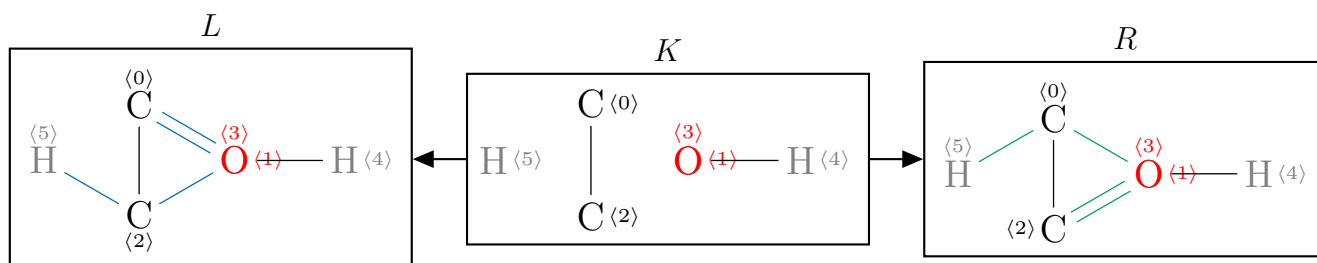


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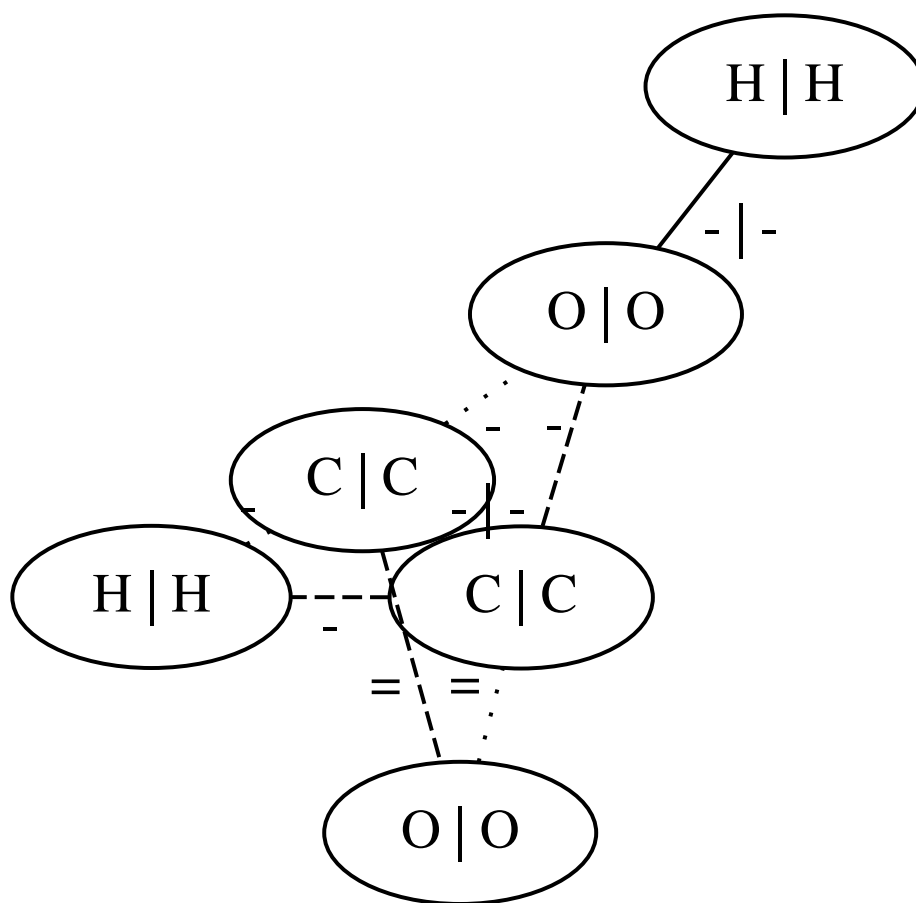
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& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.5 Keto-enol migration twice



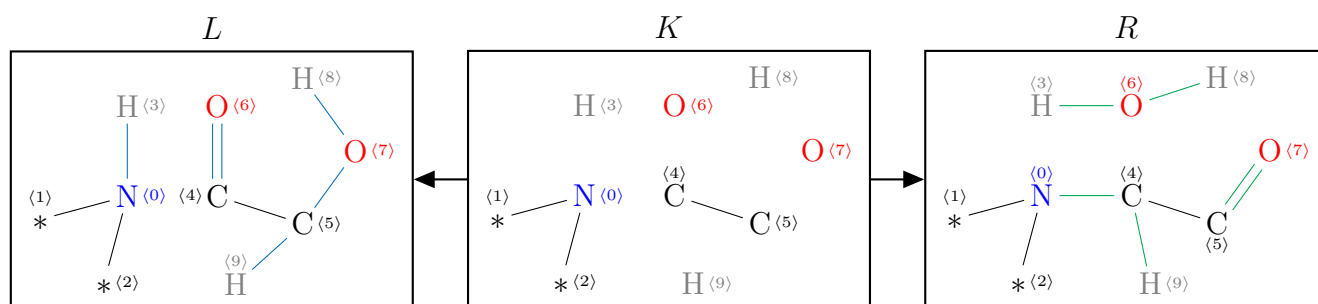
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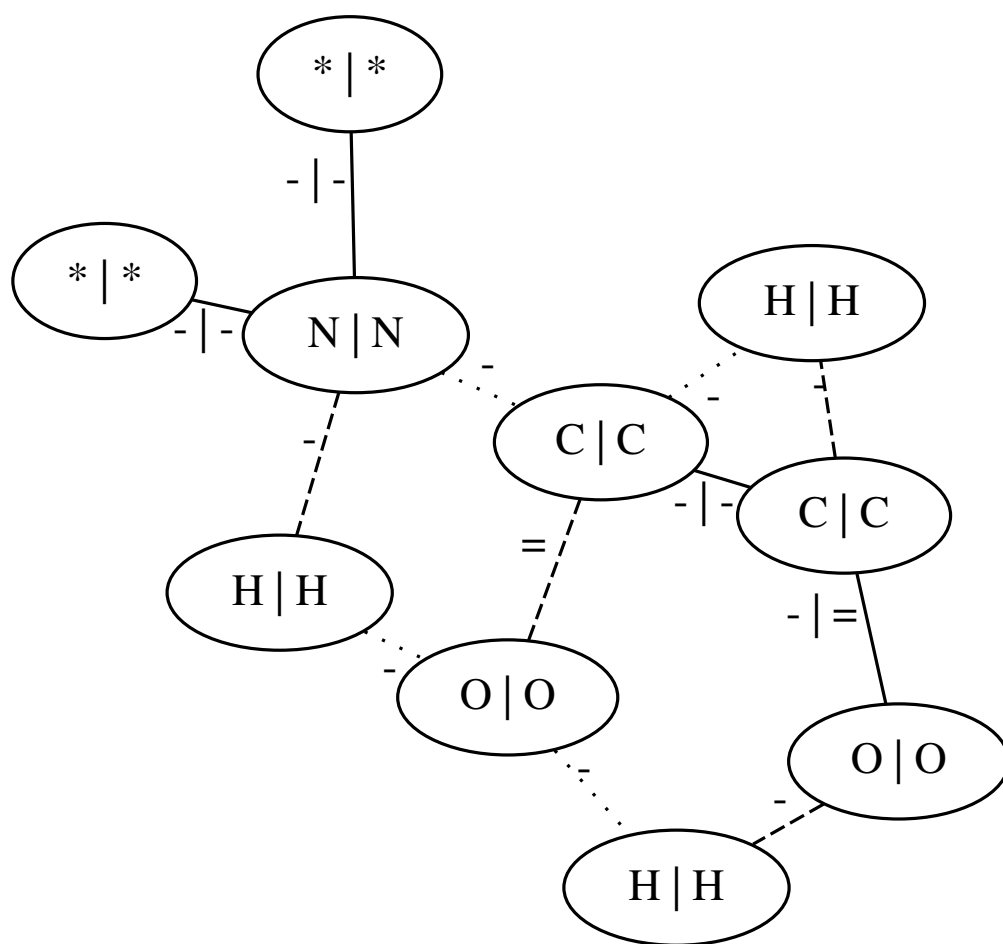
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 \end{aligned}$$

1.0.6 Amadori/Heyns Rearrangement



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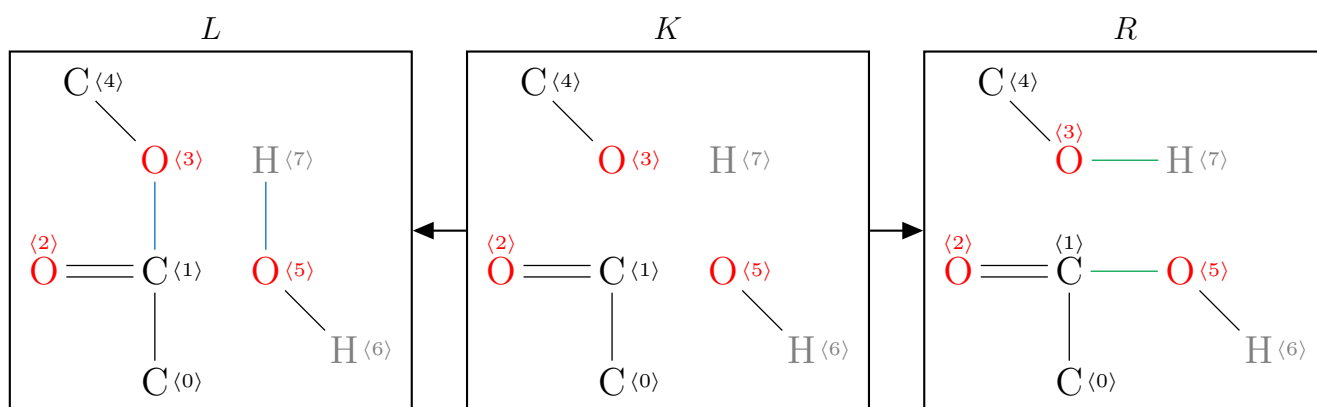
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$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
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& \quad \}| = 0
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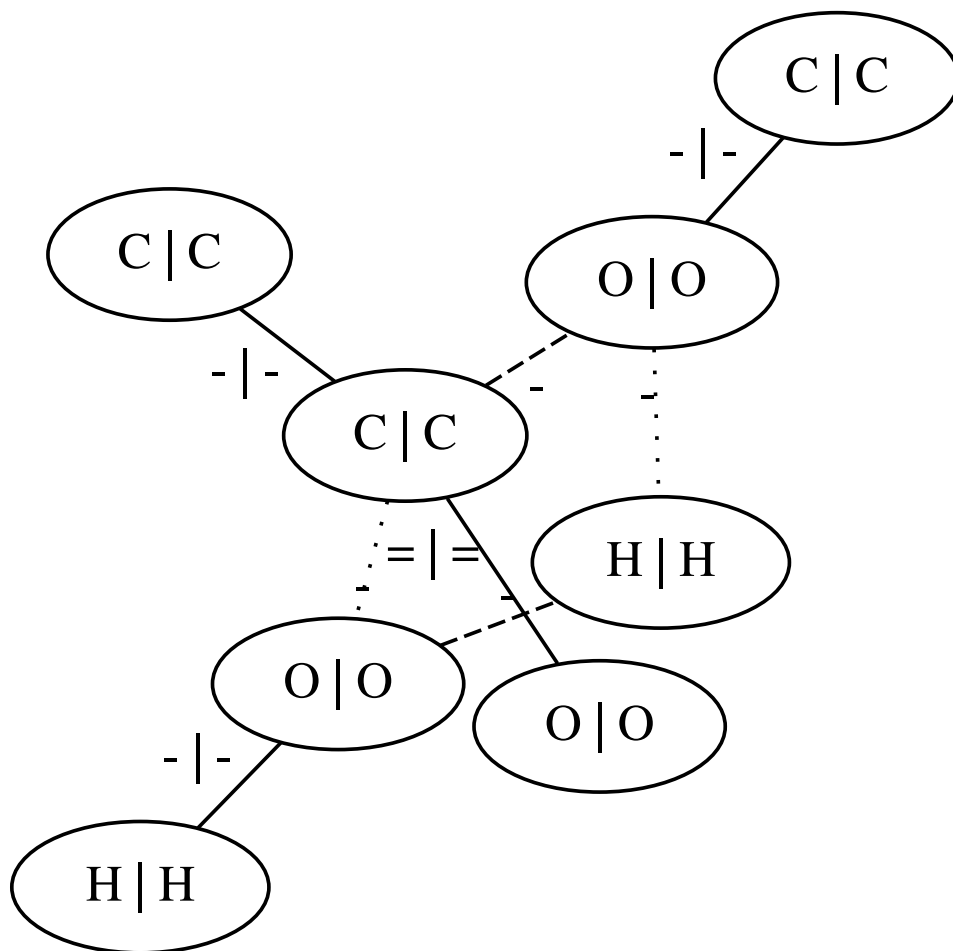
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& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.7 Ester Hydrolysis



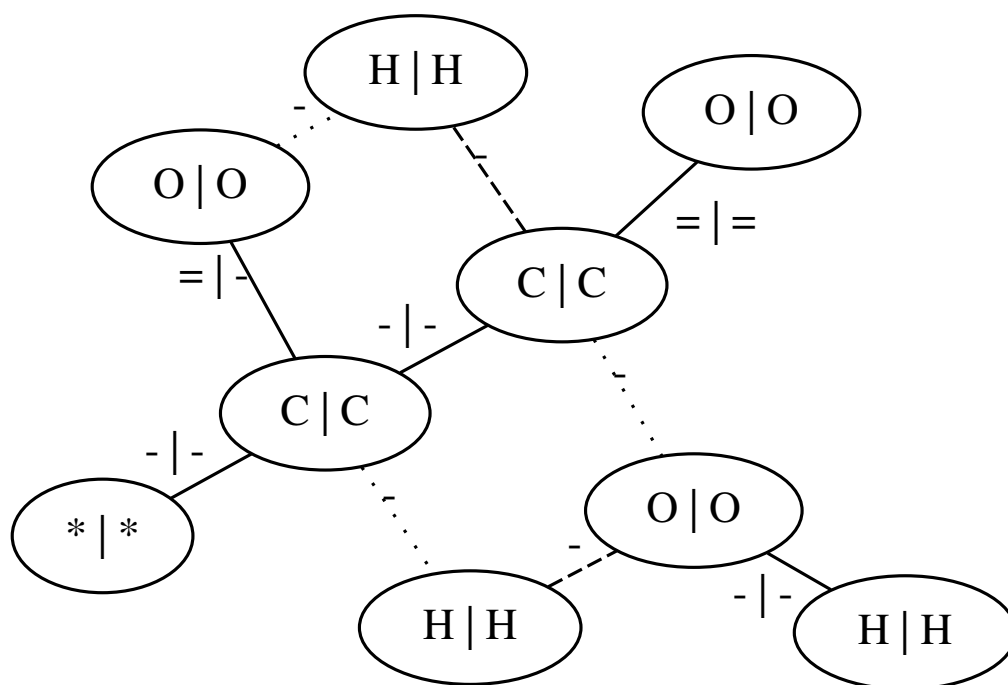
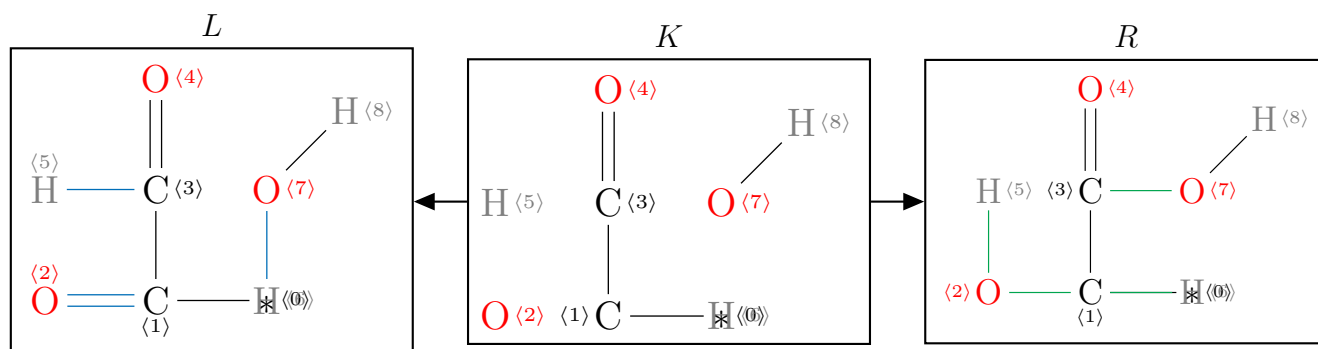
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File: out/026_r_6_combined

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1.0.8 Cannizzaro 1



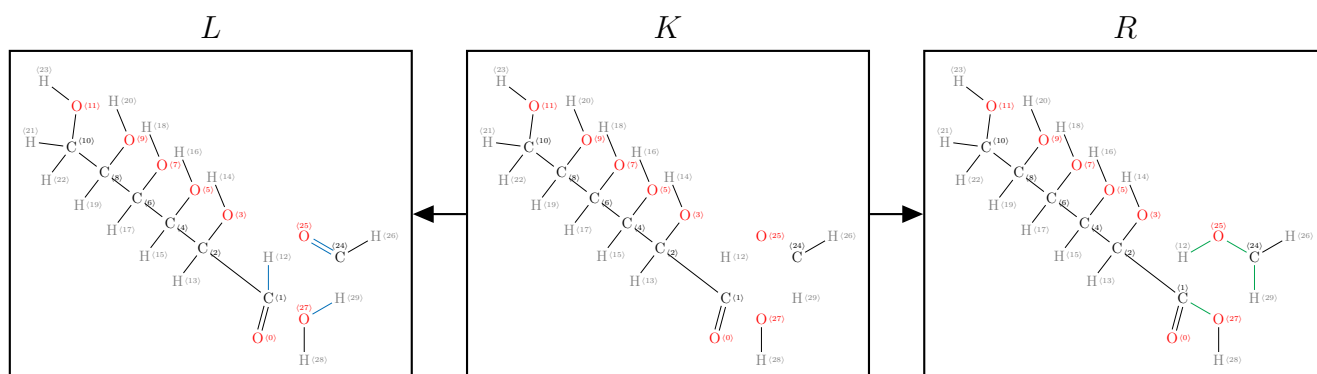
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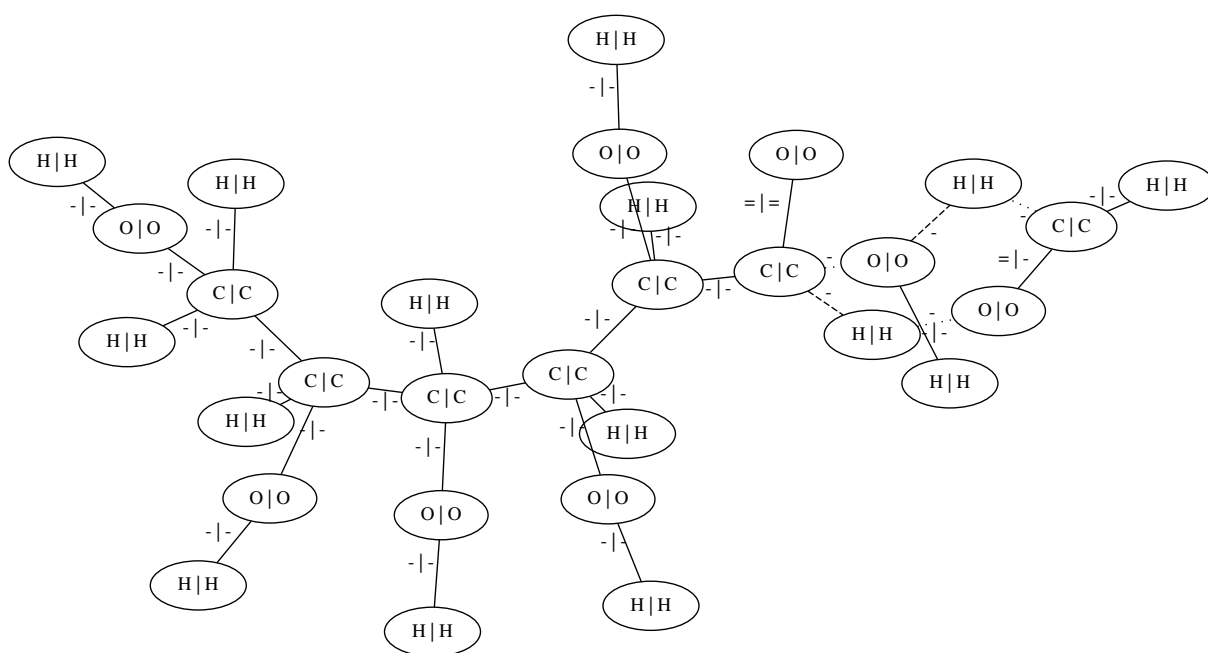
|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'-'}
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1.0.9 Cannizzaro 2, glucose (oxidation)



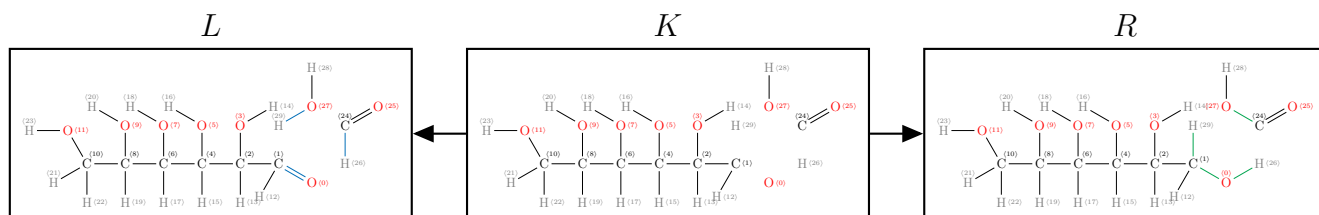
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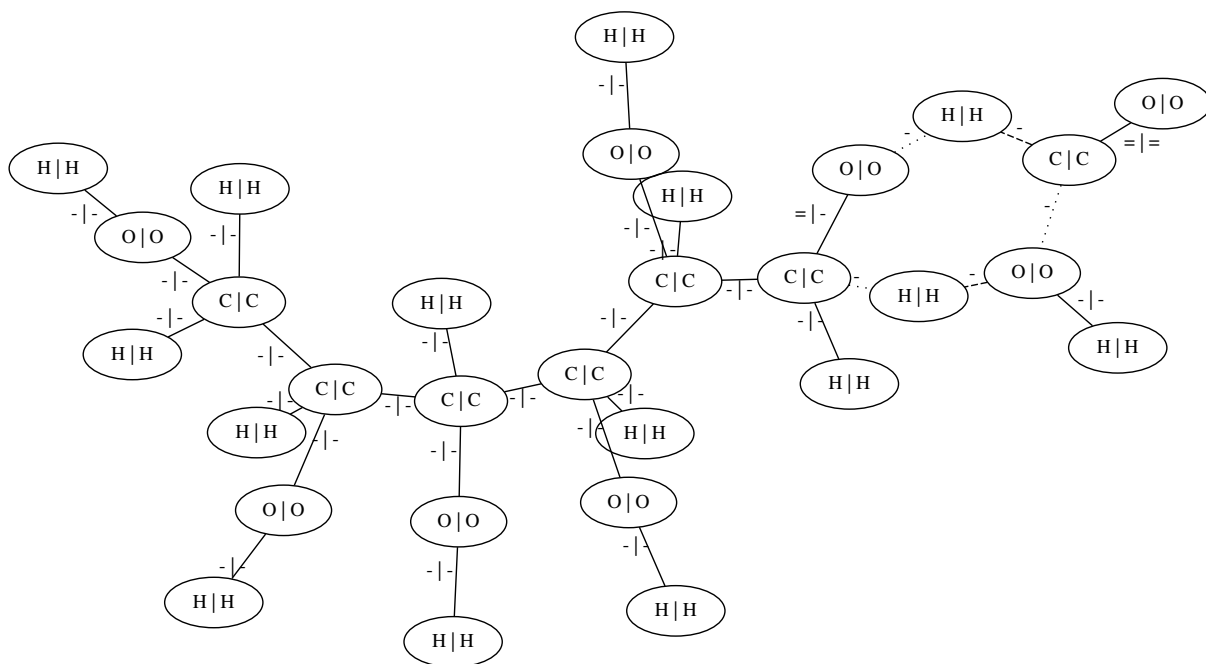
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 &\quad \} = 0
 \end{aligned}$$

1.0.10 Cannizzarro 2, glucose (reduction)



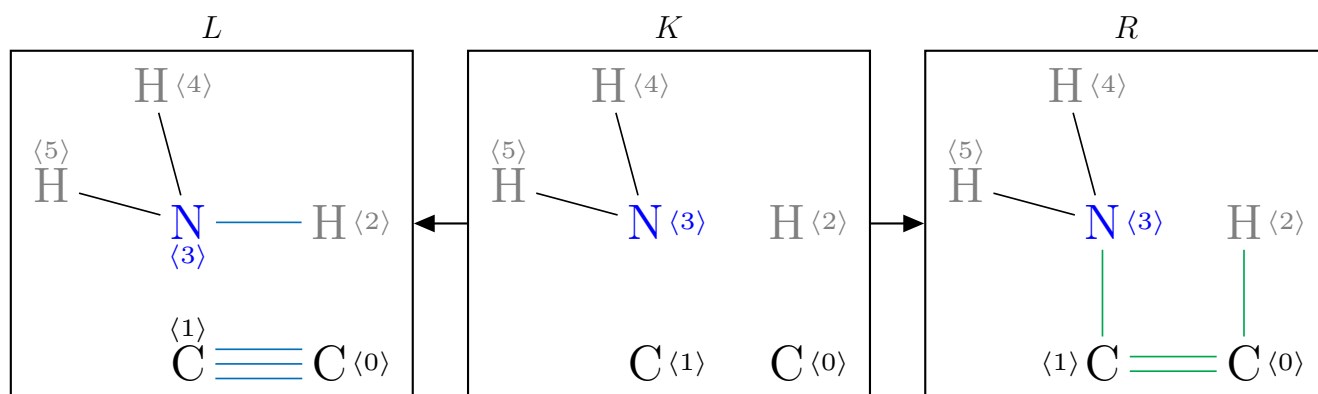
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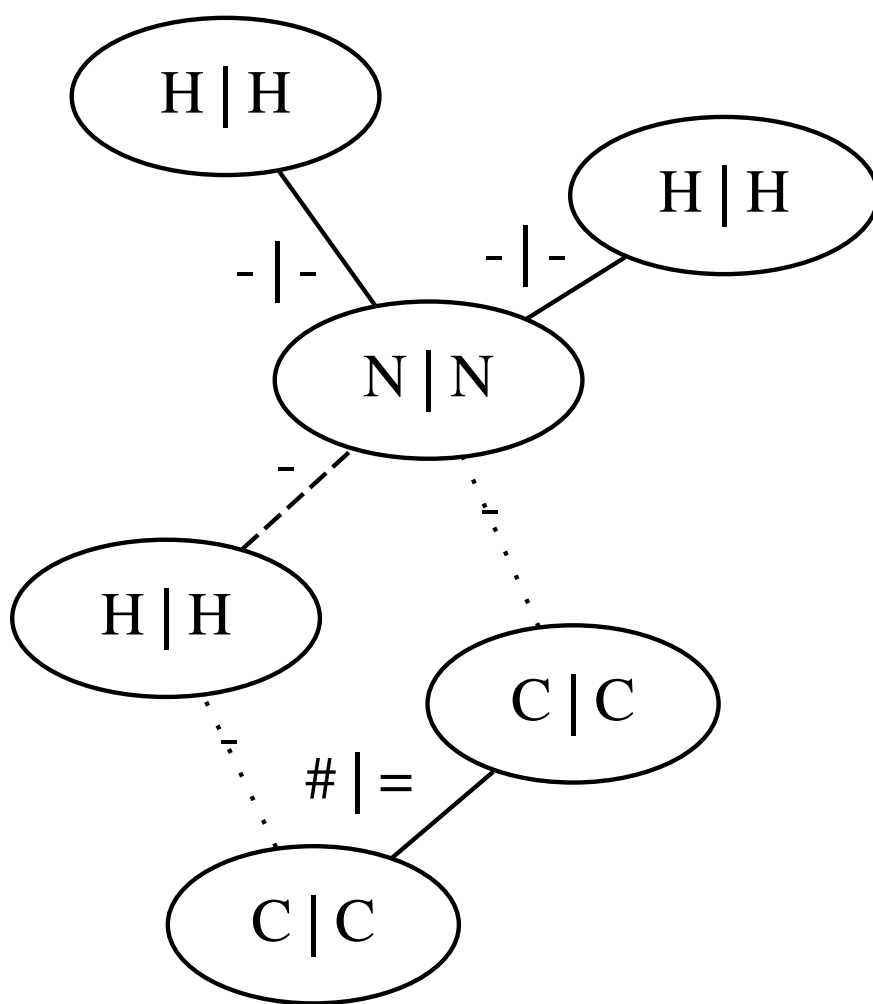
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 \end{aligned}$$

1.0.11 Alkyne Addition, N, HH

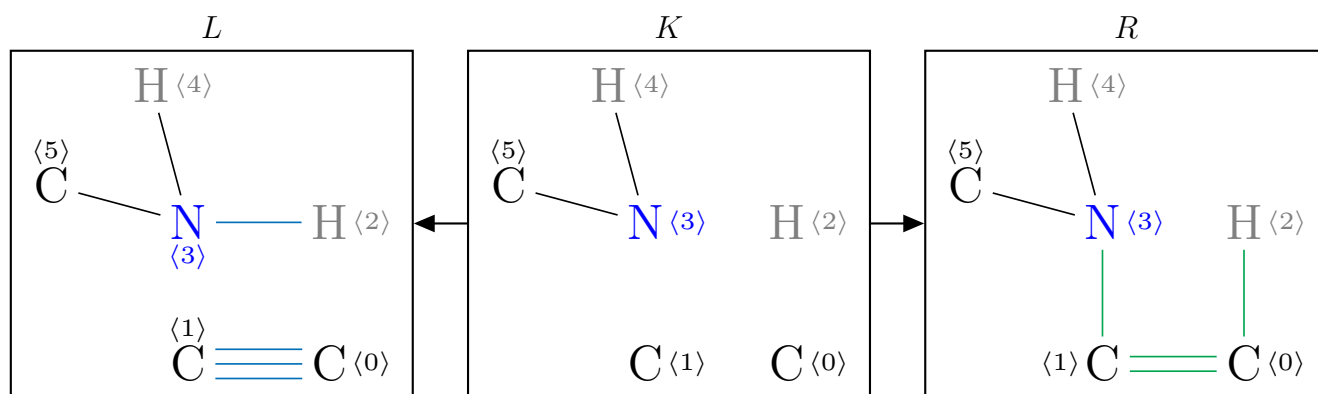


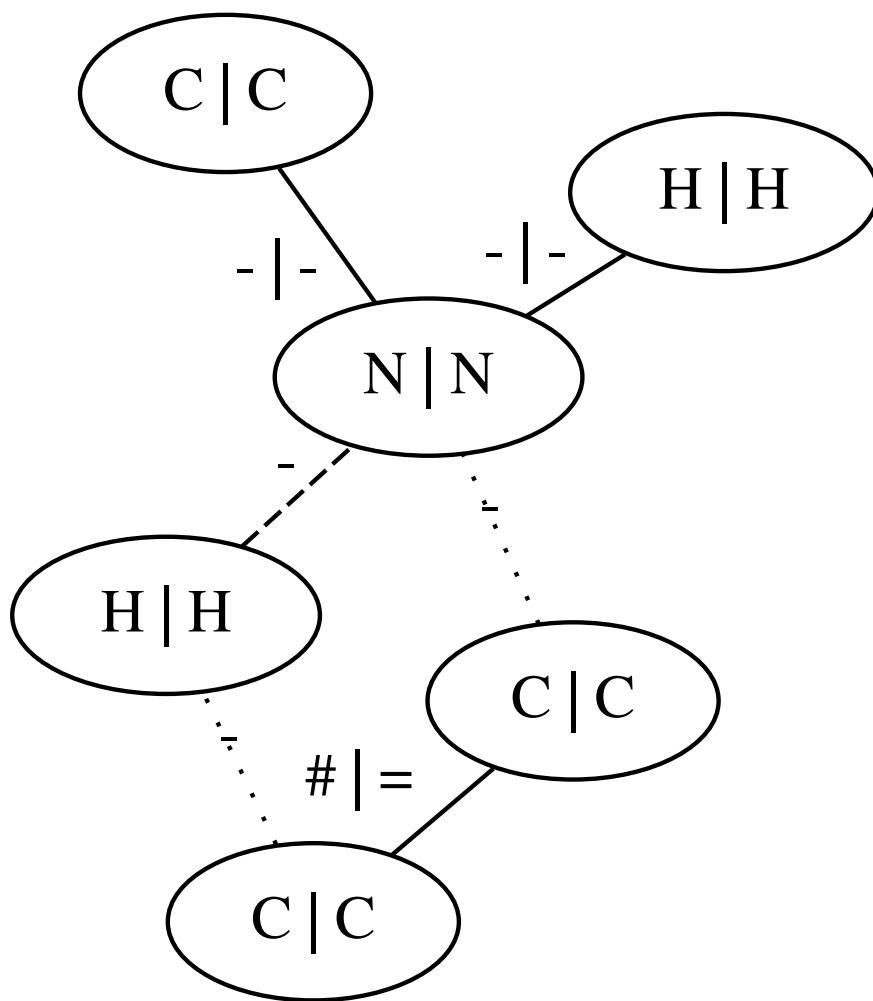
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1.0.12 Alkyne Addition, N, HC

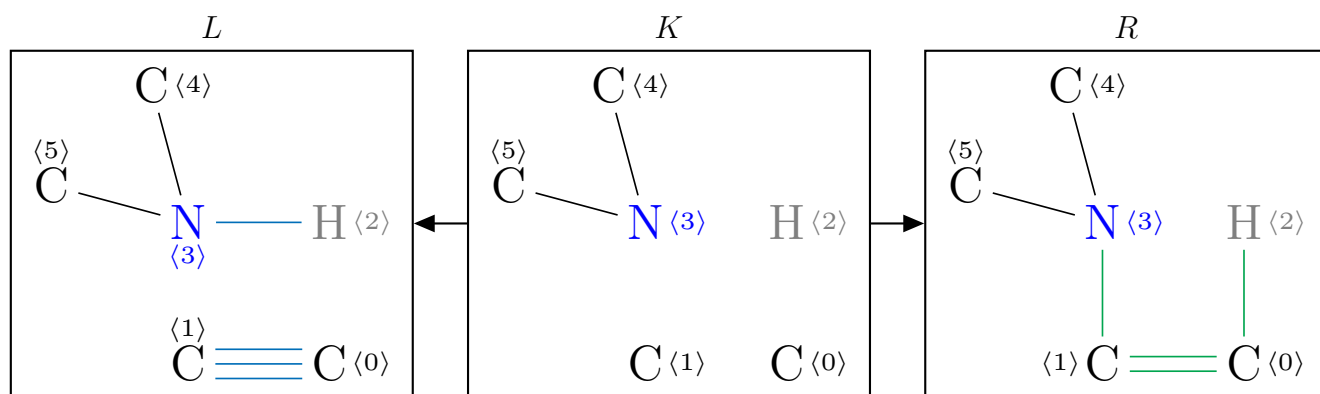




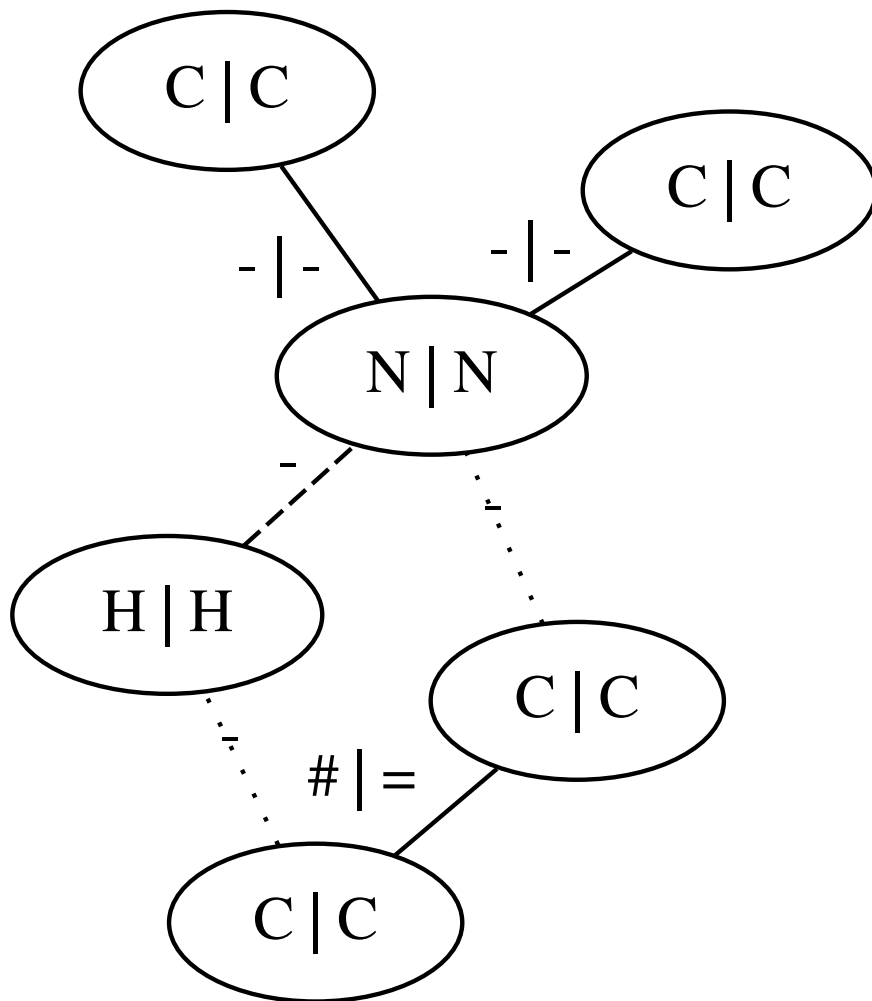
File: out/046_r_11_combined

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

1.0.13 Alkyne Addition, N, CC



Files: out/049_r_12_10300110_{L, K, R}

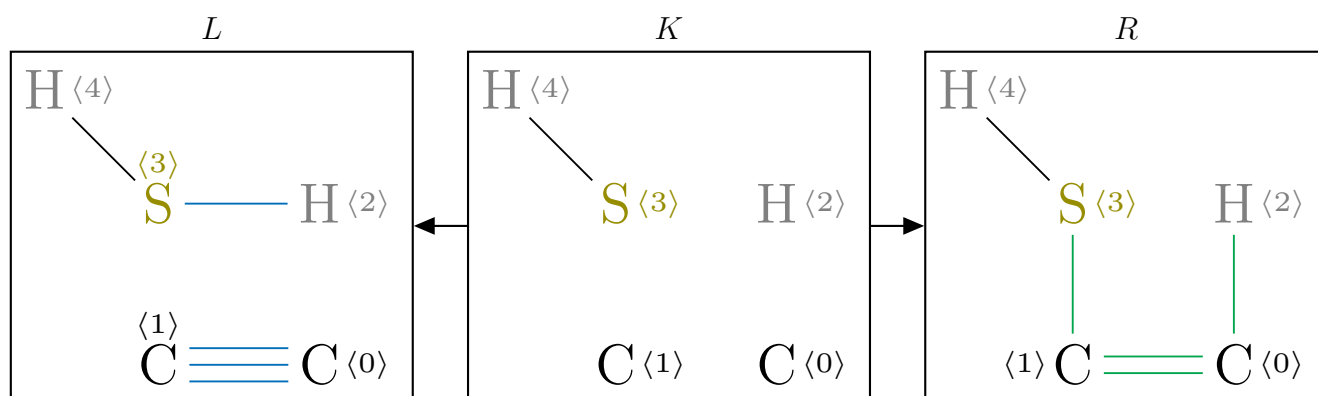


File: out/050_r_12_combined

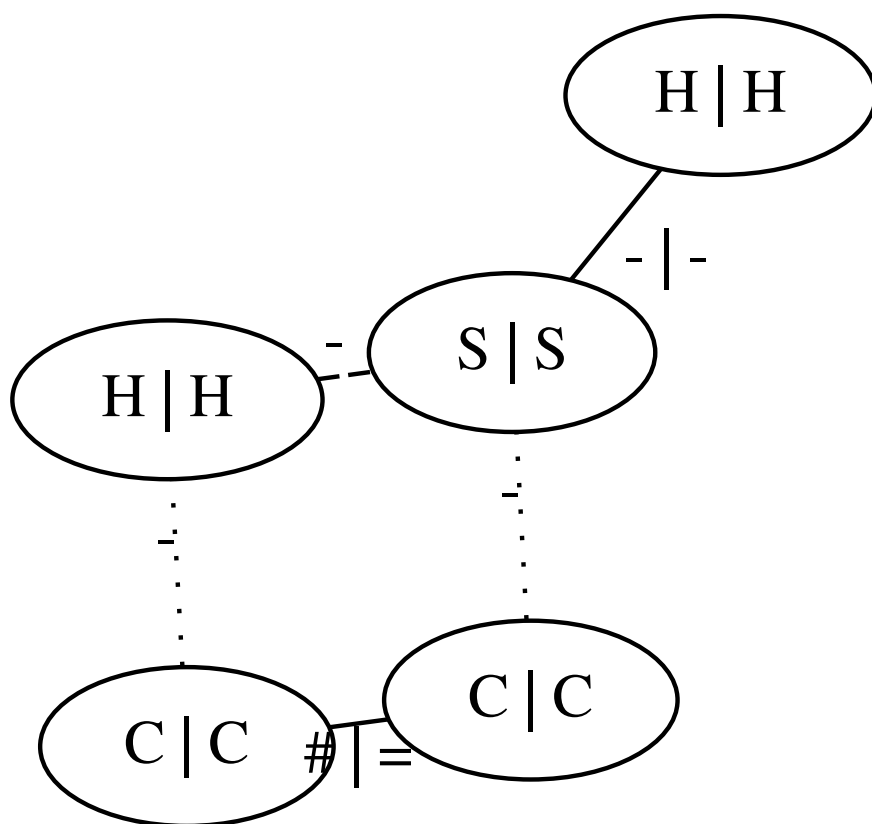
$$\begin{aligned}
 & |\{e \in \text{outEdges}(4) \mid \\
 & \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 & \quad \wedge \\
 & \quad \text{label}(e) \in \{'=\'} \\
 & \quad \}| = 0
 \end{aligned}$$

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

1.0.14 Alkyne Addition, S, H

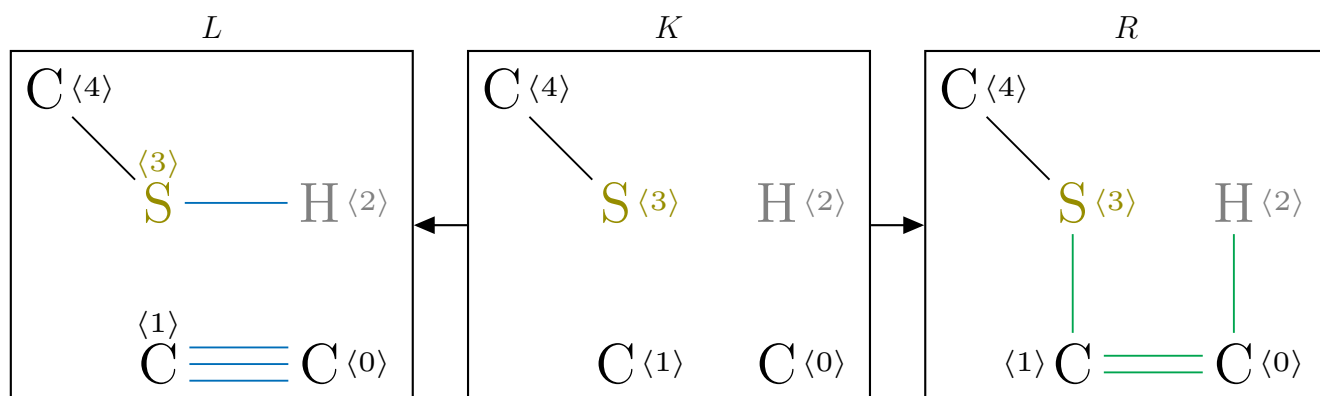


Files: out/053_r_13_10300110_{L, K, R}

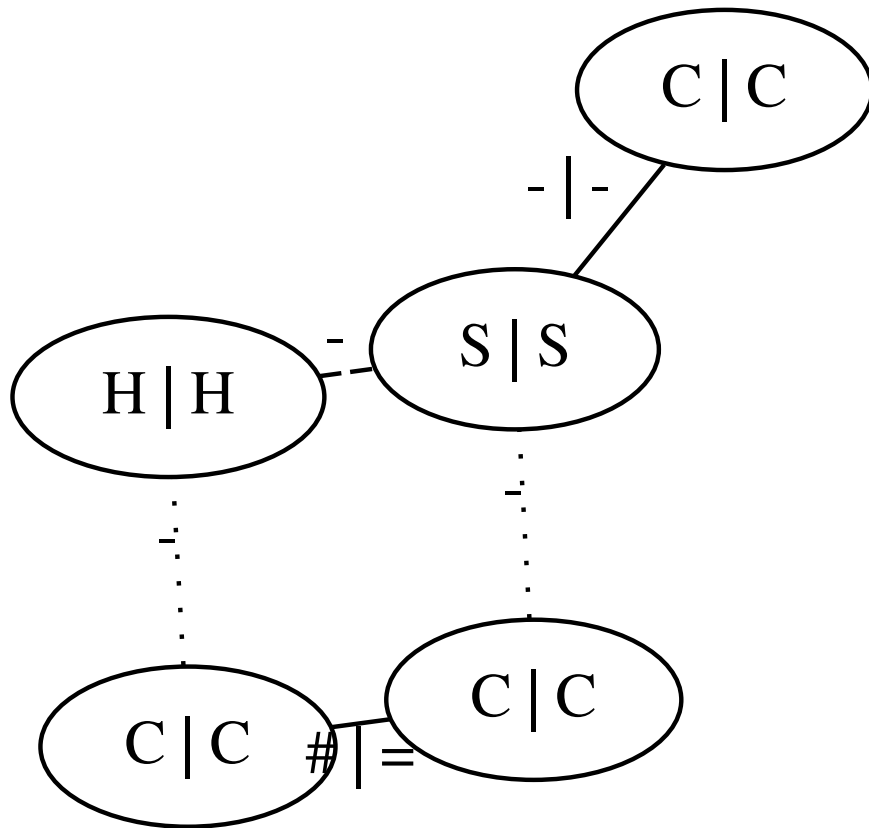


File: out/054_r_13_combined

1.0.15 Alkyne Addition, S, C



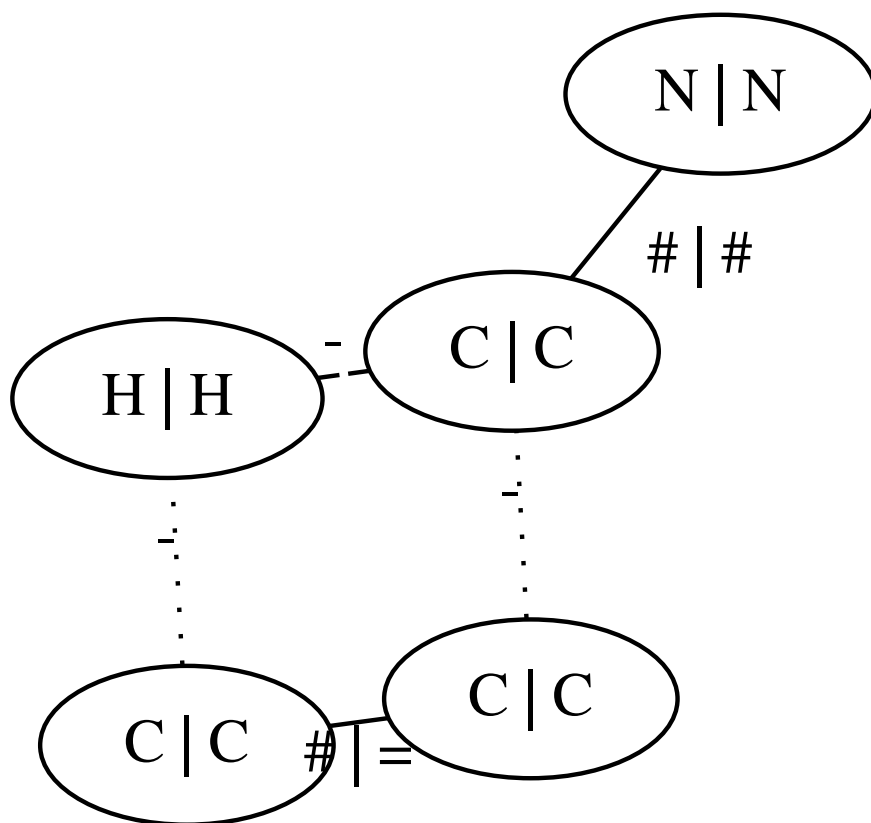
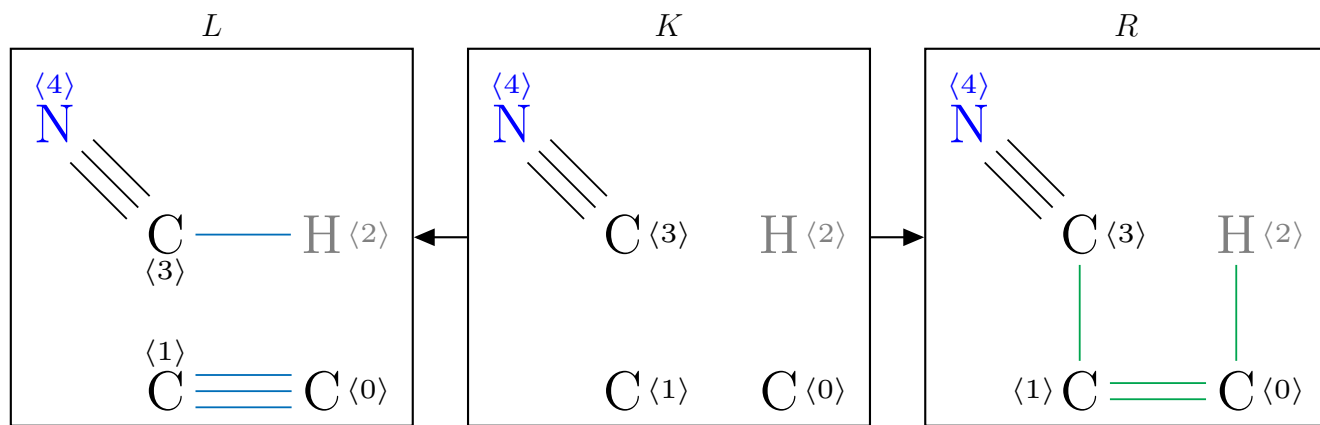
Files: out/057_r_14_10300110_{L, K, R}



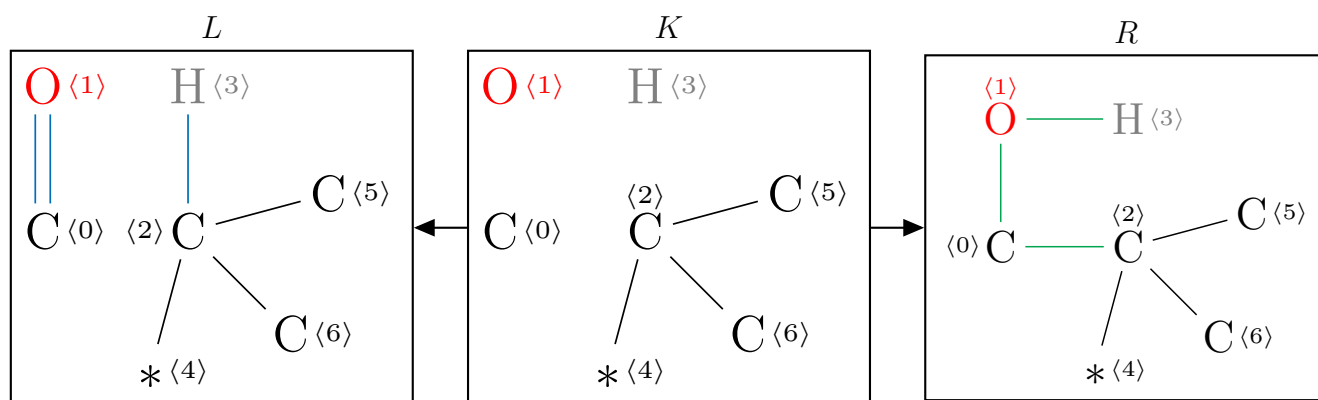
File: out/058_r_14_combined

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

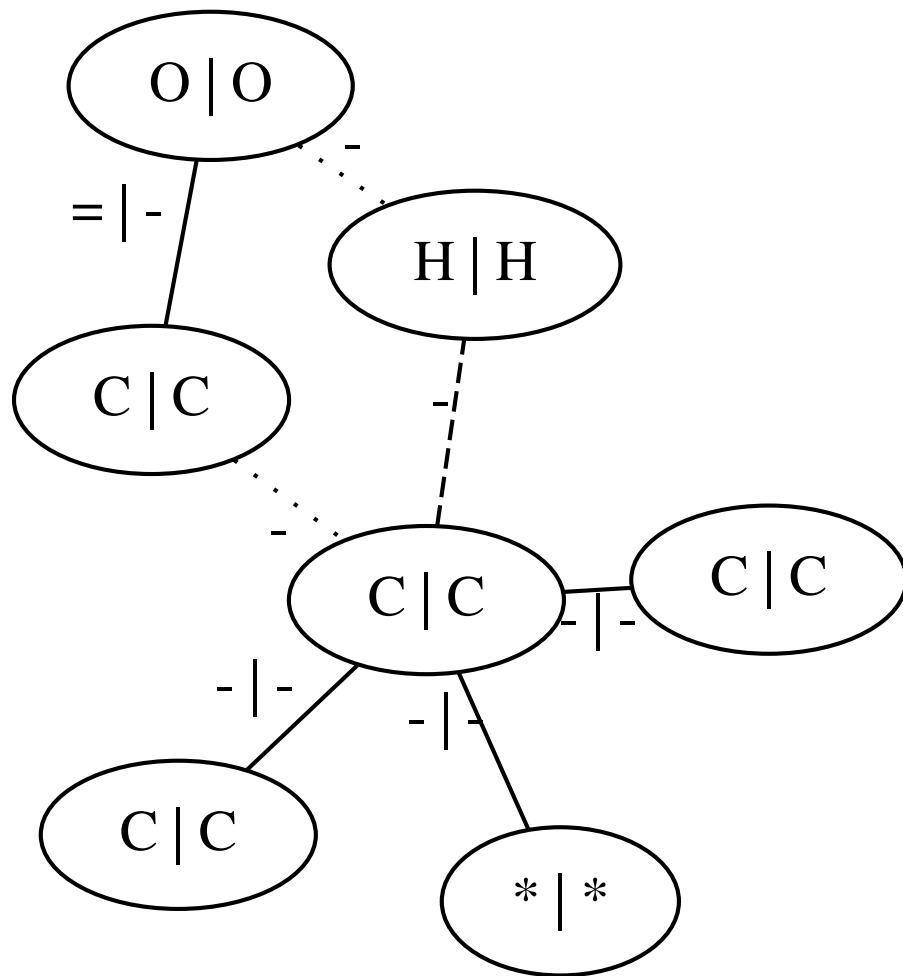
1.0.16 Alkyne Addition, C



1.0.17 Knoevenagel C



Files: out/065_r_16_10300110_{L, K, R}



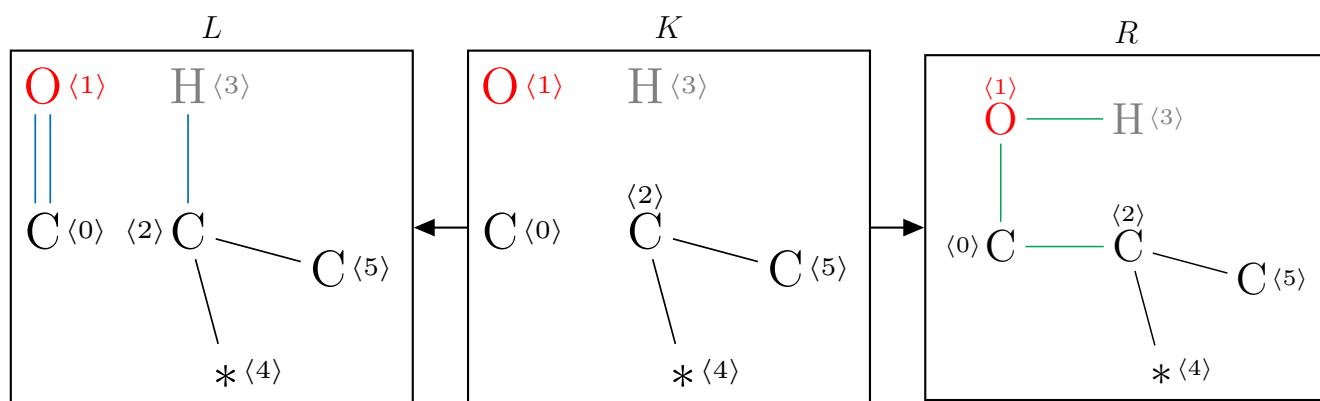
File: out/066_r_16_combined

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

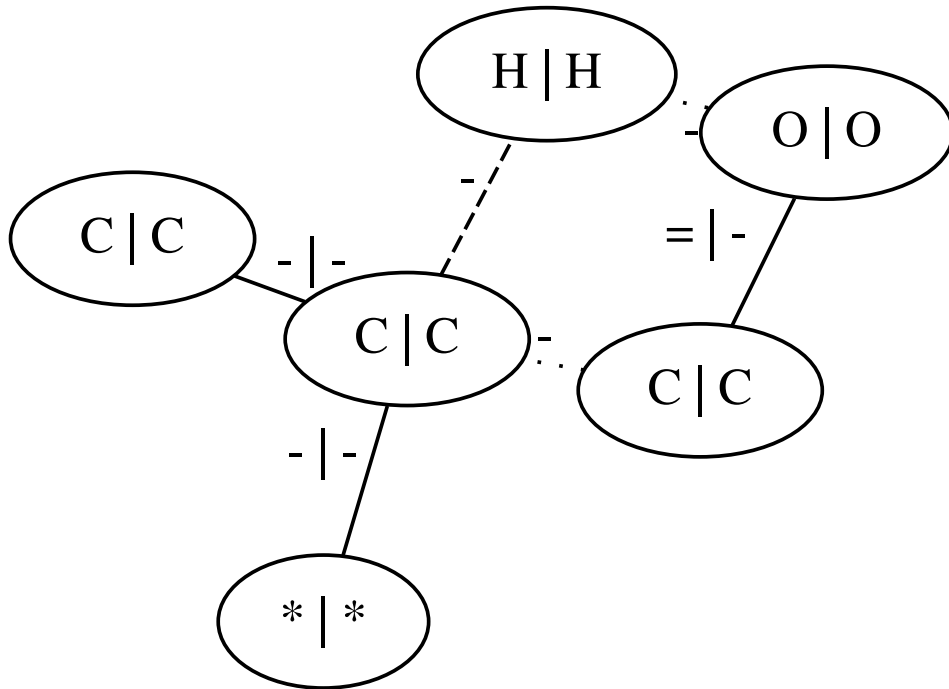
$$\begin{aligned}
& |\{e \in \text{outEdges}(5) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'\#'}, \text{'='}\} \\
& \quad \}| = 1
\end{aligned}$$

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

1.0.18 Knoevenagel H



Files: out/069_r_17_10300110_{L, K, R}



File: out/070_r_17_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

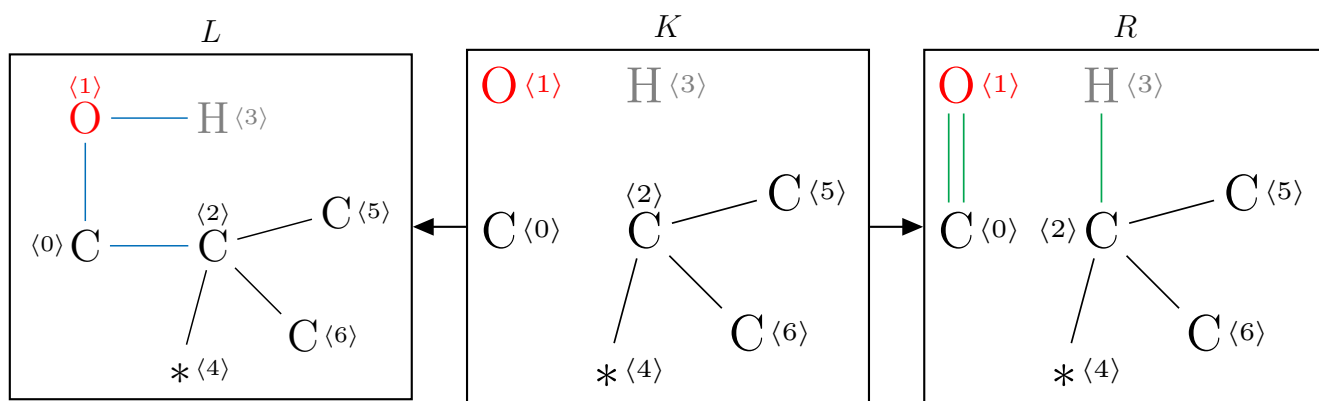
$$\wedge$$

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

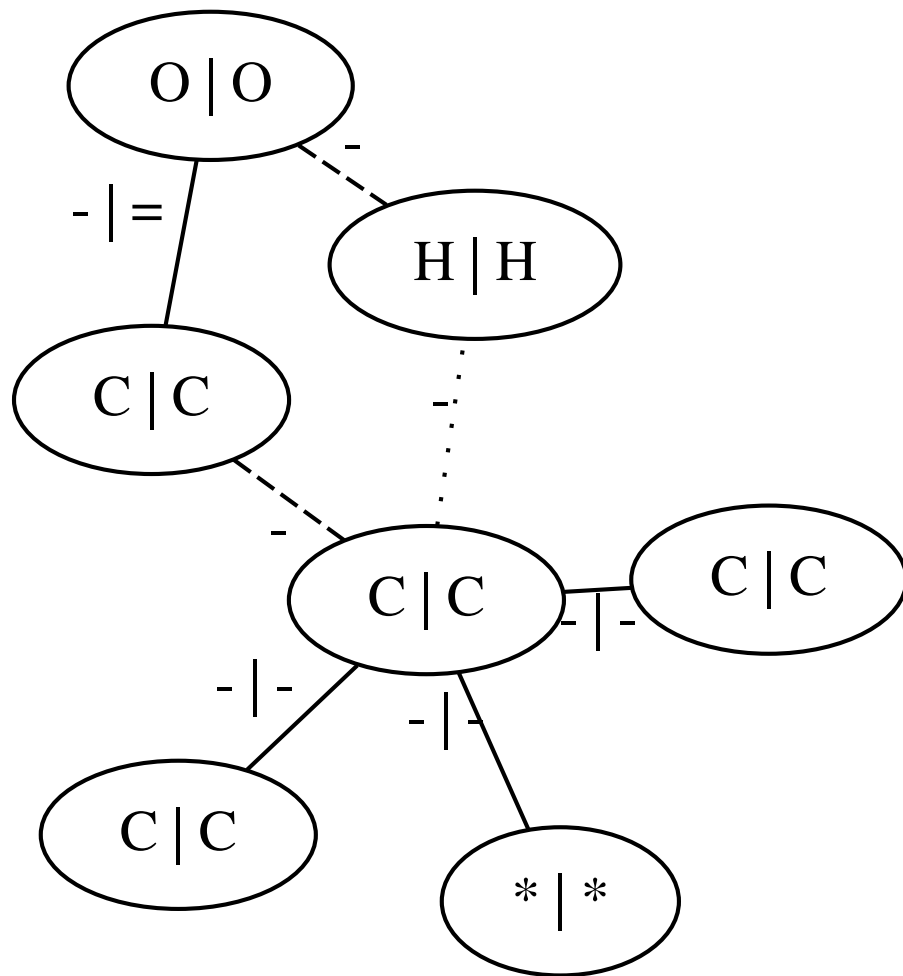
$$\}| = 1$$

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

1.0.19 Knoevenagel C (inverse)



Files: out/073_r_18_10300110_{L, K, R}



File: out/074_r_18_combined

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

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

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

$$\wedge$$

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

$$\}| = 1$$

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

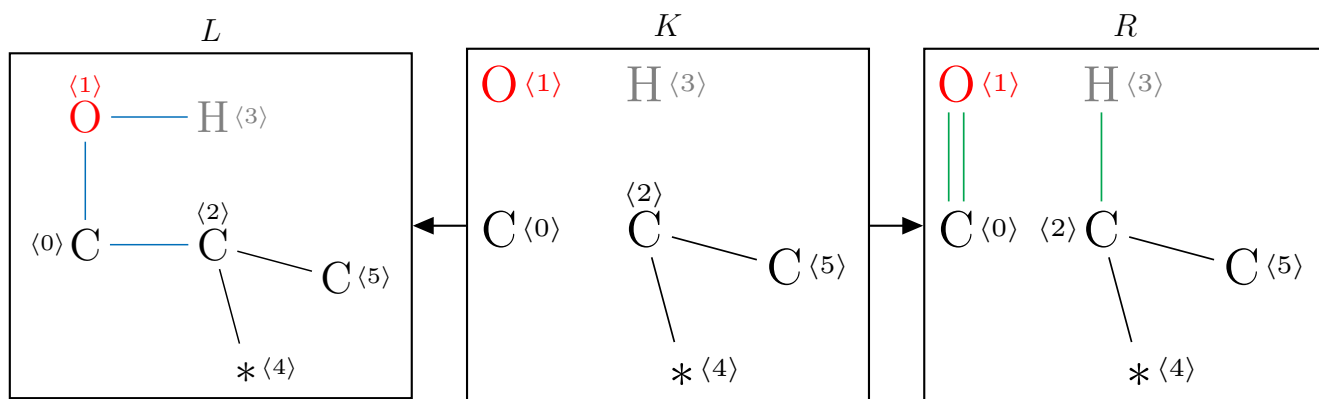
$$\text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\}$$

$$\wedge$$

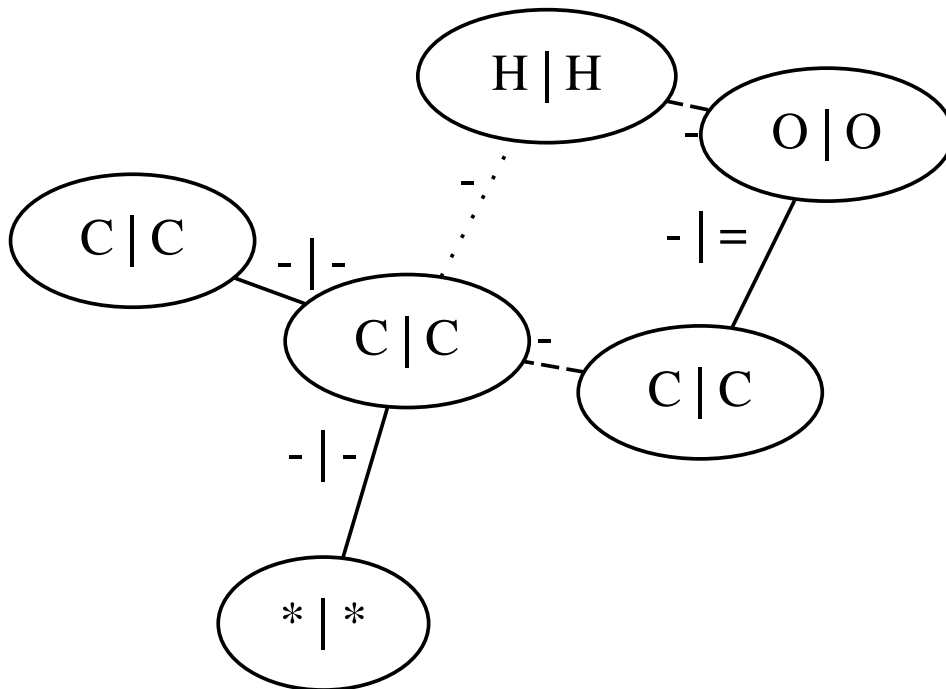
$$\text{label}(e) \in \{\text{'\#'}, \text{'-'}, \text{'='}\}$$

$$\}| \geq 1$$

1.0.20 Knoevenagel H (inv)



Files: out/077_r_19_10300110_{L, K, R}



File: out/078_r_19_combined

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

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

$$\wedge$$

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

$$| = 0$$

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

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

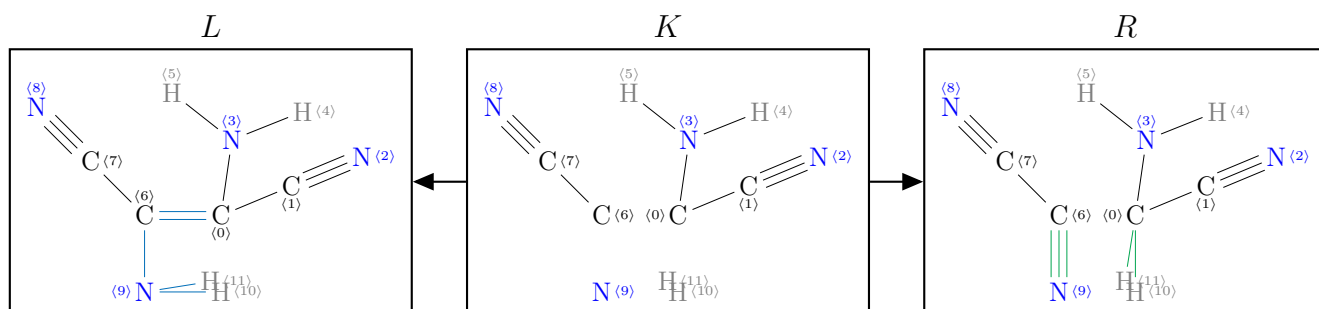
$$\wedge$$

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

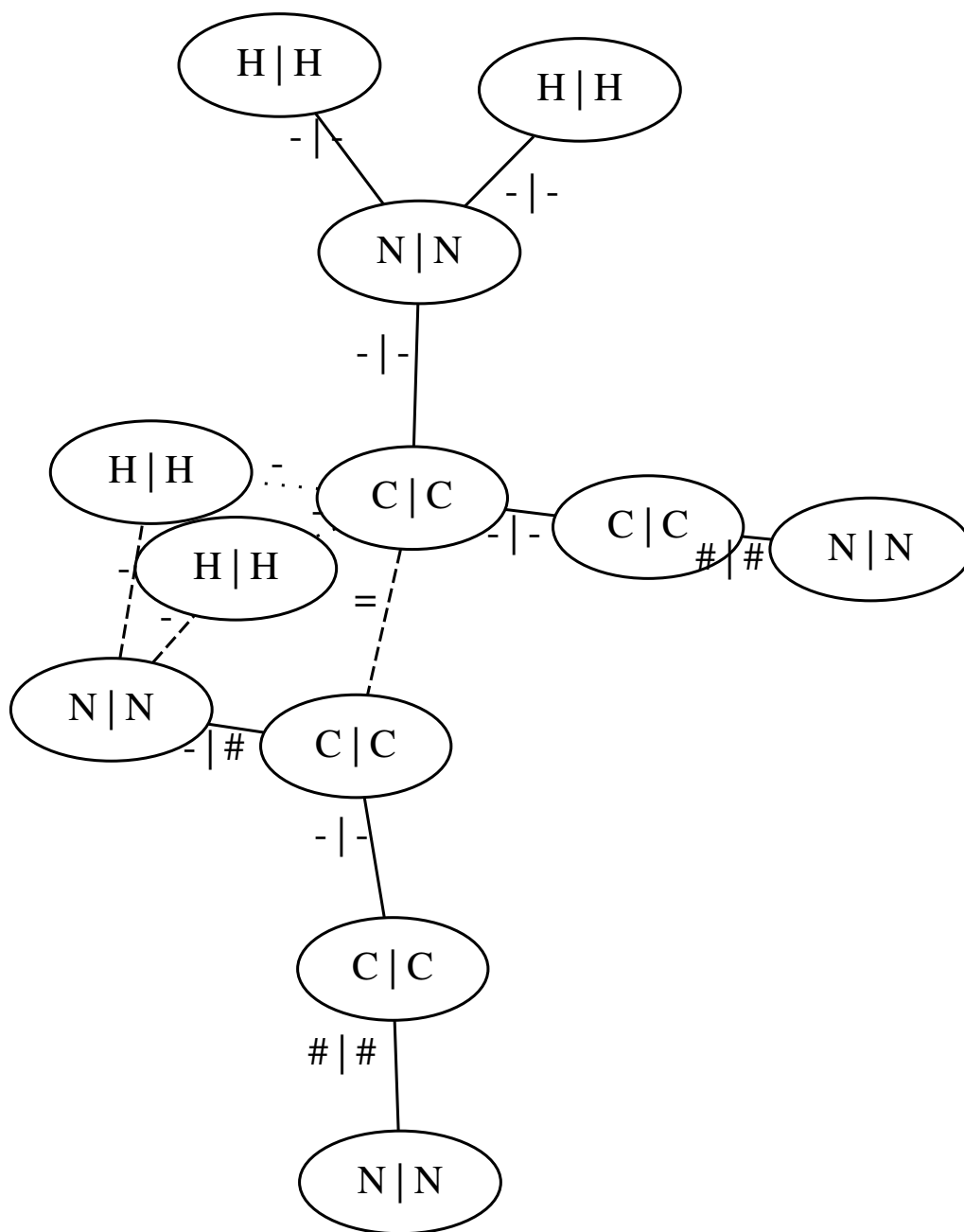
$$| = 1$$

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

1.0.21 DAMN Scission

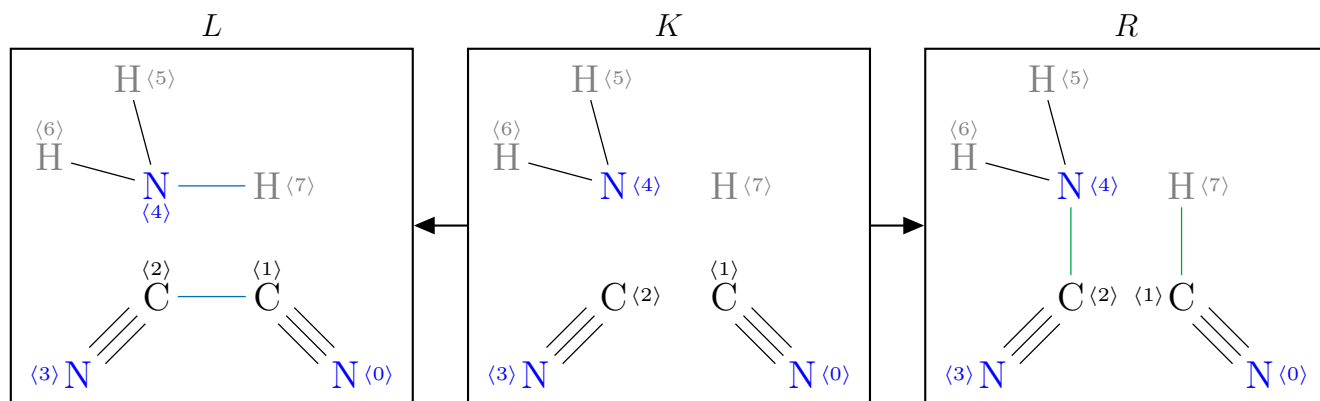


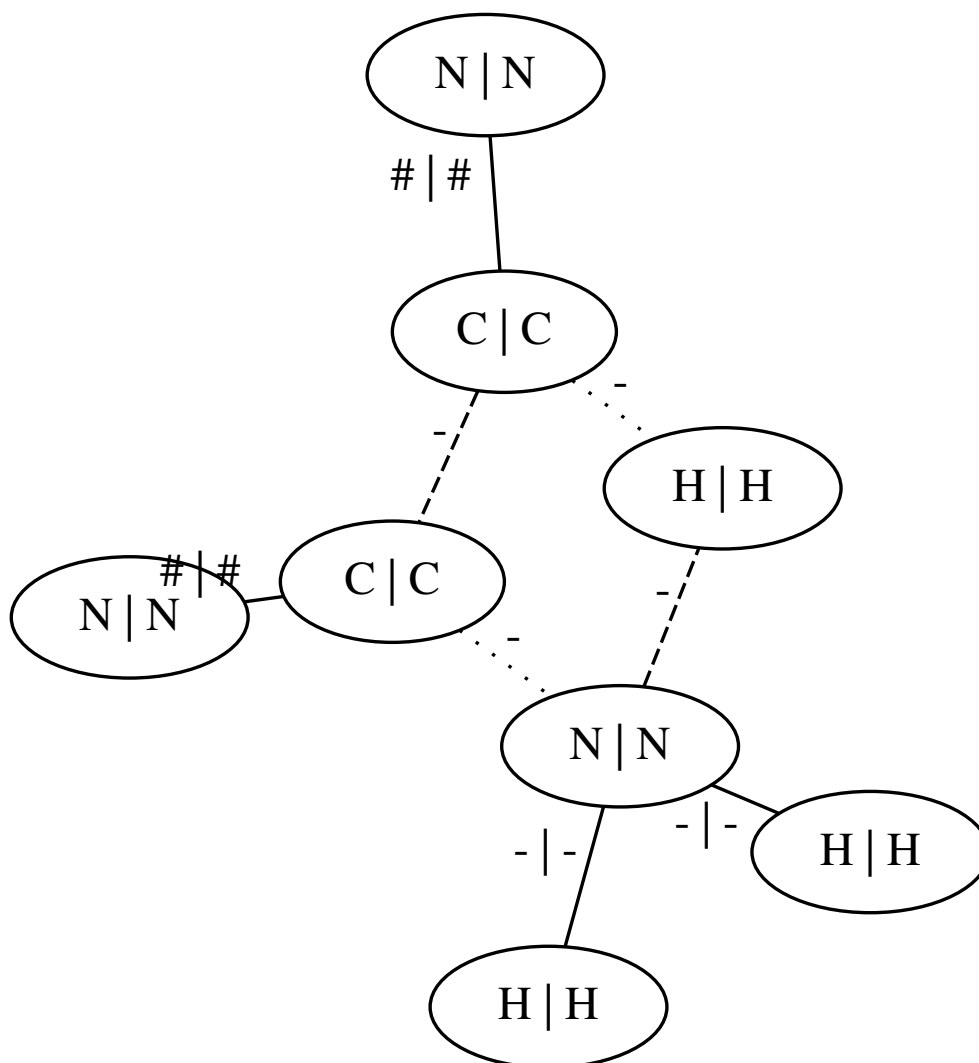
Files: out/081_r_20_10300110_{L, K, R}



File: out/082_r_20_combined

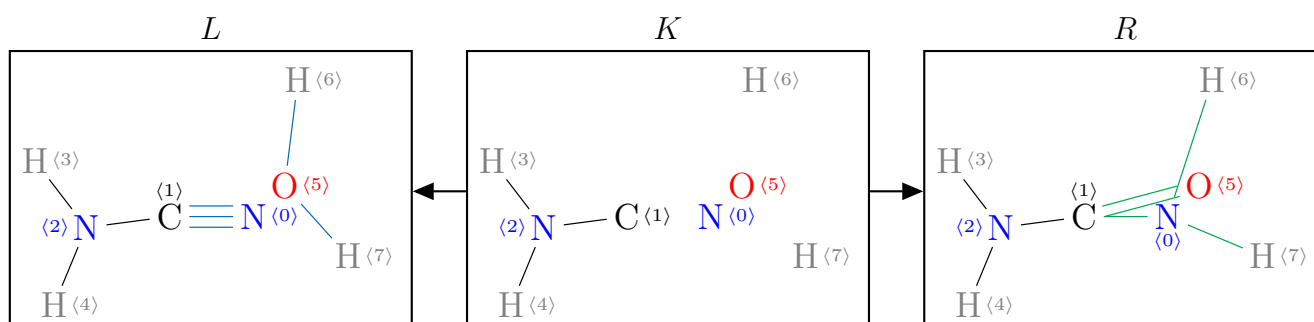
1.0.22 Cyanogen Ammonolysis

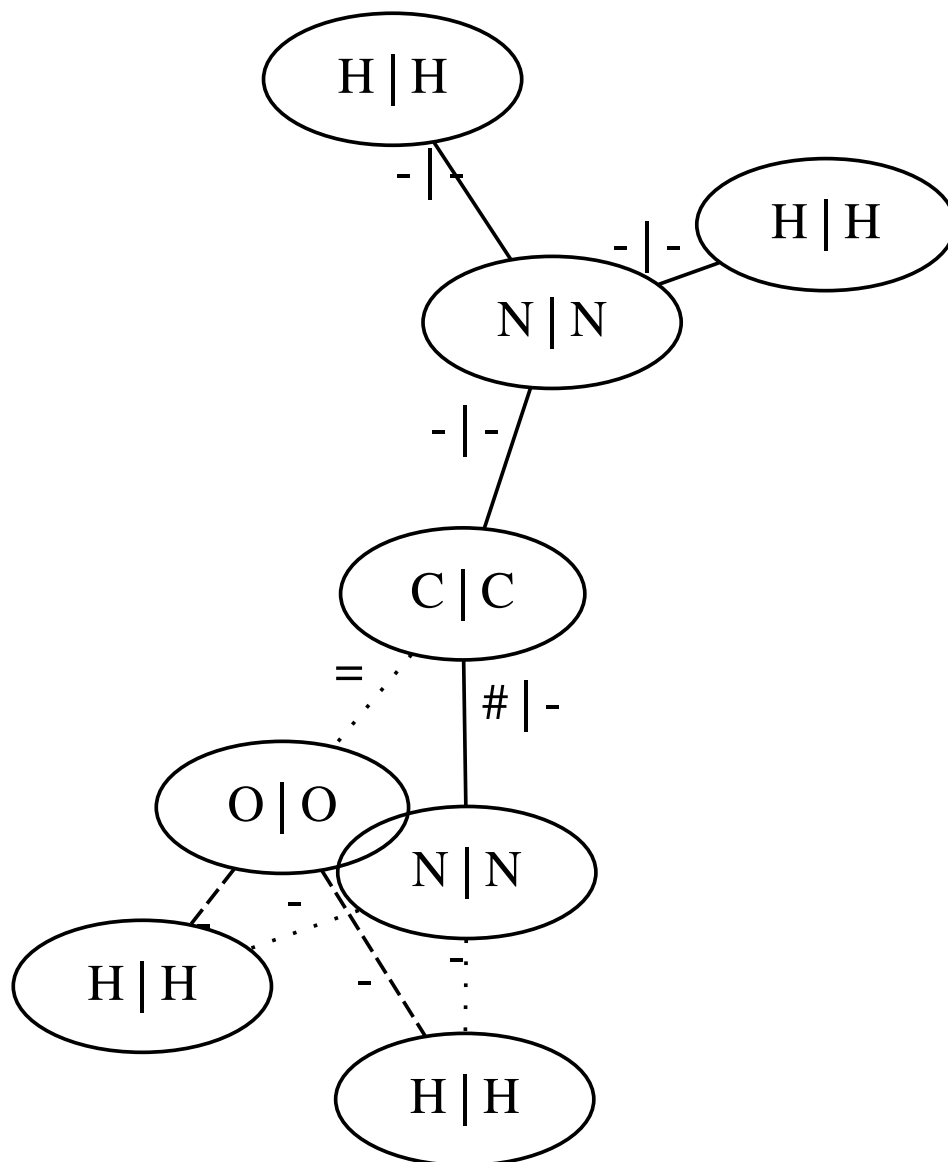




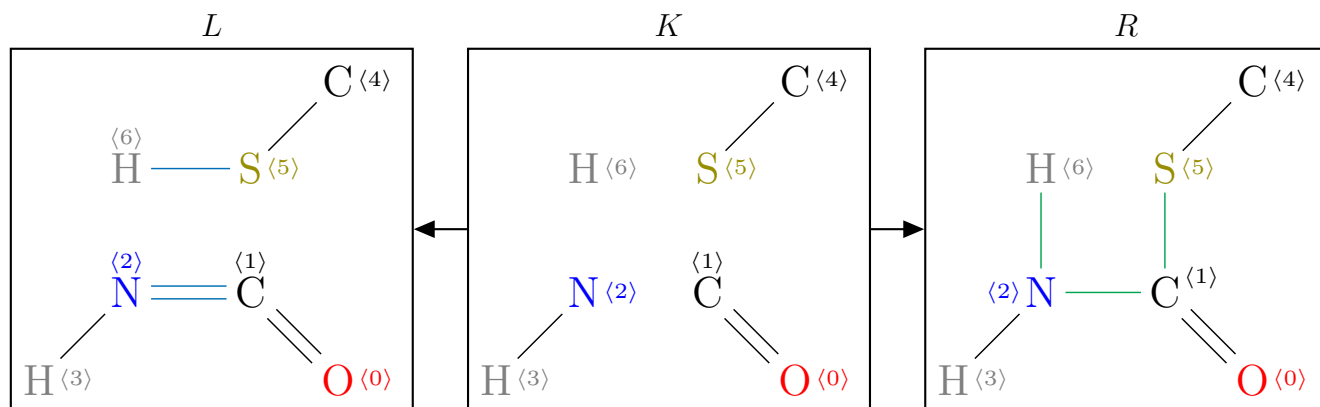
File: out/086_r_21_combined

1.0.23 Cyanamide Hydration

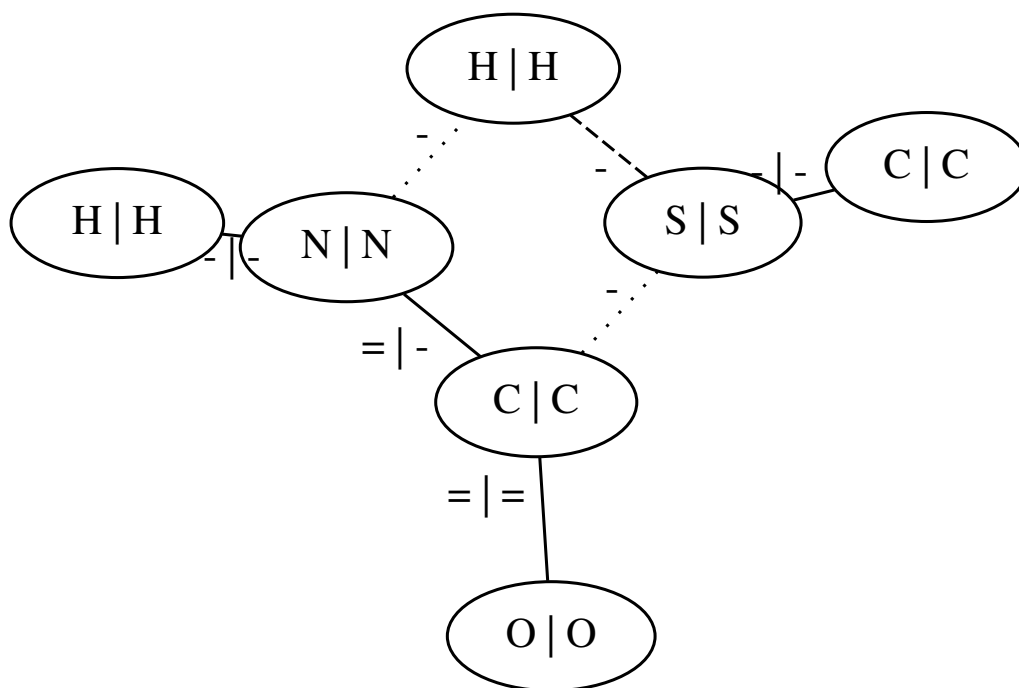




1.0.24 Carbamylation, SC

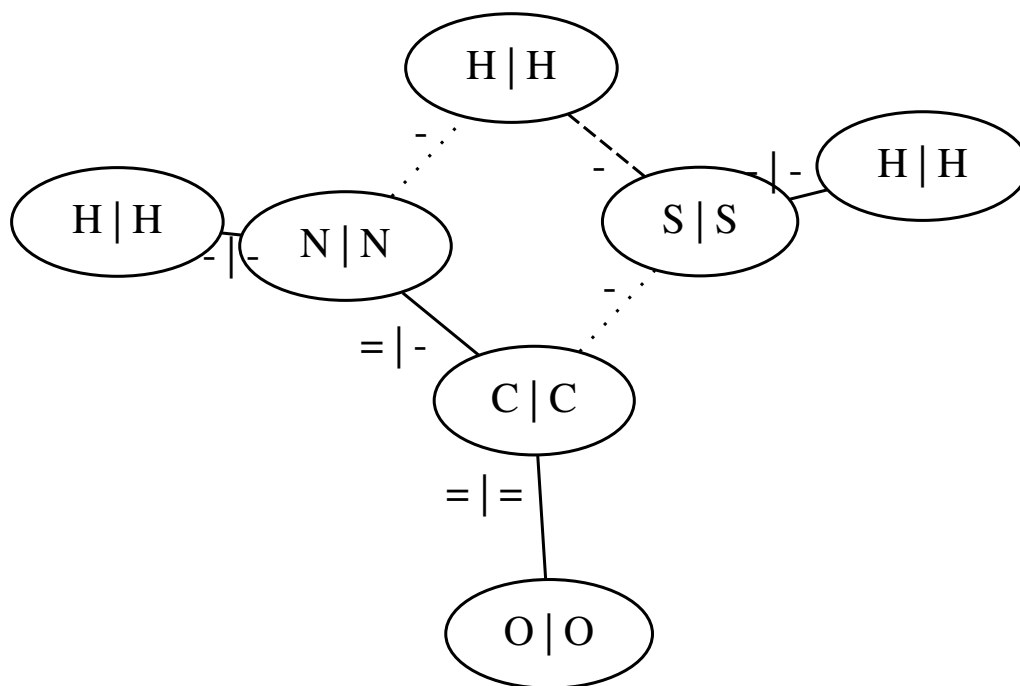
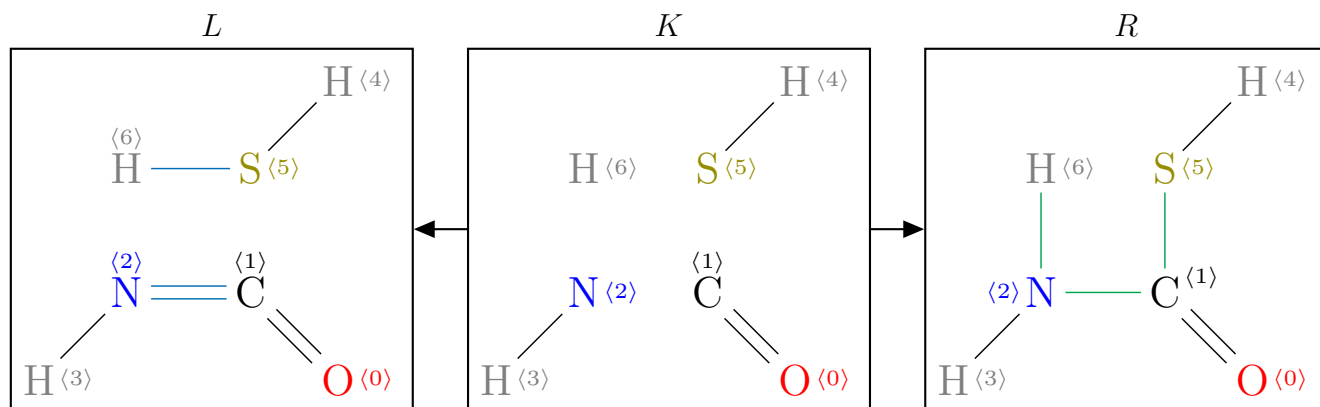


Files: out/093_r_23_10300110_{L, K, R}



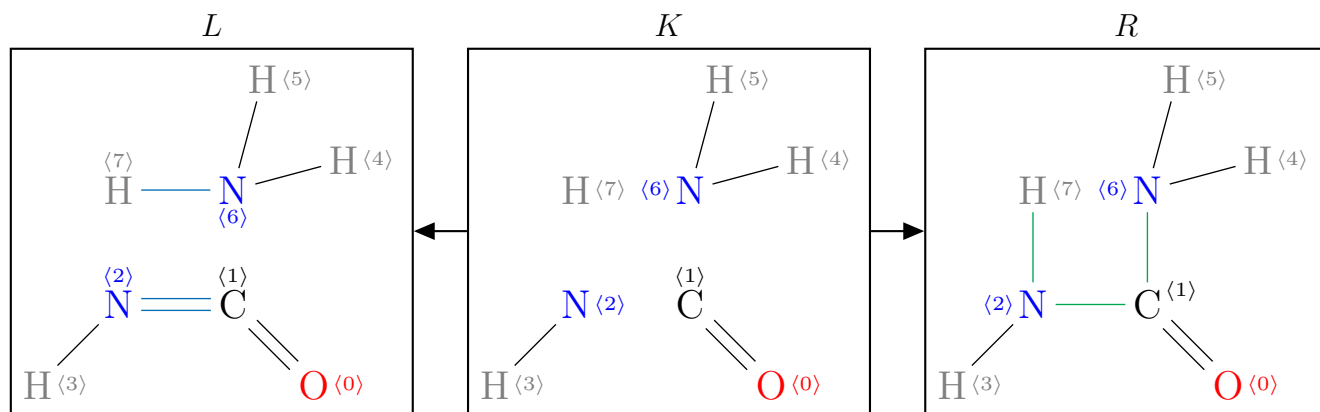
File: out/094_r_23_combined

1.0.25 Carbamylation, SH

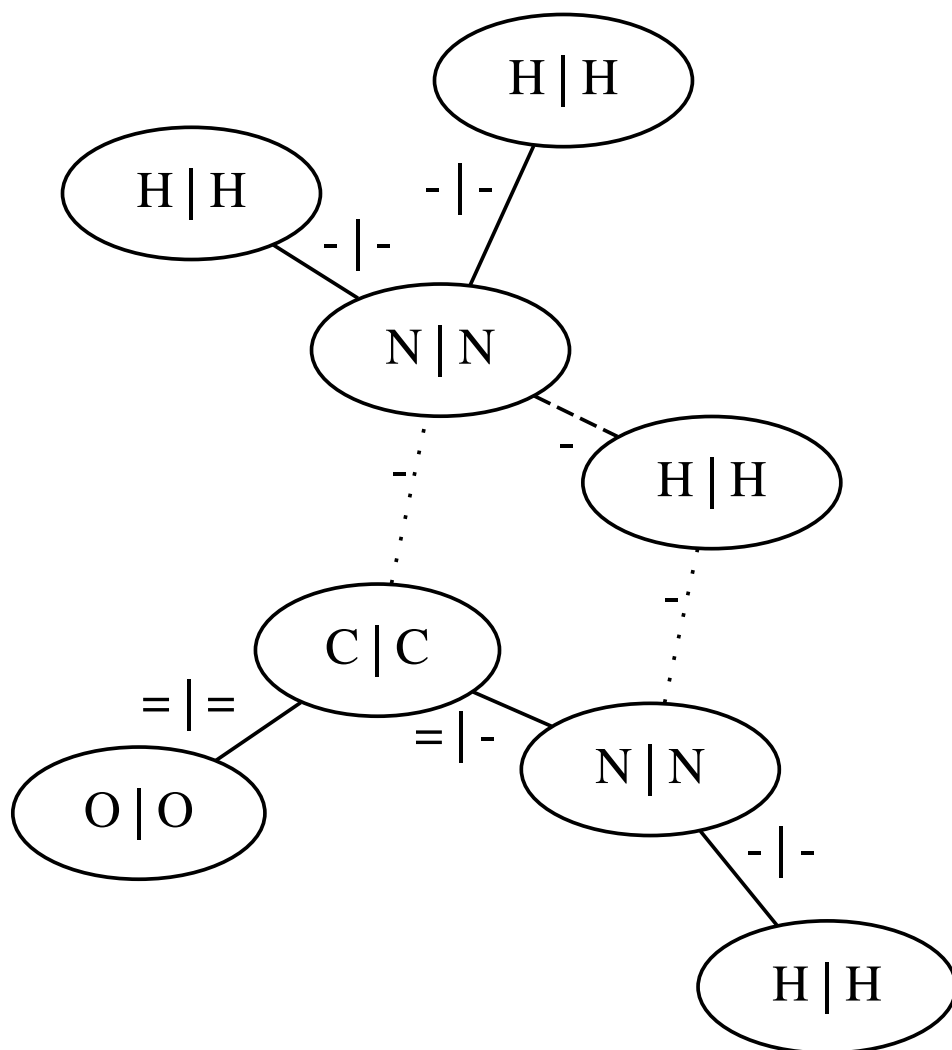


File: out/098_r_24_combined

1.0.26 Carbamylation, N, HH

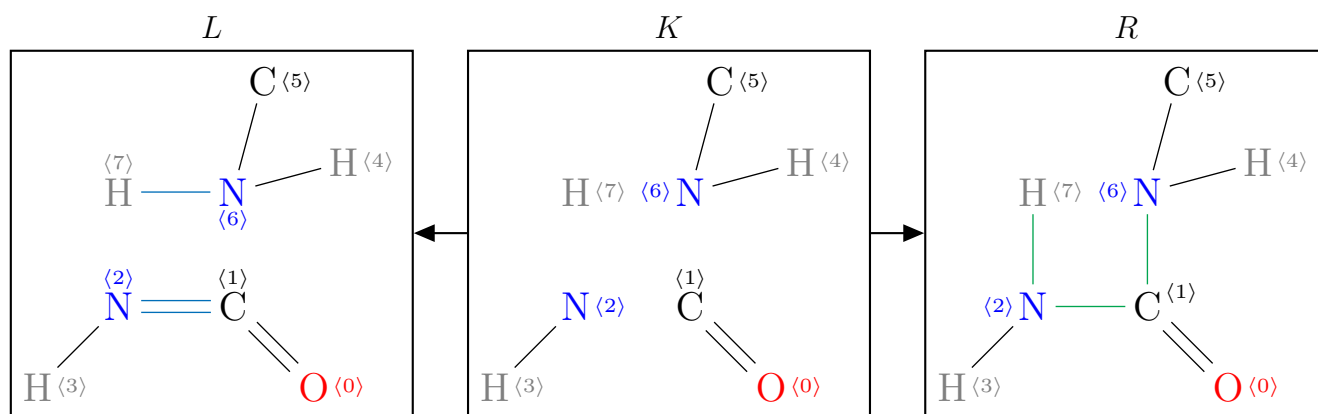


Files: out/101_r_25_10300110_{L, K, R}

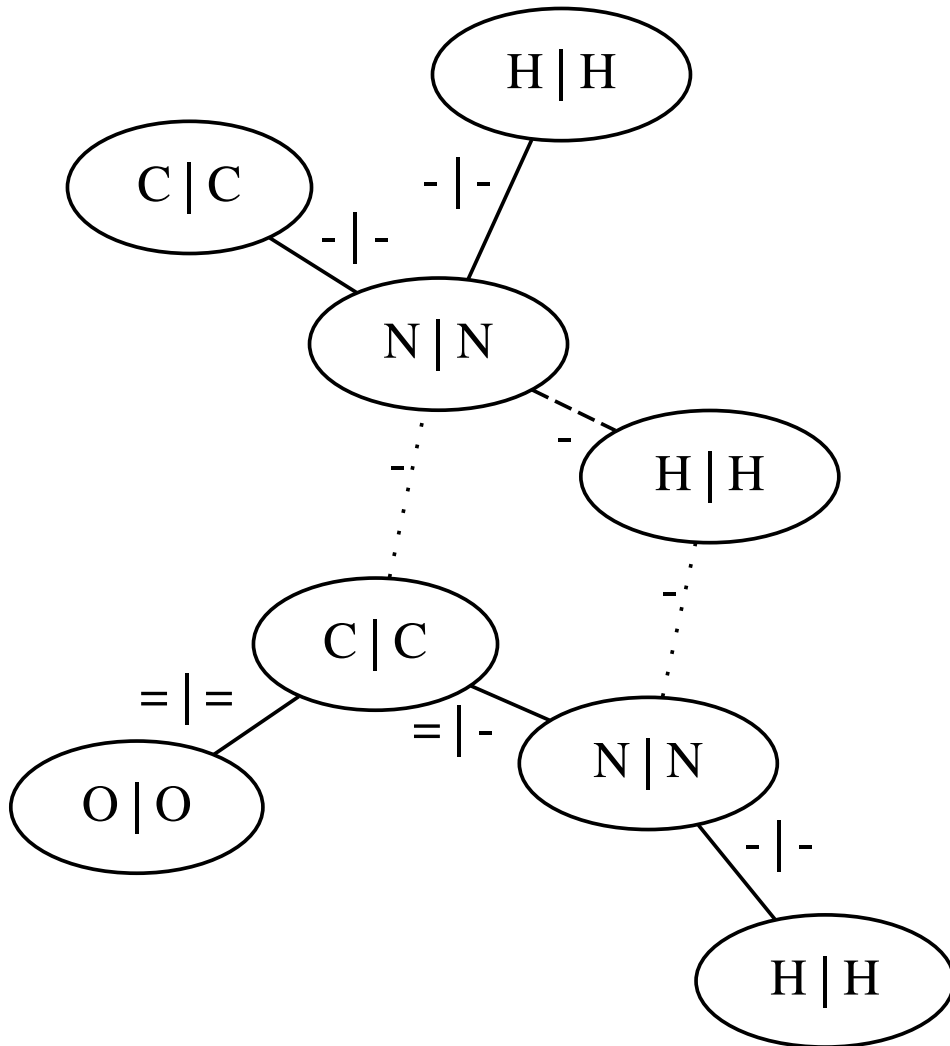


File: out/102_r_25_combined

1.0.27 Carbamylation, N, HC



Files: out/105_r_26_10300110_{L, K, R}



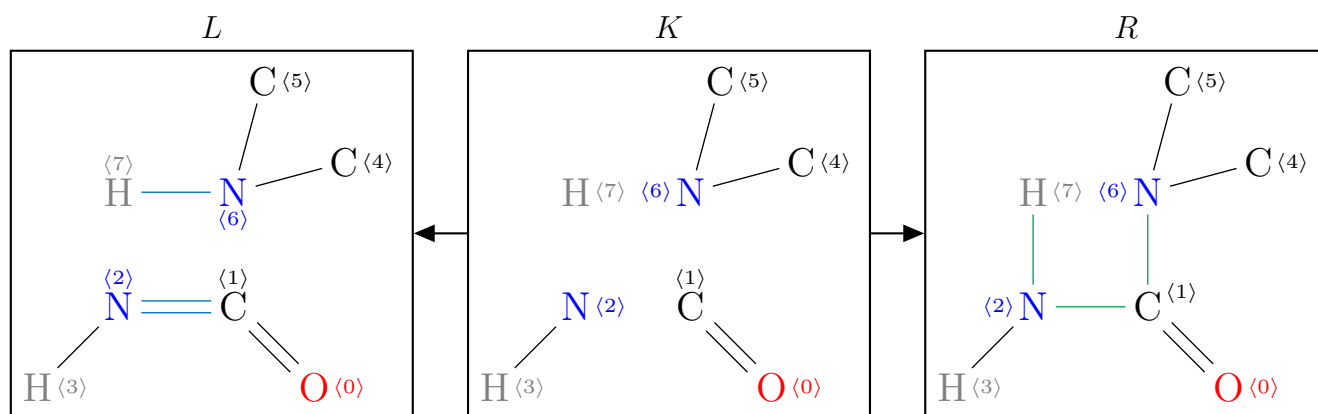
File: out/106_r_26_combined

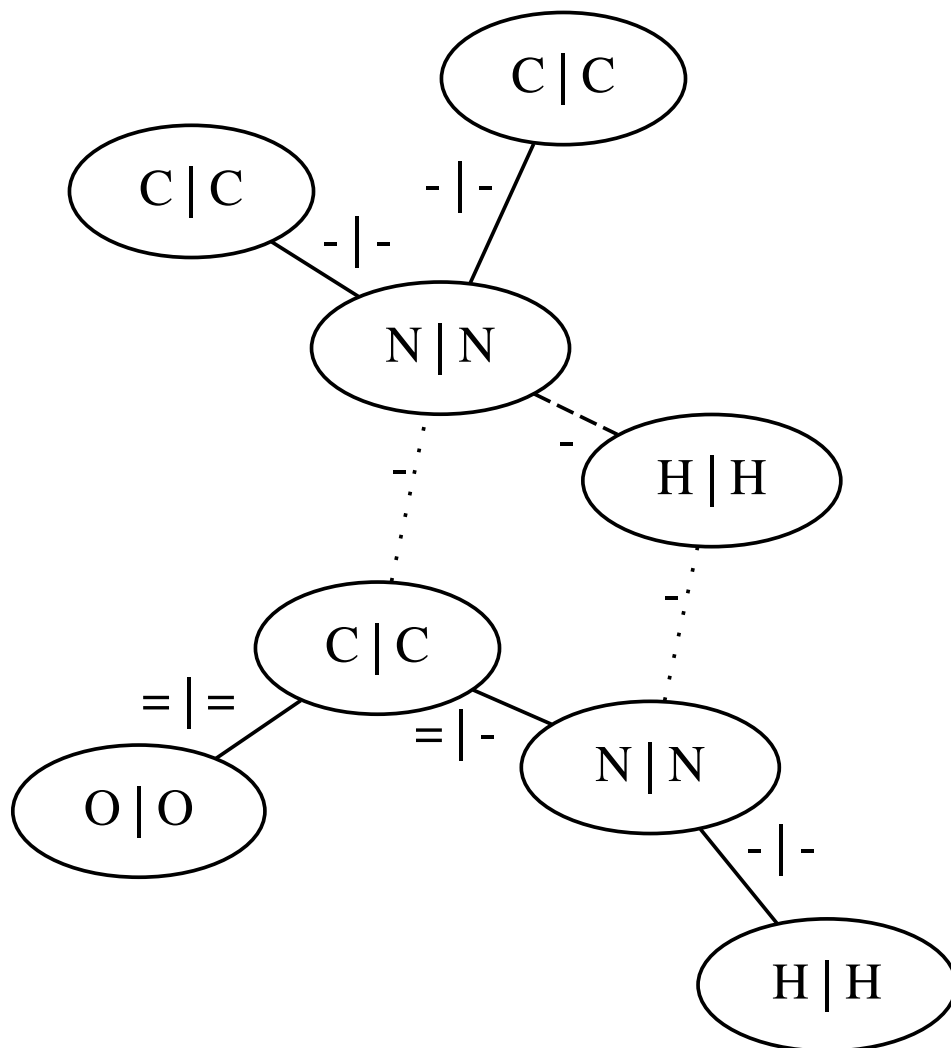
```

|{e ∈ outEdges(5) |
  label(target(e)) ∈ {'0'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

1.0.28 Carbamylation, N, CC





File: out/110_r_27_combined

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

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

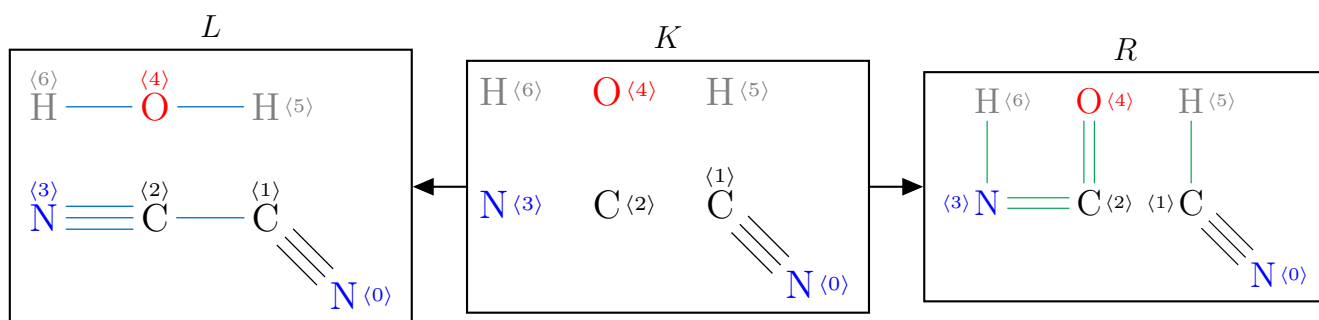
$$\wedge$$

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

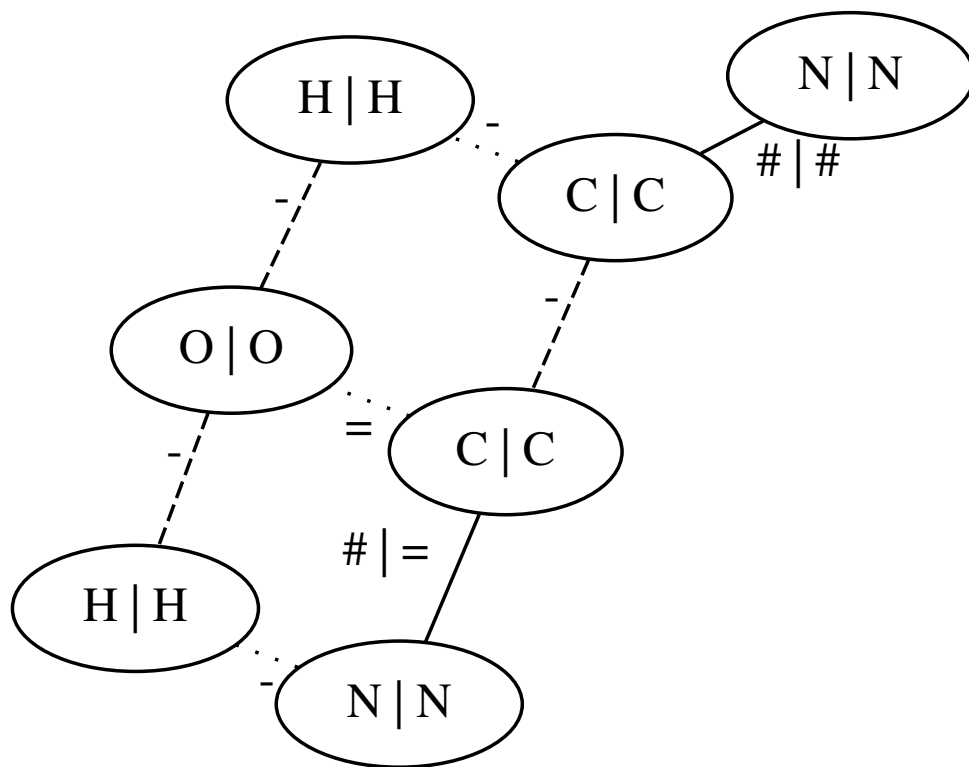
$$| = 0$$

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

1.0.29 Cyanate from cyanogen

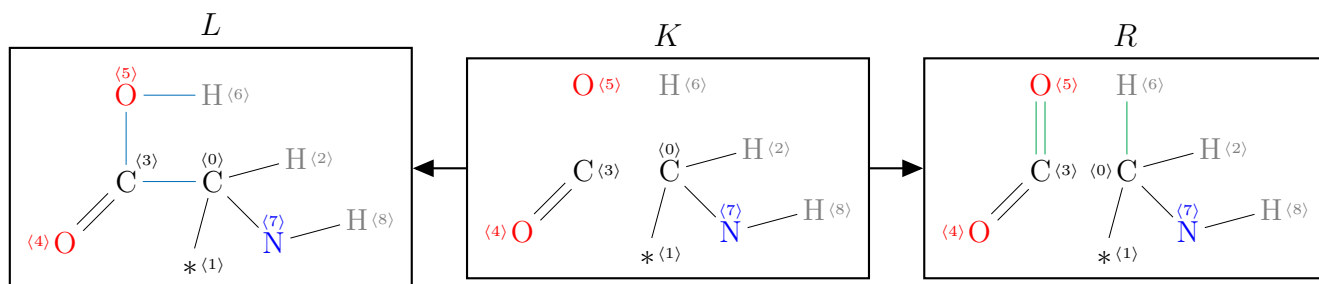


Files: out/113_r_28_10300110_{L, K, R}

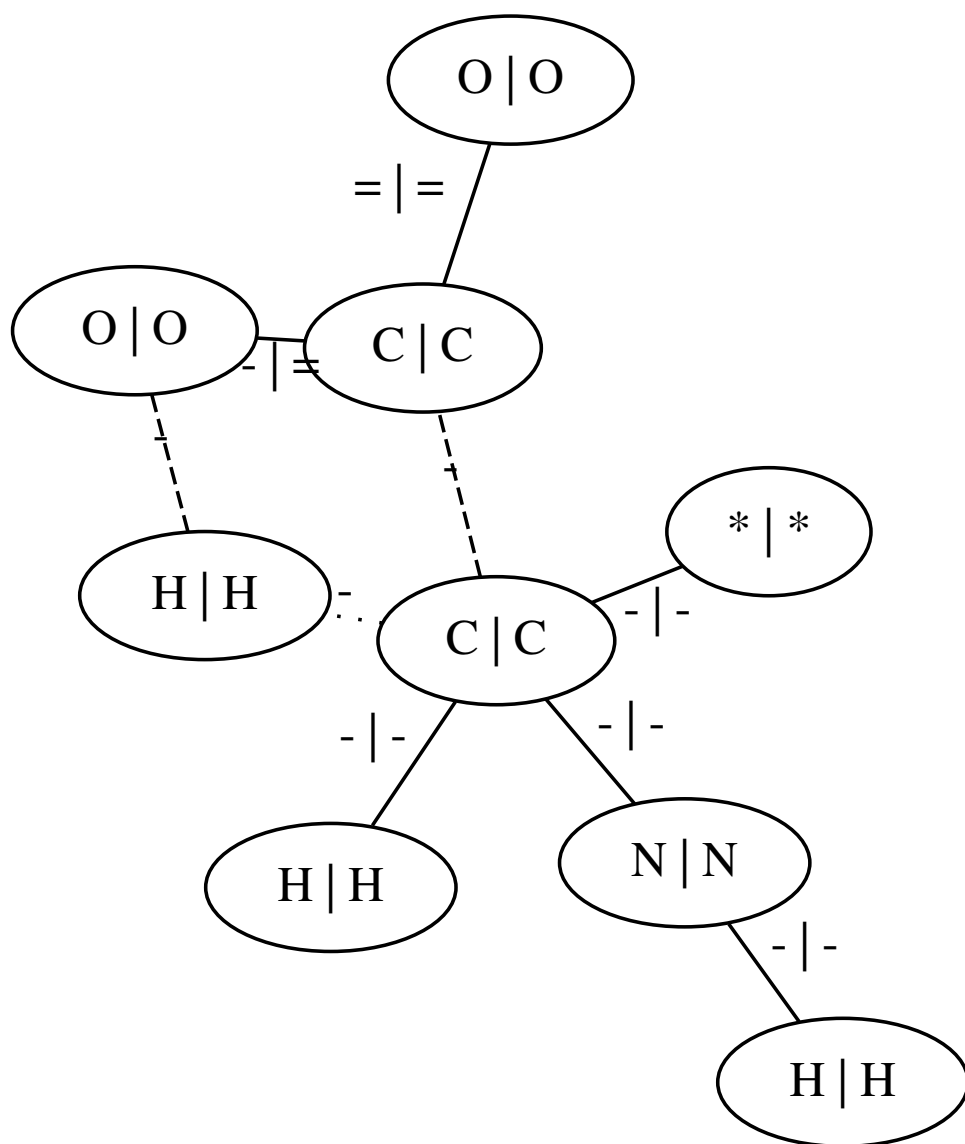


File: out/114_r_28_combined

1.0.30 Ketone-Catalyzed Decarboxylation

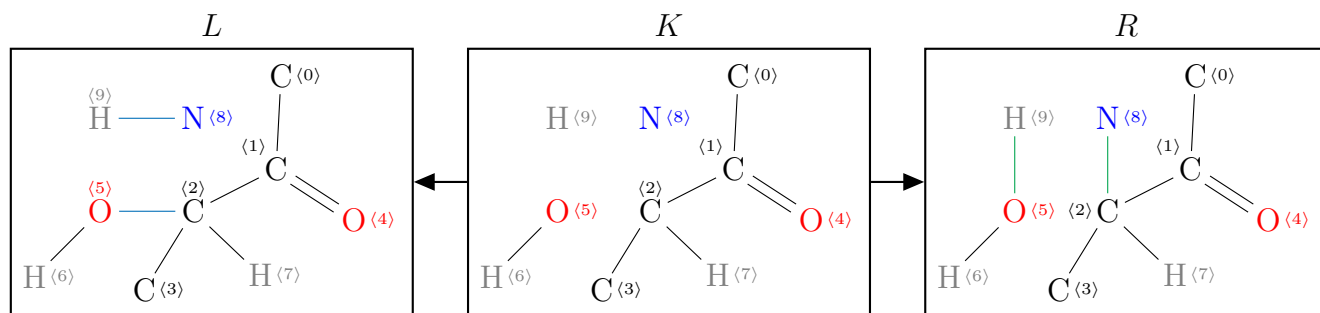


Files: out/117_r_29_10300110_{L, K, R}

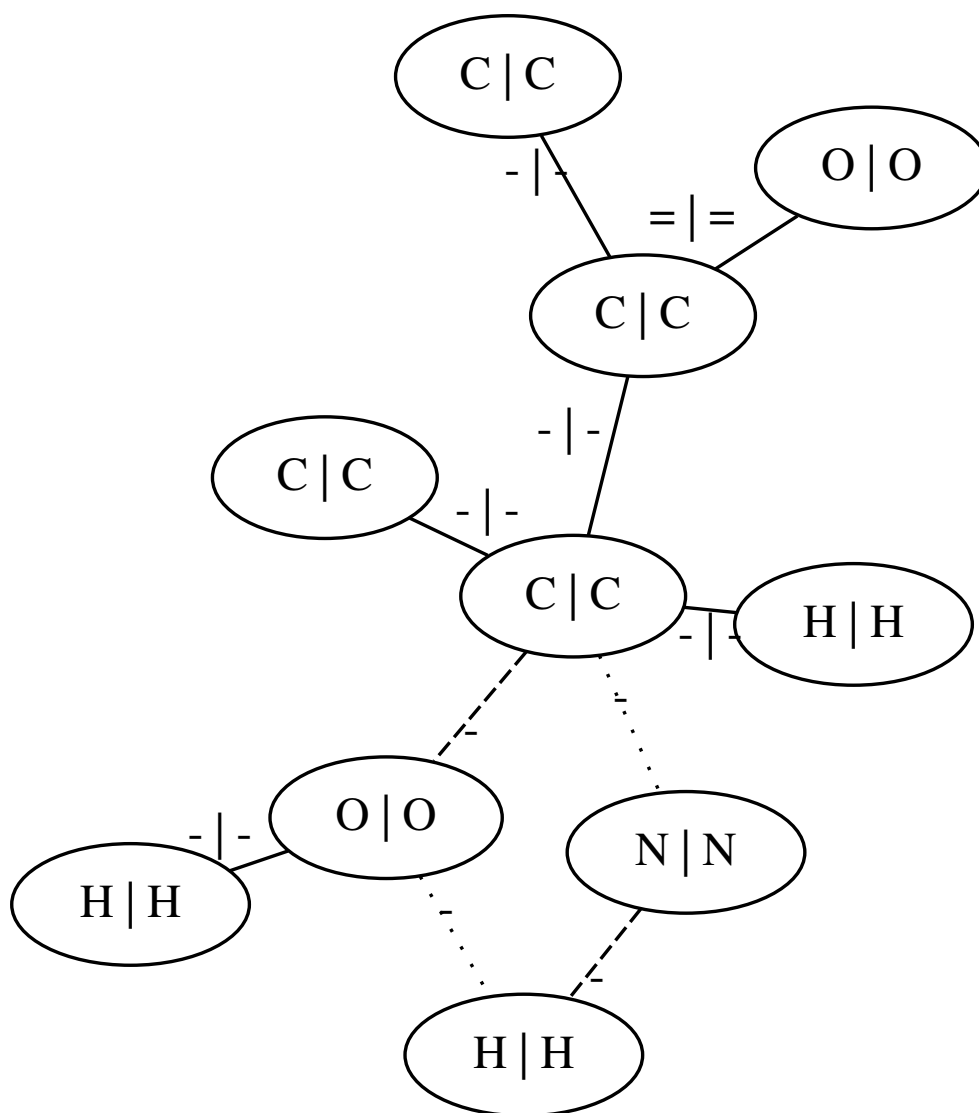


File: out/118_r_29_combined

1.0.31 Amadori Rearrangement

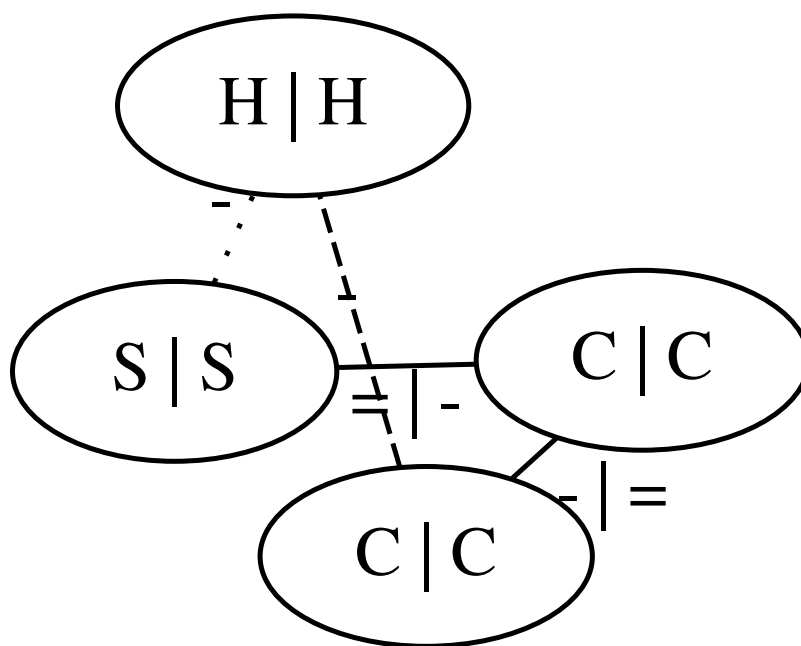
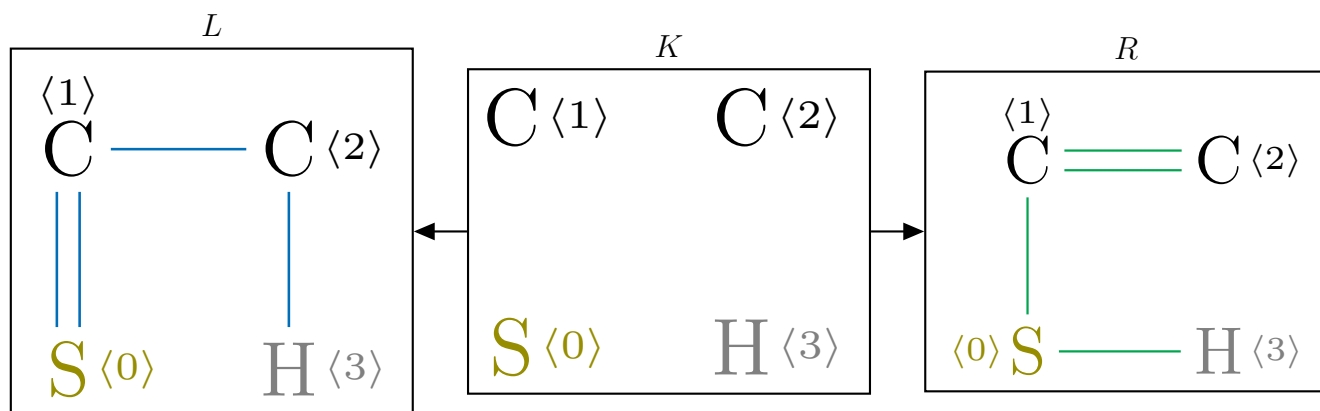


Files: out/121_r_30_10300110_{L, K, R}



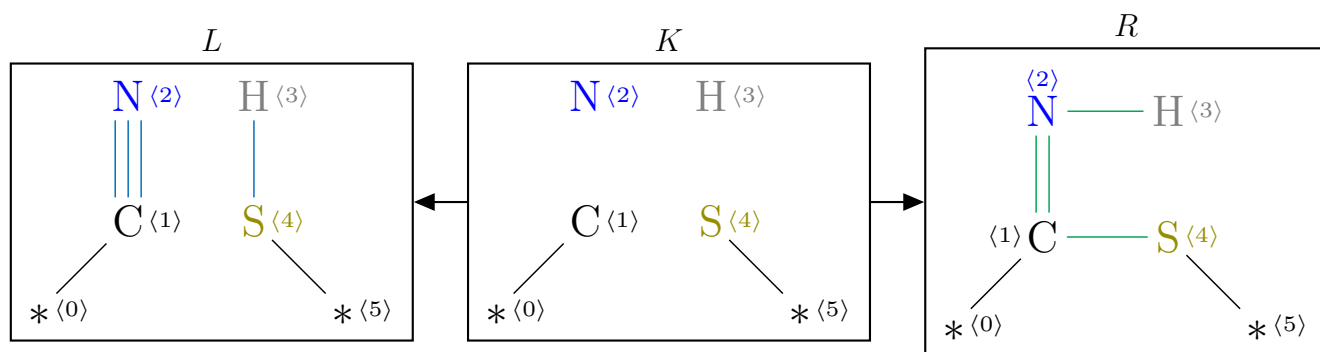
File: out/122_r_30_combined

1.0.32 Thial -> Thiene

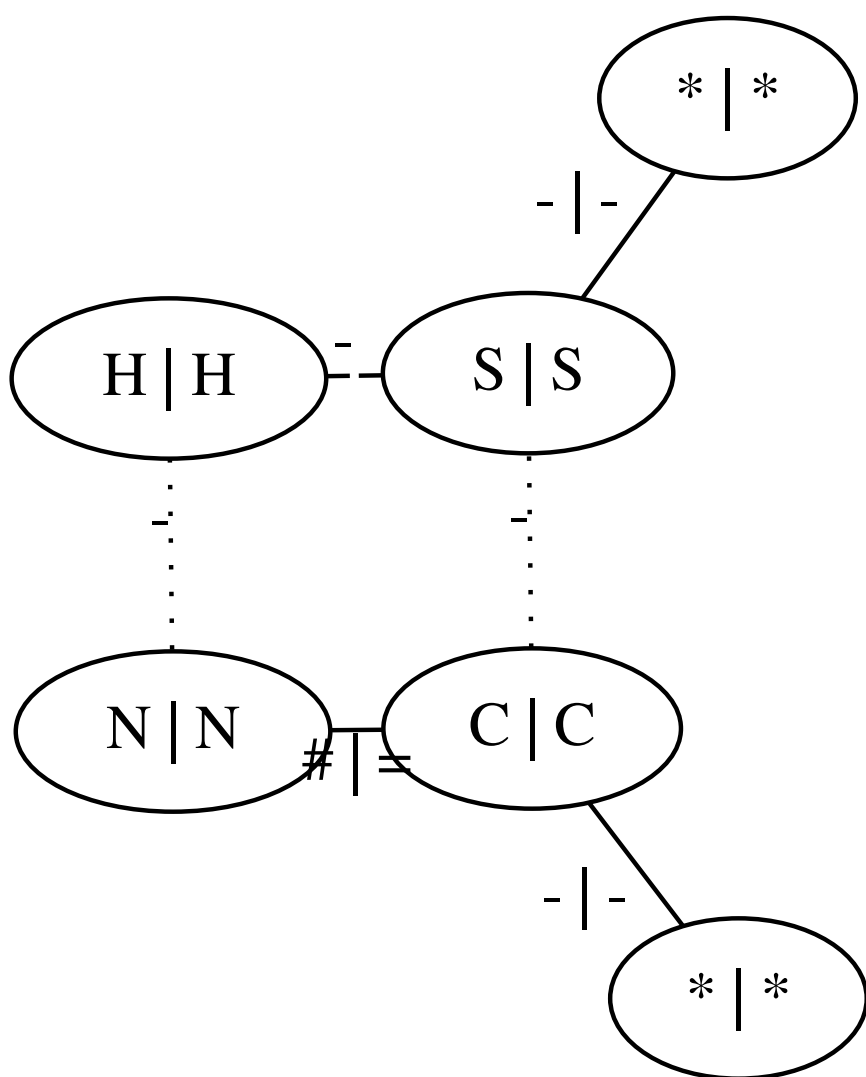


File: out/126_r_31_combined

1.0.33 Sulfide to Nitrile Addition

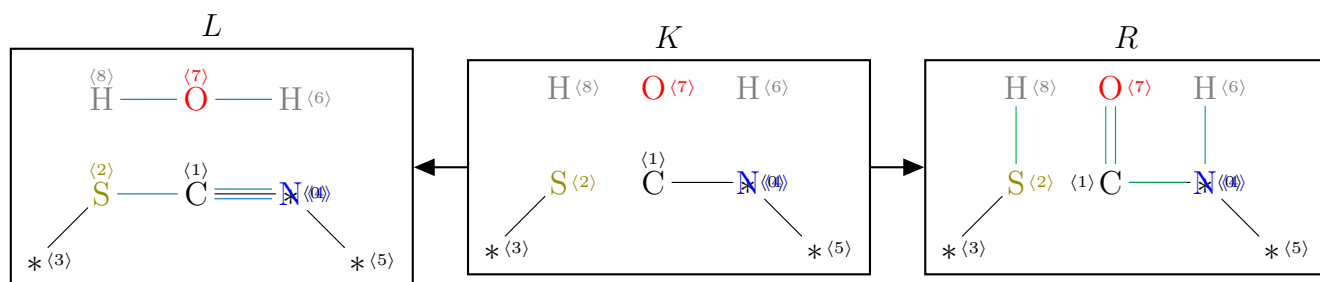


Files: out/129_r_32_10300110_{L, K, R}

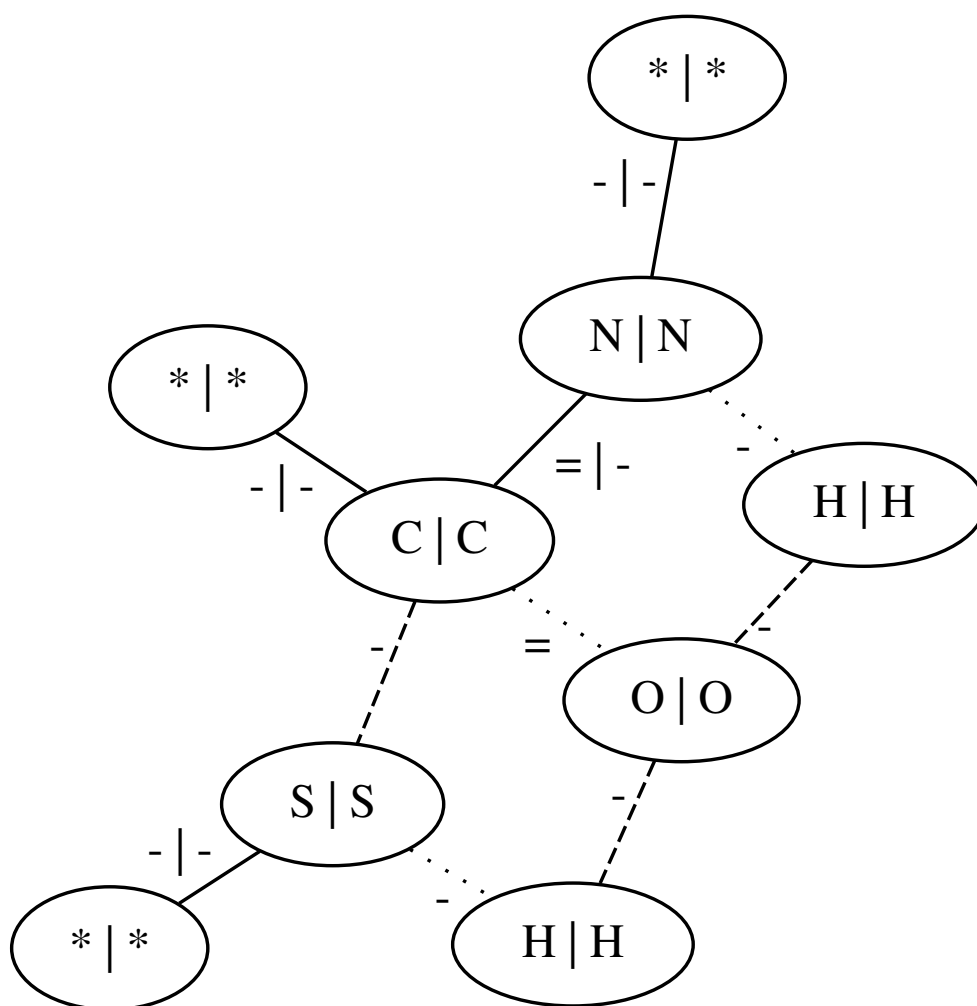


File: out/130_r_32_combined

1.0.34 Thioamidine to Amide Hydrolysis

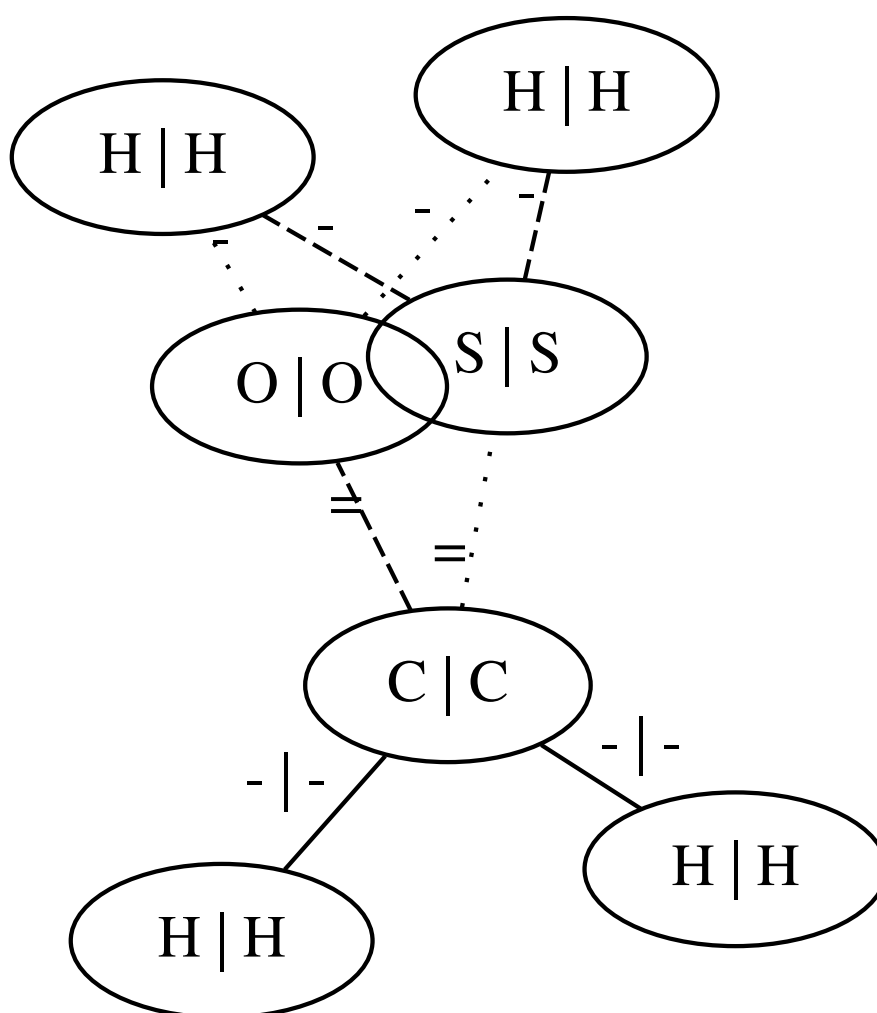
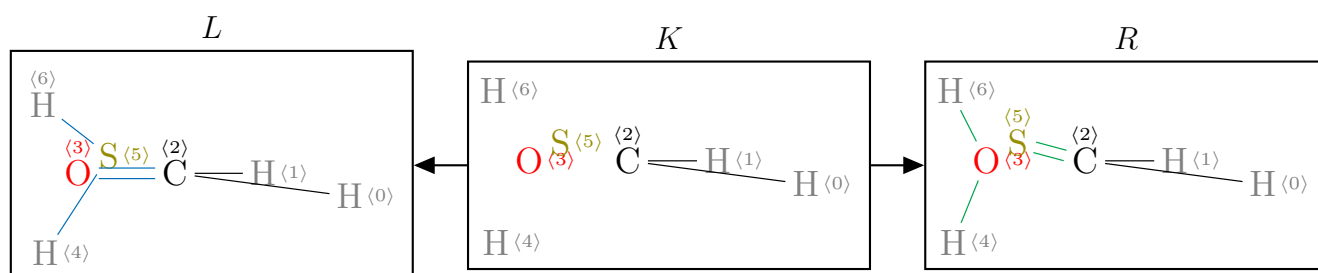


Files: out/133_r_33_10300110_{L, K, R}

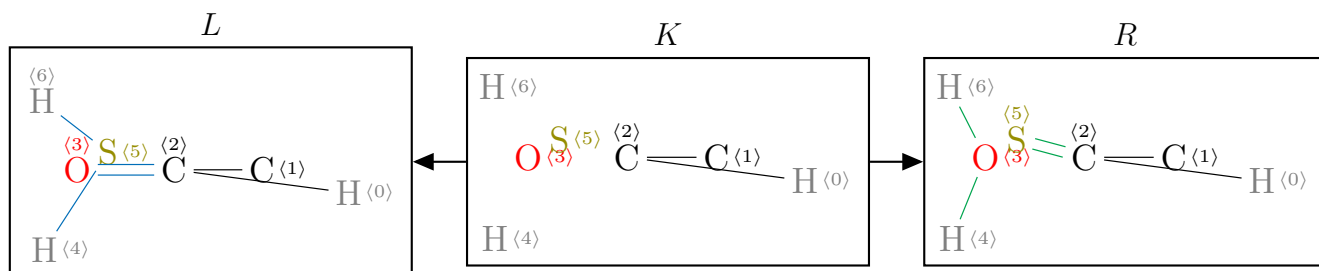


File: out/134_r_33_combined

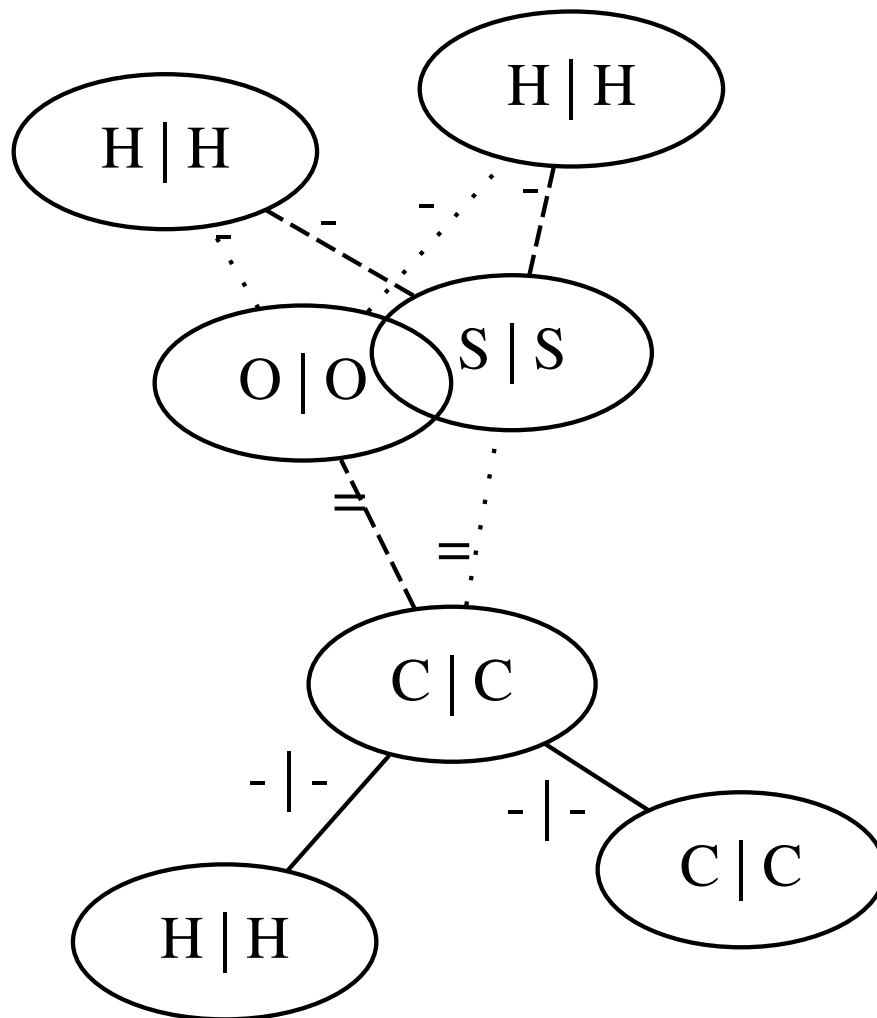
1.0.35 Ketone/Aldehyde to Thioketone/Thial, HH



1.0.36 Ketone/Aldehyde to Thioketone/Thial, HC



Files: out/141_r_35_10300110_{L, K, R}



File: out/142_r_35_combined

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

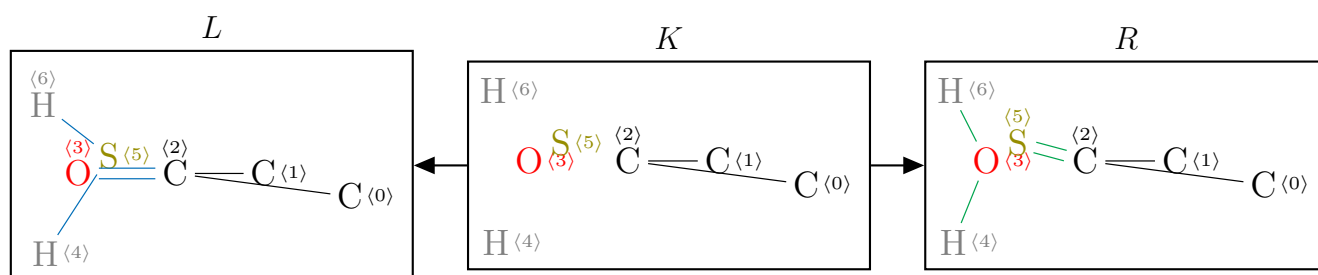
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

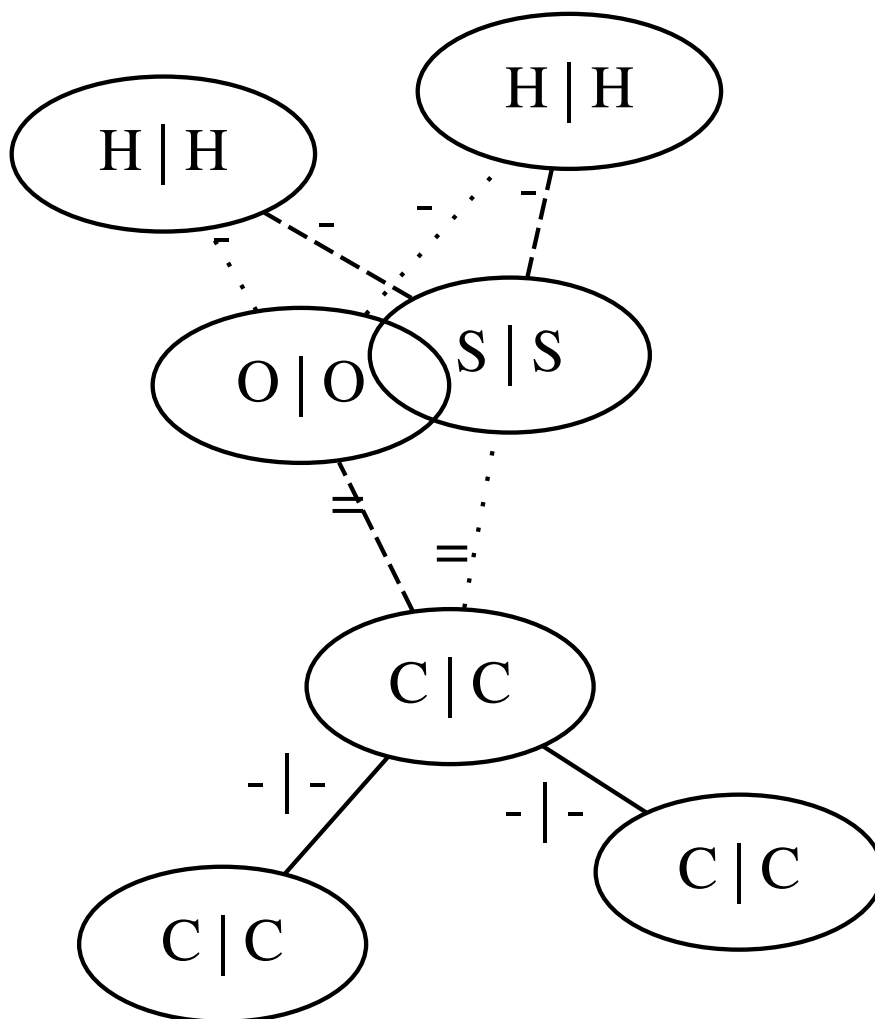
$$\text{label}(e) \in \{'=\'}\}$$

$$\} = 0$$

1.0.37 Ketone/Aldehyde to Thioketone/Thial, CC



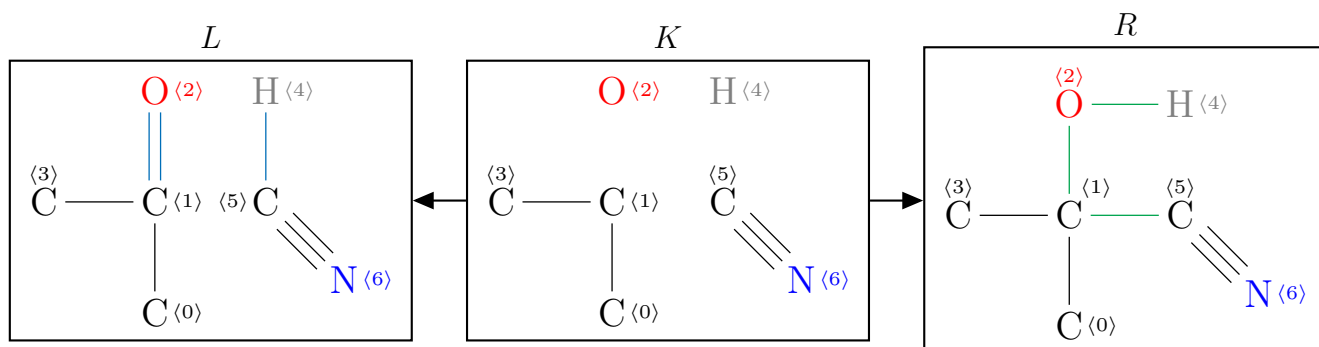
Files: out/145_r_36_10300110_{L, K, R}



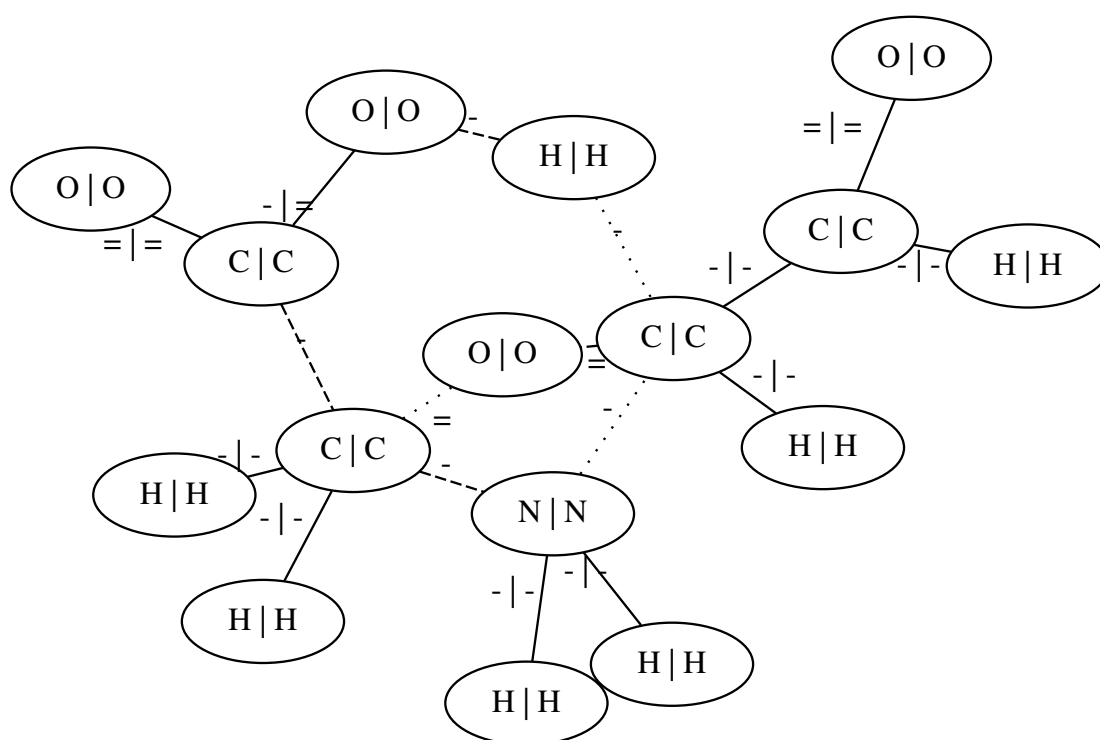
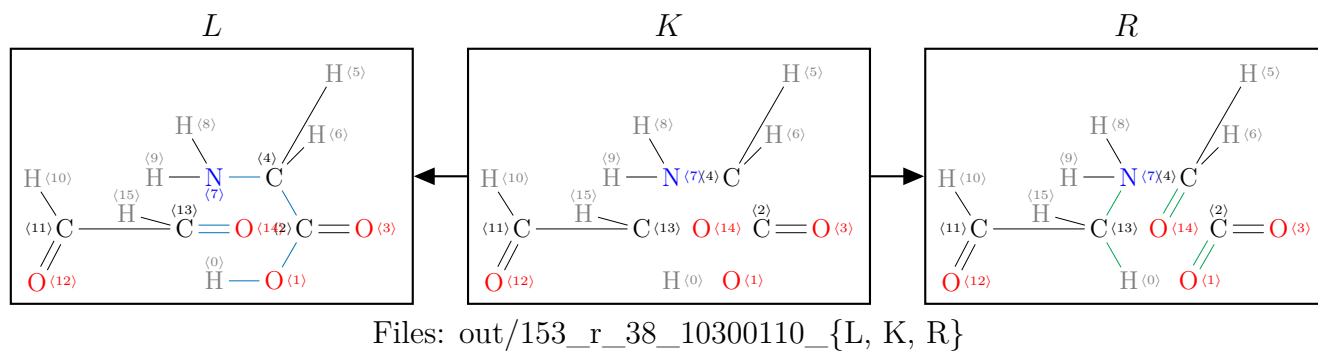
$$\begin{aligned}
 &|\{e \in \text{outEdges}(0) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{'=\'} \\
 &\}\} = 0
 \end{aligned}$$

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

1.0.38 HCN to Ketone

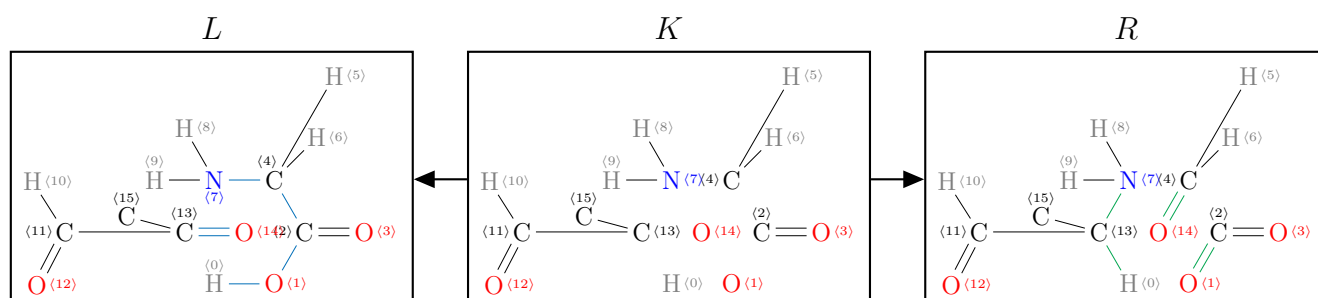


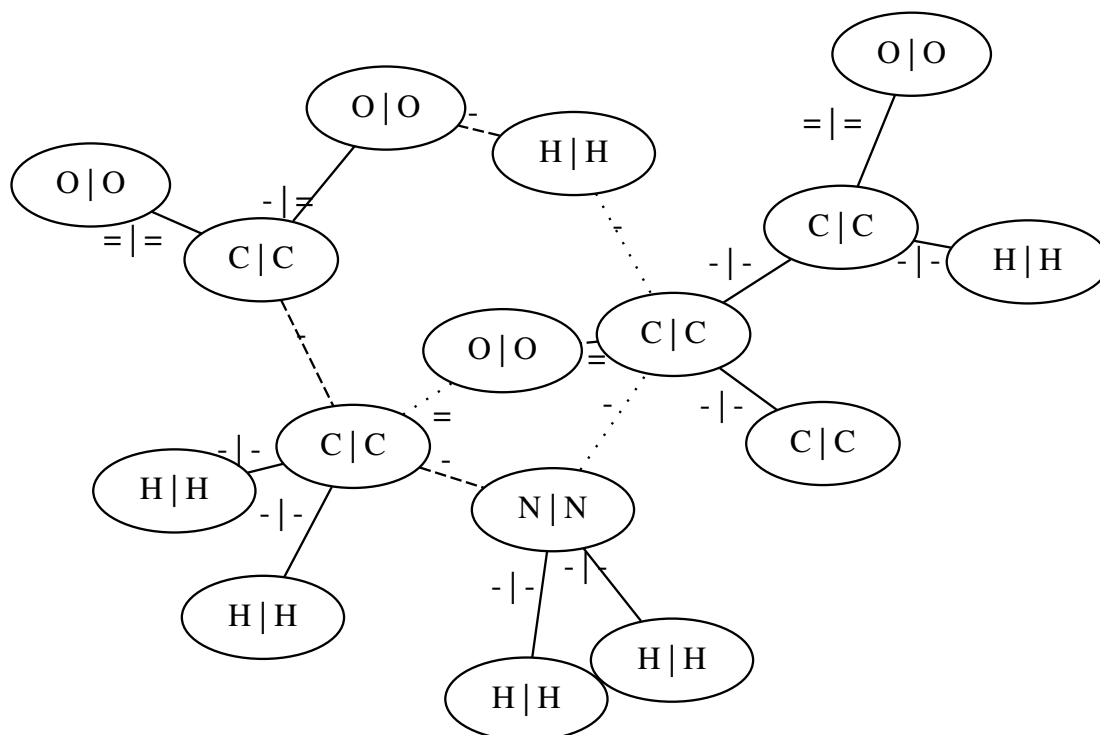
1.0.39 Strecker Degradation Dicarbonyl, H, H, H, H



File: out/154_r_38_combined

1.0.40 Strecker Degradation Dicarbonyl, H, H, H, C

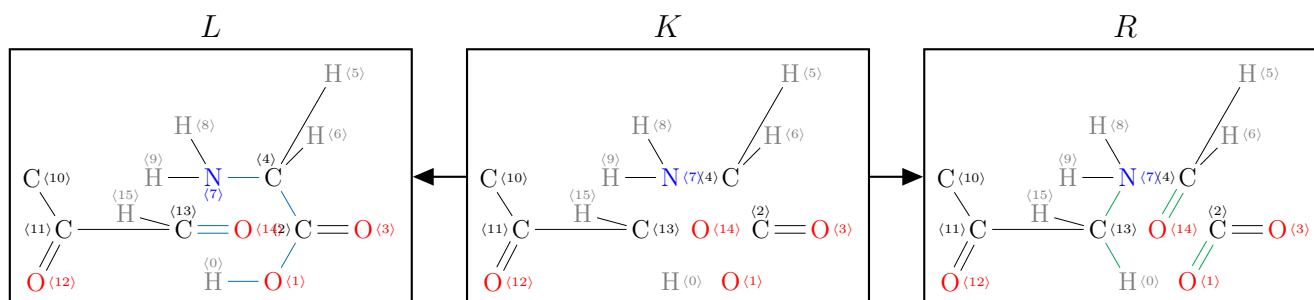




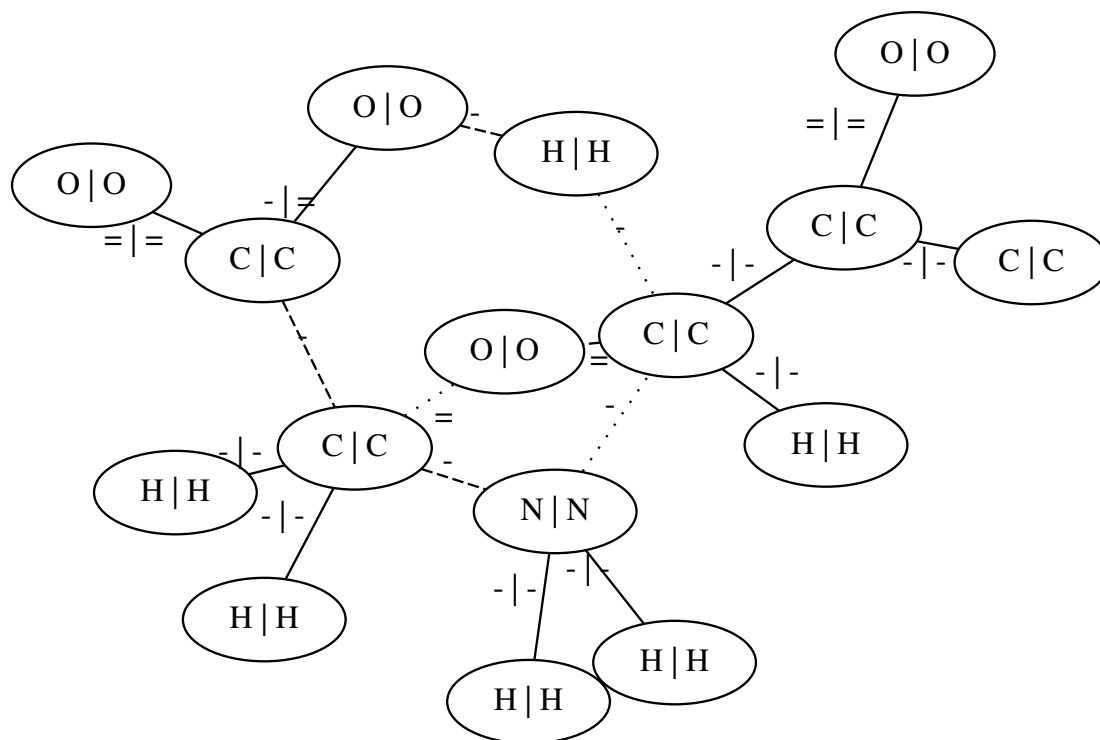
File: out/158_r_39_combined

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

1.0.41 Strecker Degradation Dicarbonyl, H, H, C, H



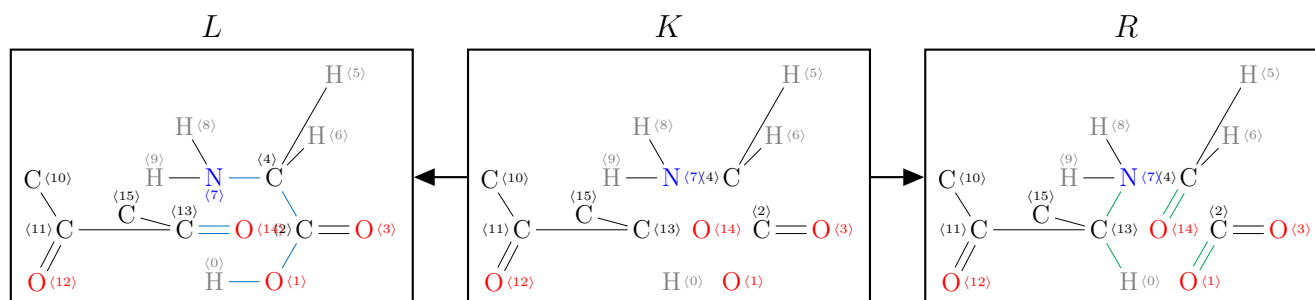
Files: out/161_r_40_10300110_{L, K, R}



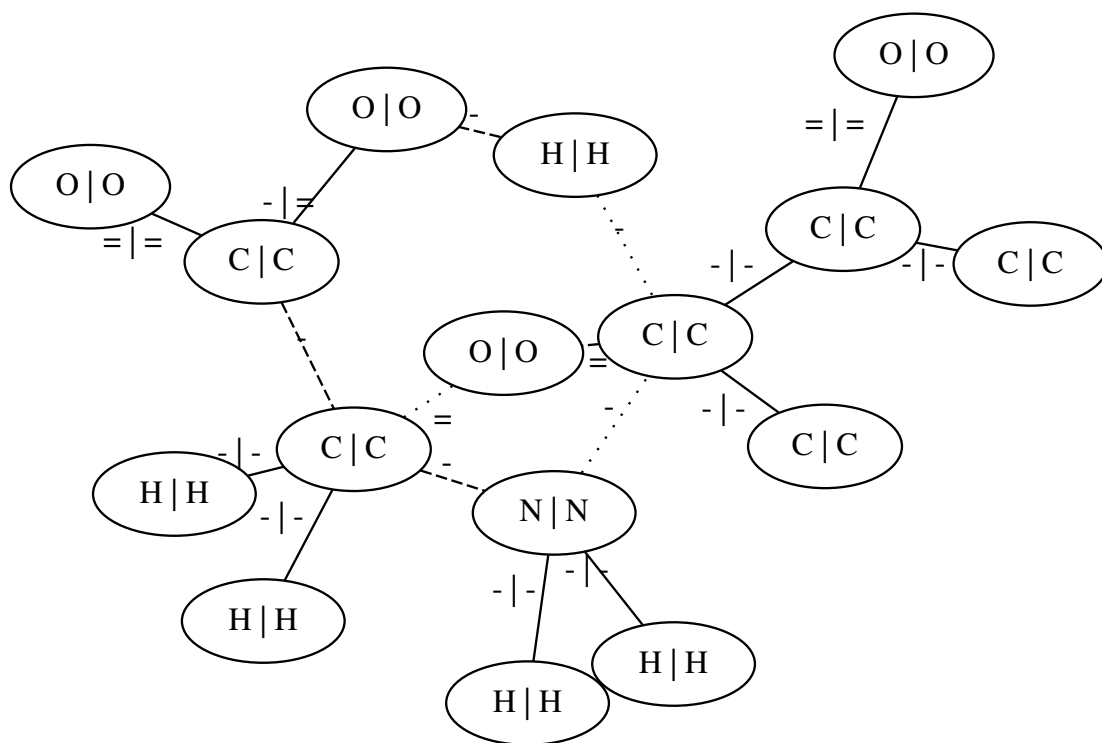
File: out/162_r_40_combined

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

1.0.42 Strecker Degradation Dicarbonyl, H, H, C, C



Files: out/165_r_41_10300110_{L, K, R}



File: out/166_r_41_combined

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

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

$$\wedge$$

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

$$\} = 0$$

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

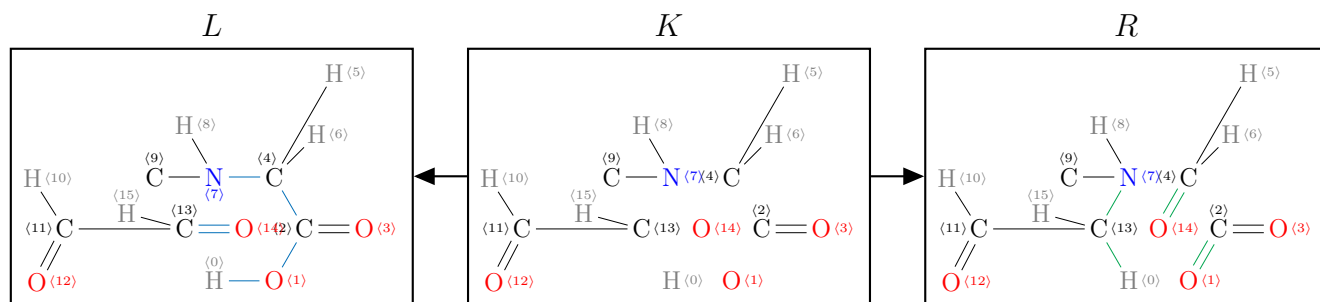
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

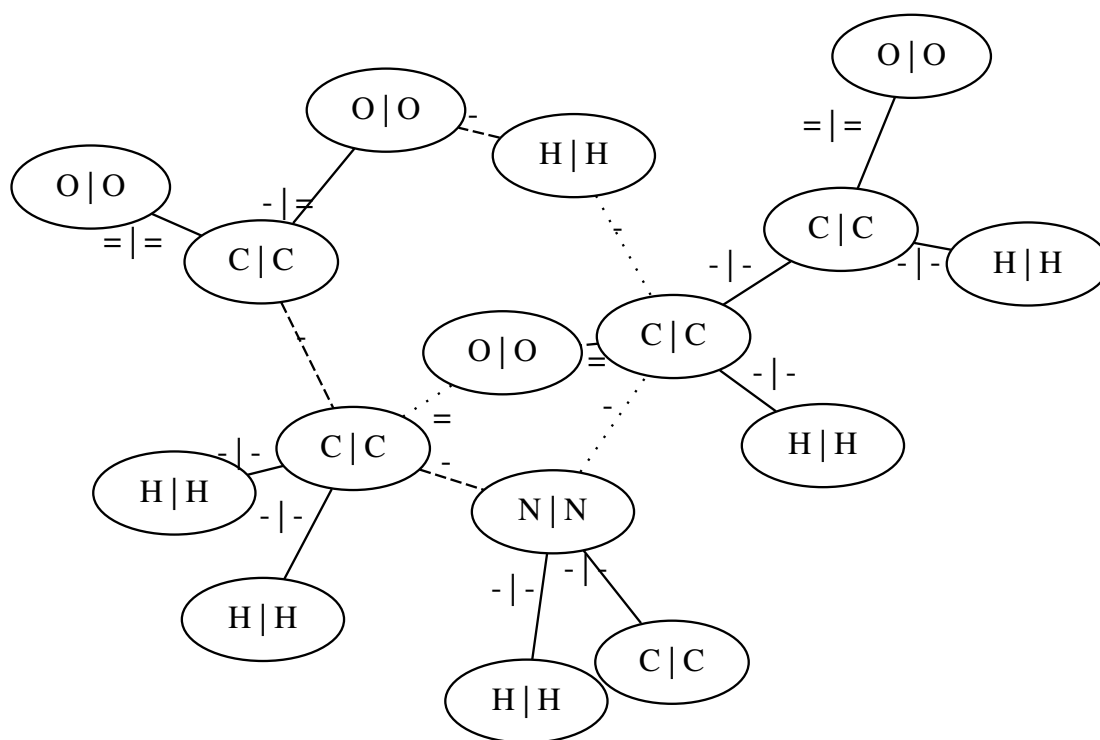
$$\text{label}(e) \in \{'=\'}\}$$

$$\} = 0$$

1.0.43 Strecker Degradation Dicarbonyl, H, C, H, H



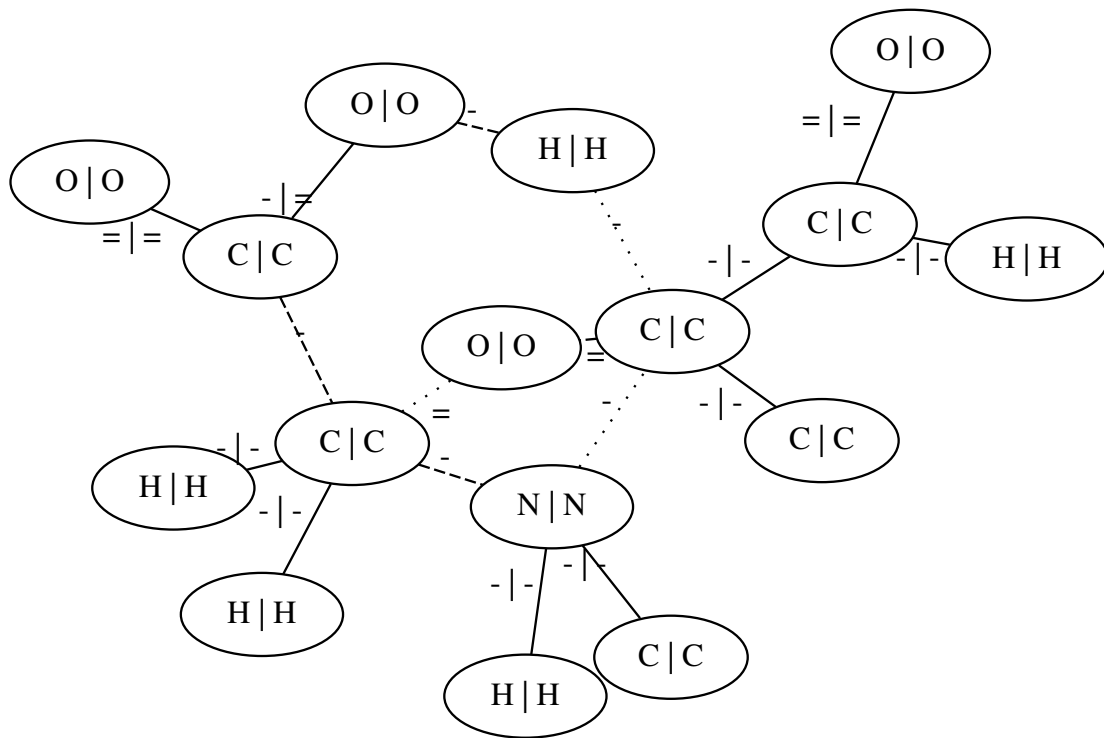
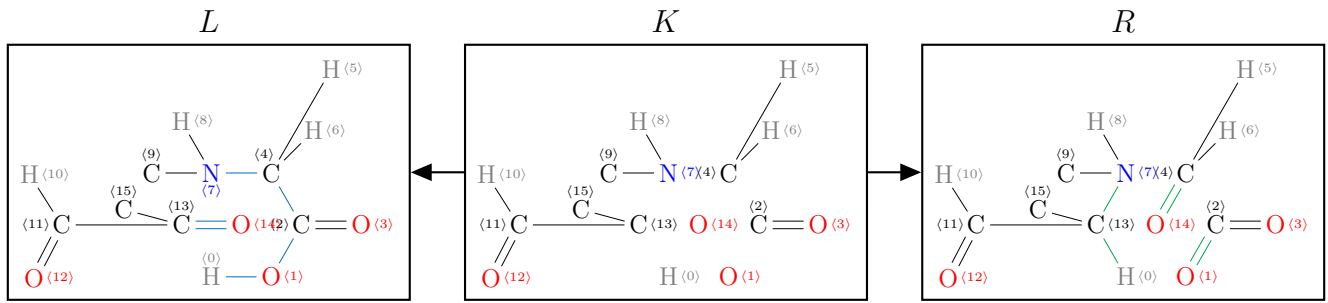
Files: out/169_r_42_10300110_{L, K, R}



File: out/170_r_42_combined

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

1.0.44 Strecker Degradation Dicarbonyl, H, C, H, C

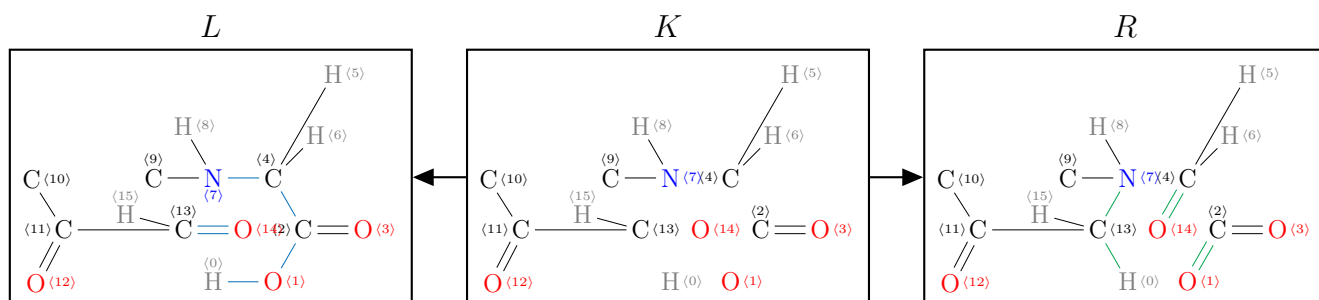


File: out/174_r_43_combined

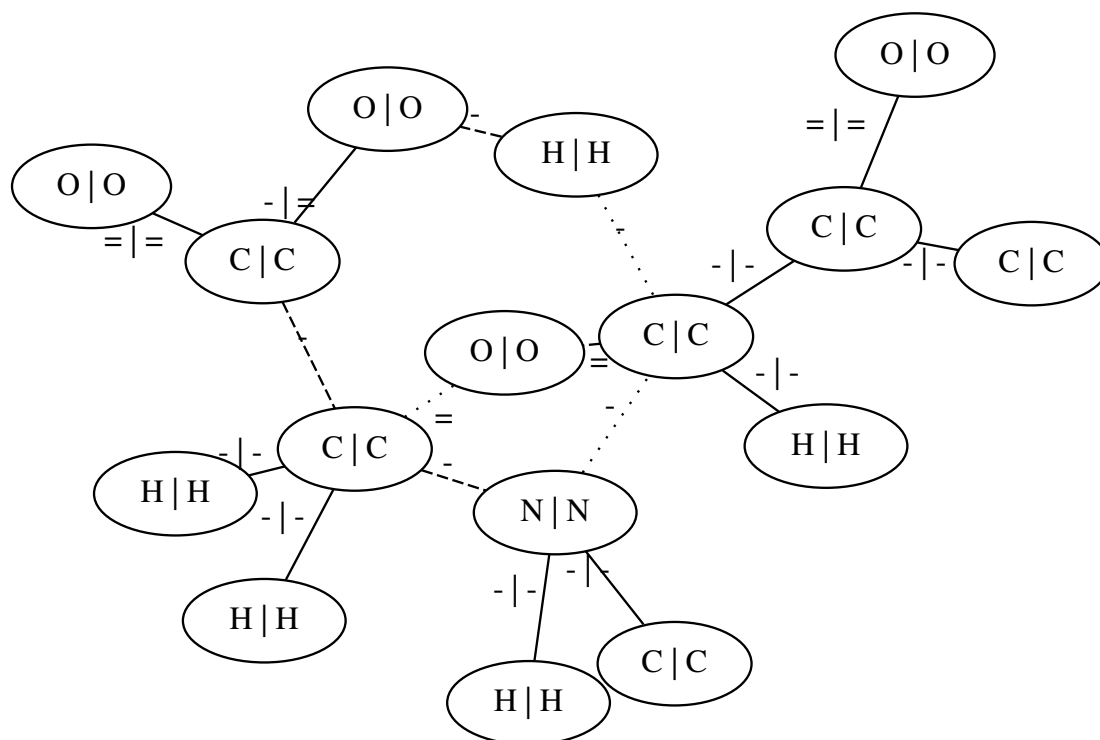
$$\begin{aligned}
 &|\{e \in \text{outEdges}(9) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{'=\'} \\
 &\}\} = 0
 \end{aligned}$$

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

1.0.45 Strecker Degradation Dicarbonyl, H, C, C, H



Files: out/177_r_44_10300110_{L, K, R}

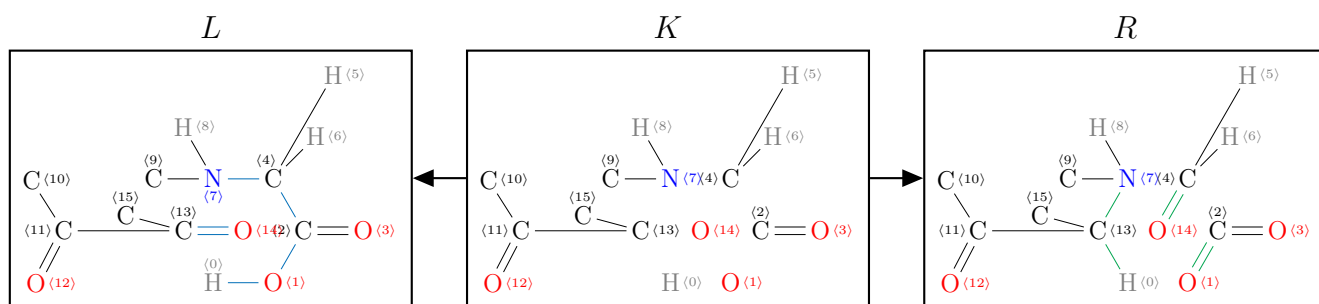


File: out/178_r_44_combined

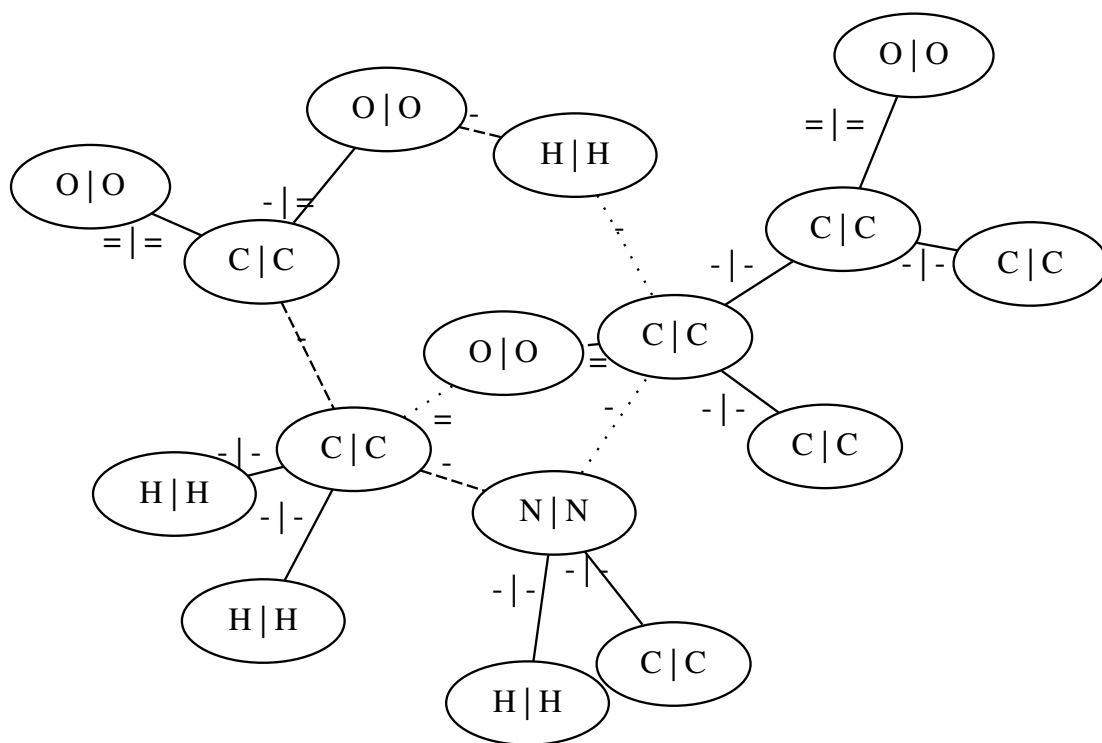
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \mid\} = 0
\end{aligned}$$

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

1.0.46 Strecker Degradation Dicarbonyl, H, C, C, C



Files: out/181_r_45_10300110_{L, K, R}



File: out/182_r_45_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

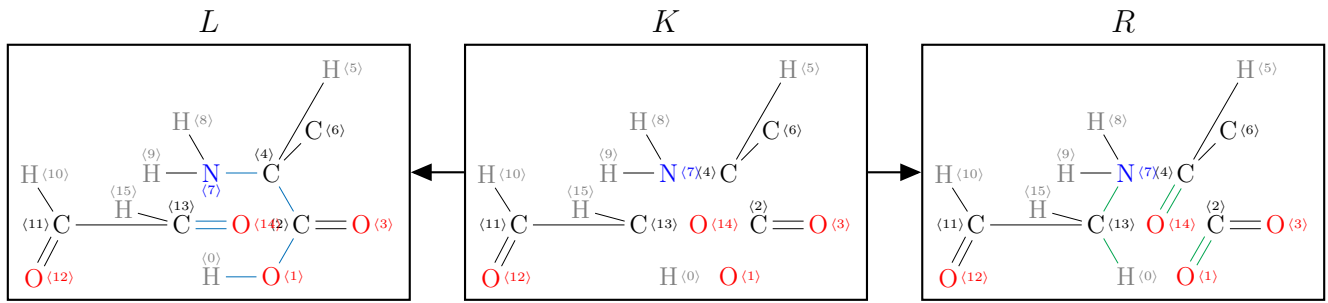
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

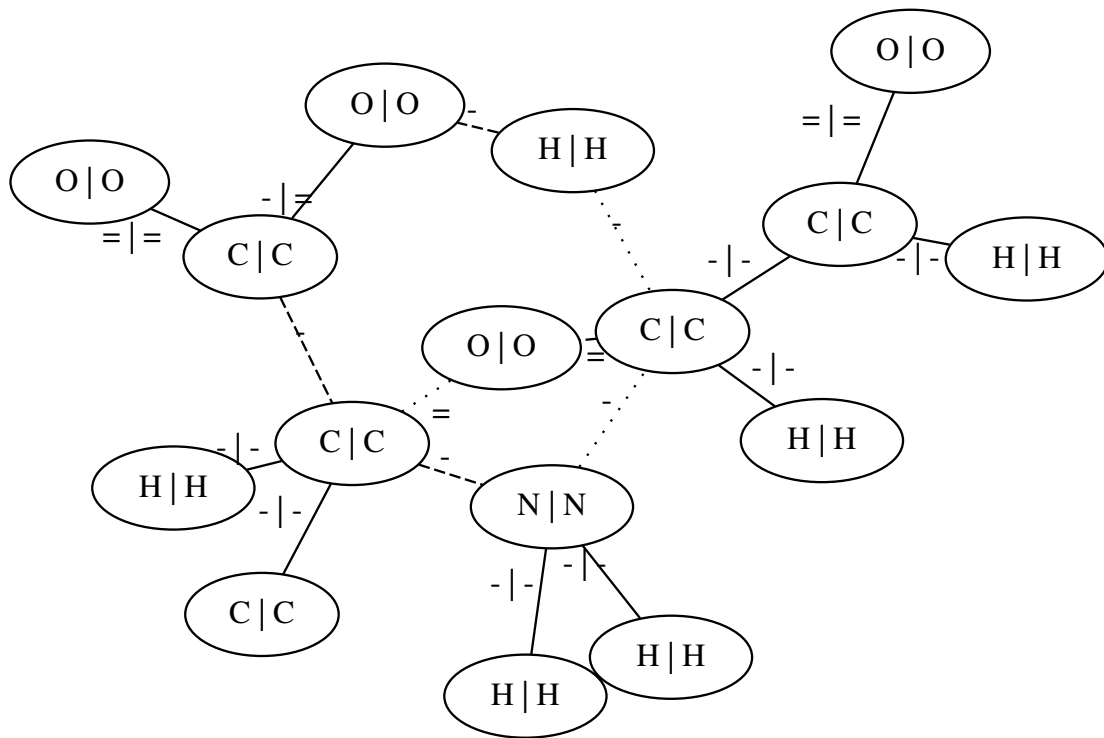
$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

1.0.47 Strecker Degradation Dicarbonyl, C, H, H, H



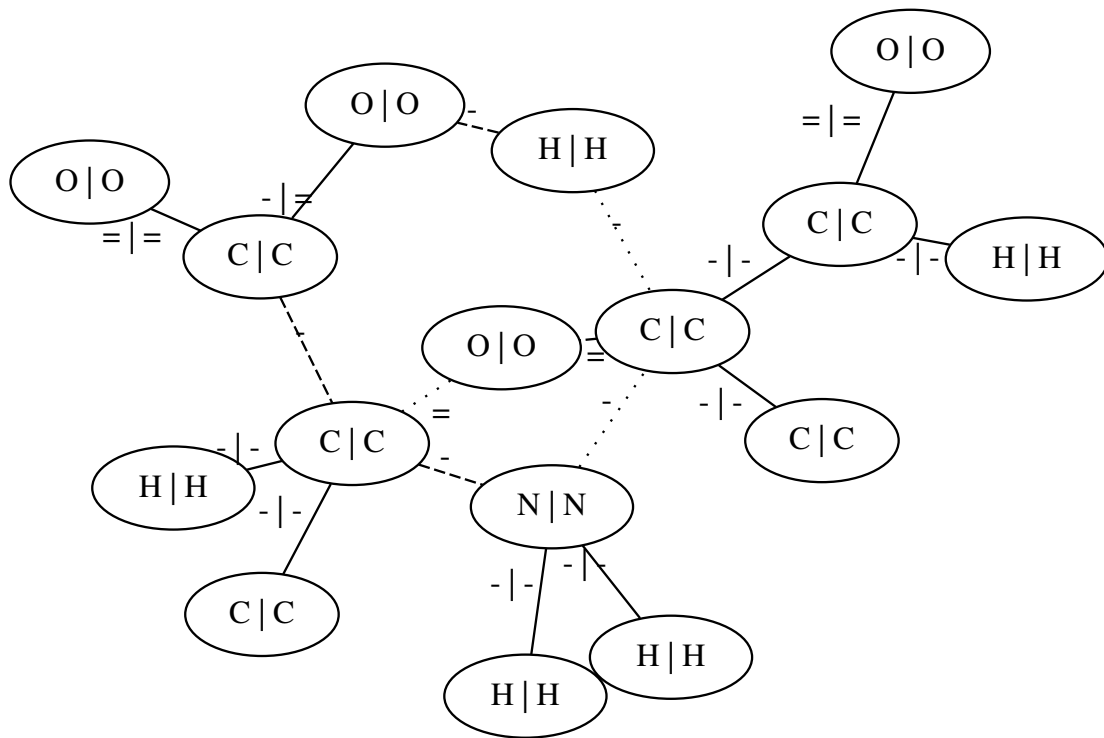
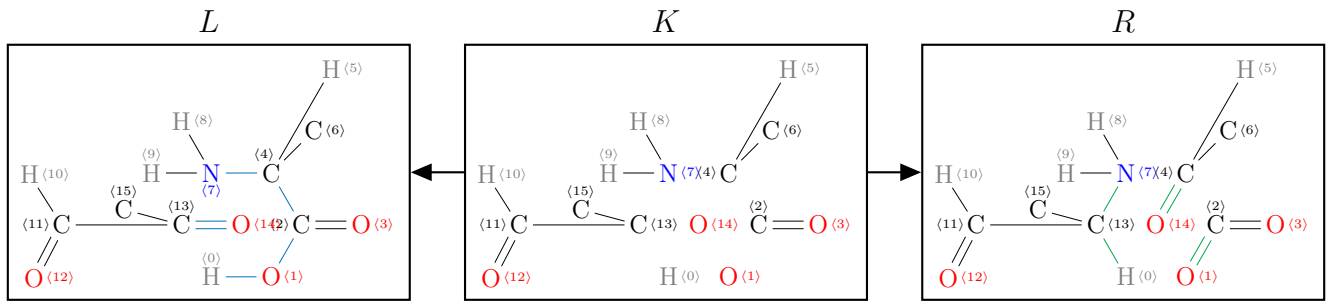
Files: out/185_r_46_10300110_{L, K, R}



File: out/186_r_46_combined

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

1.0.48 Strecker Degradation Dicarbonyl, C, H, H, C

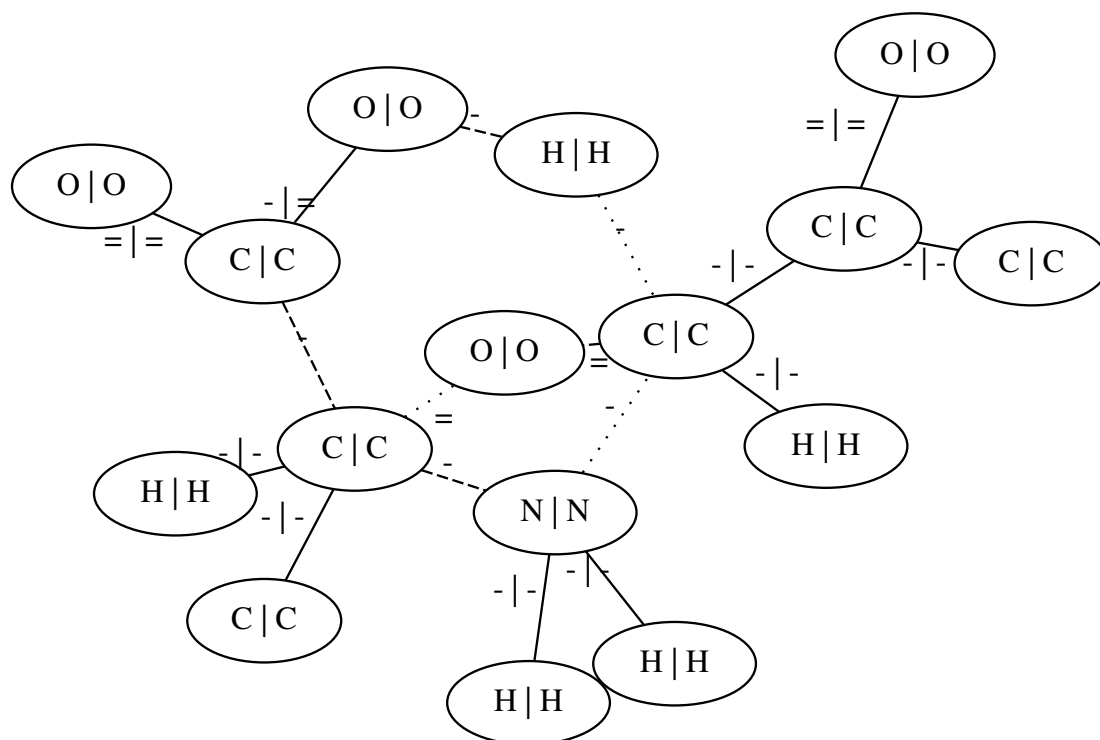
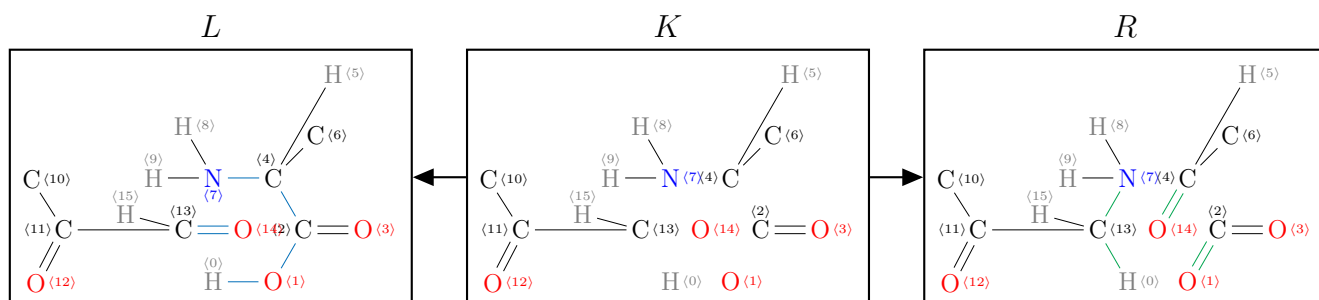


File: out/190_r_47_combined

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

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

1.0.49 Strecker Degradation Dicarbonyl, C, H, C, H

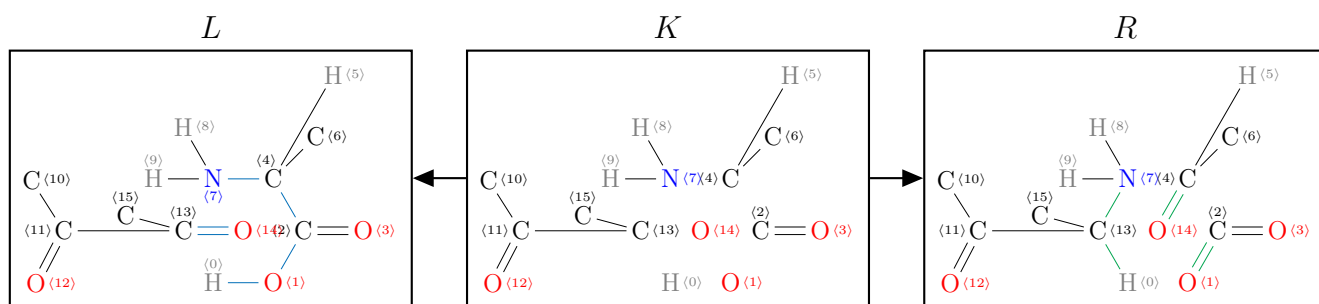


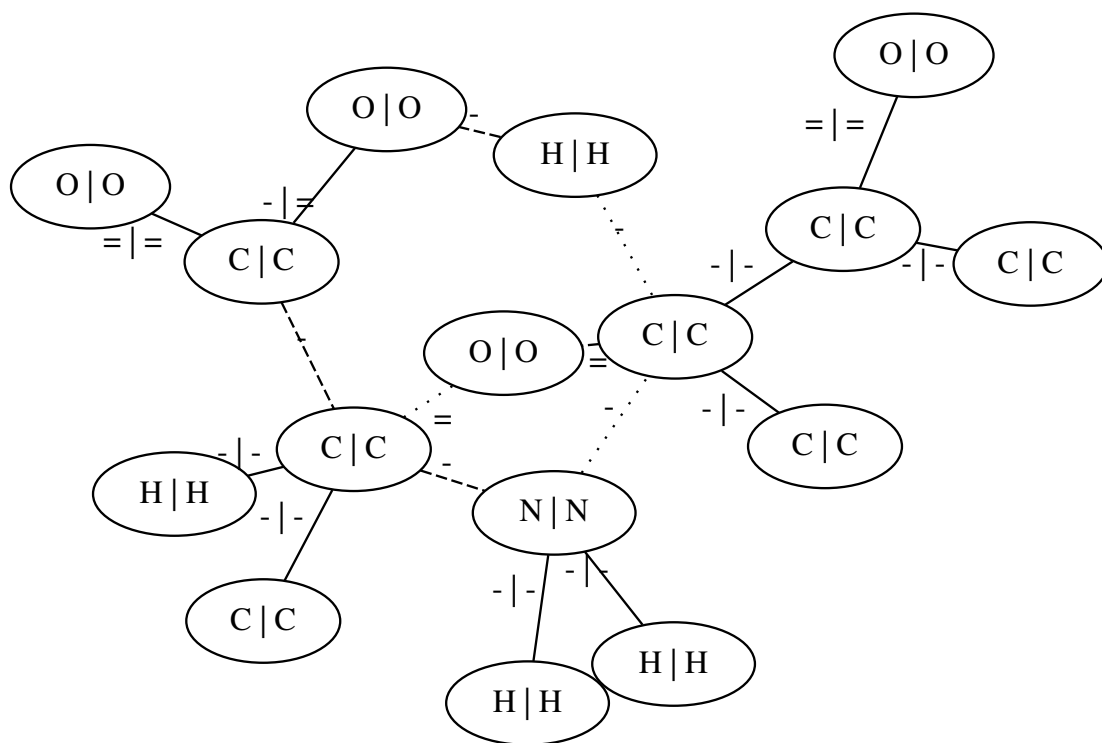
File: out/194_r_48_combined

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

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

1.0.50 Strecker Degradation Dicarbonyl, C, H, C, C





File: out/198_r_49_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

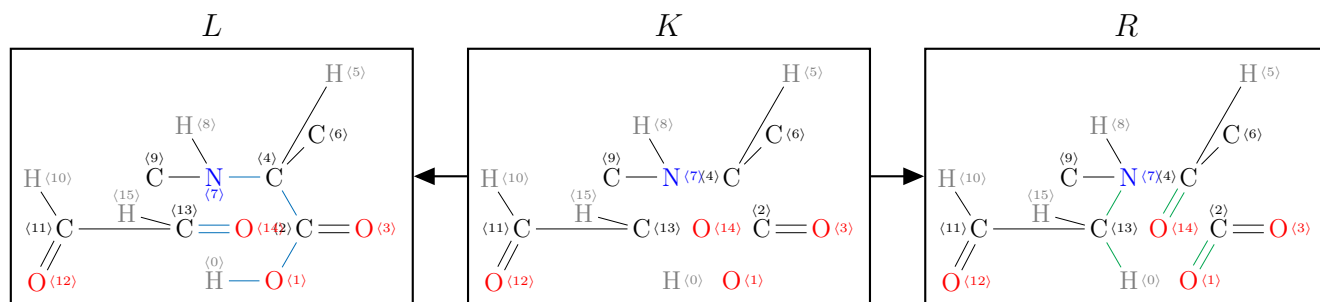
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

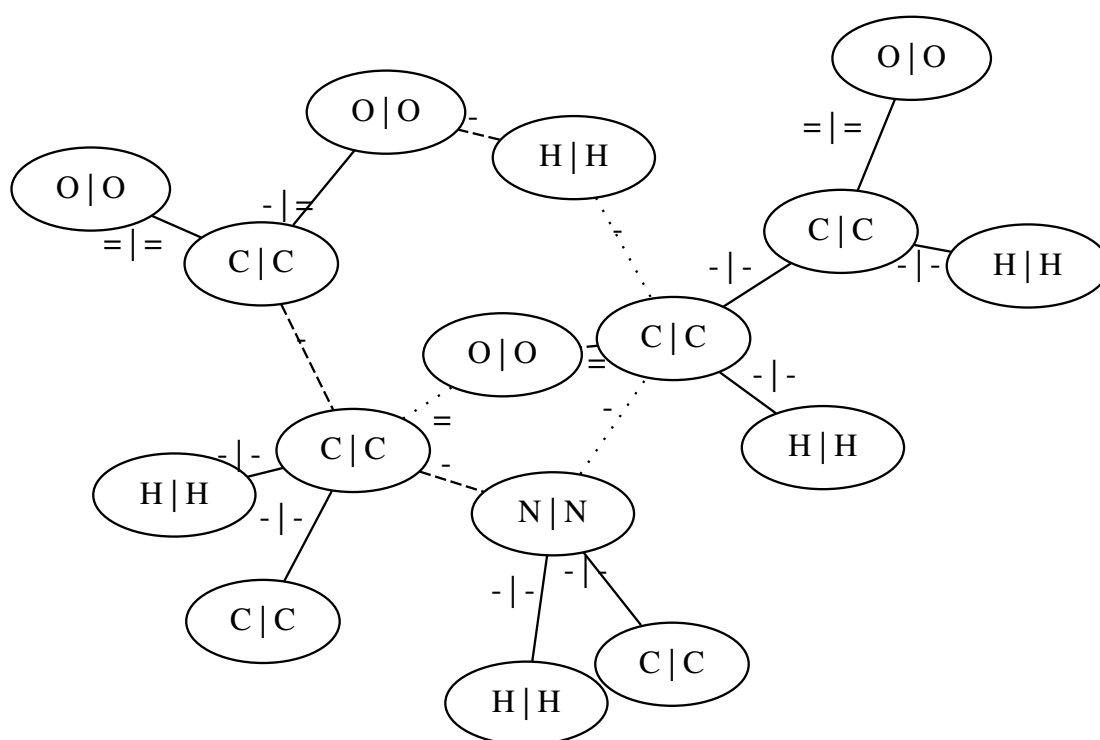
$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

1.0.51 Strecker Degradation Dicarbonyl, C, C, H, H



Files: out/201_r_50_10300110_{L, K, R}

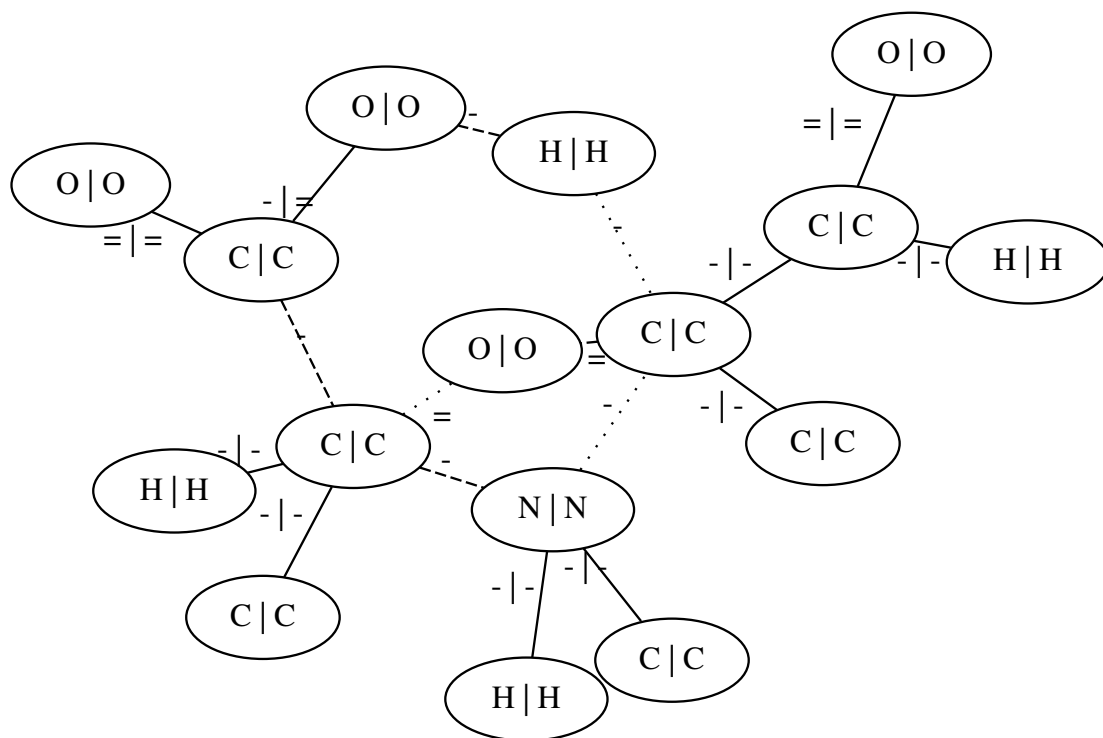
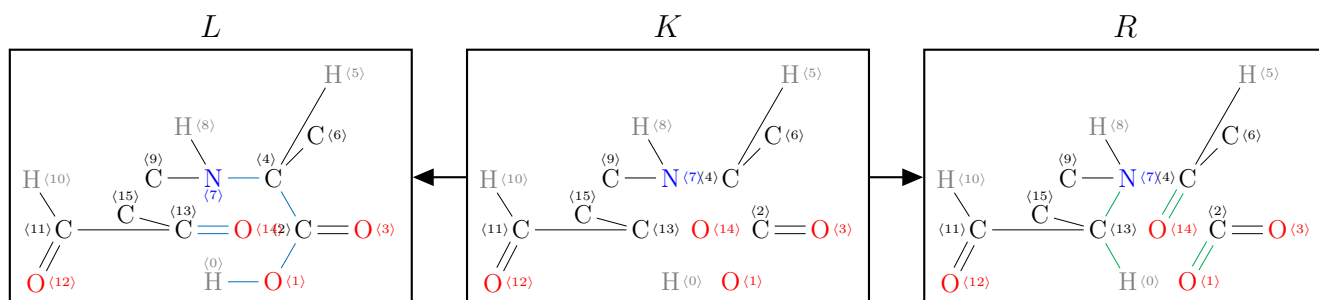


File: out/202_r_50_combined

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

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

1.0.52 Strecker Degradation Dicarbonyl, C, C, H, C



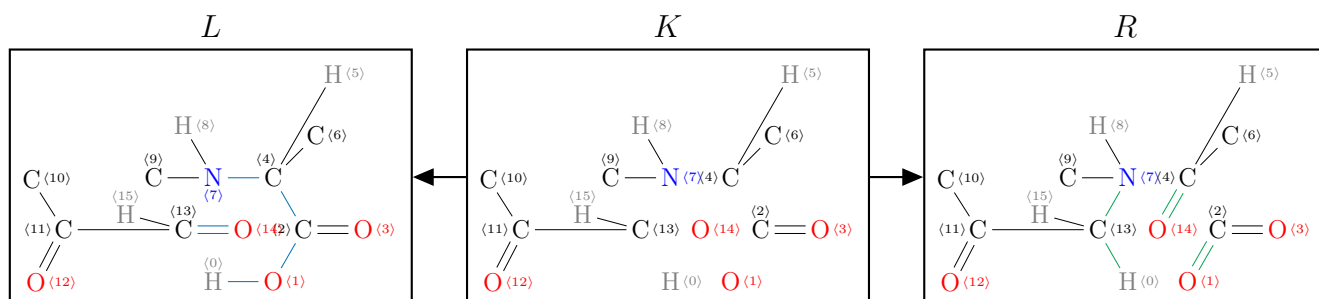
File: out/206_r_51_combined

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

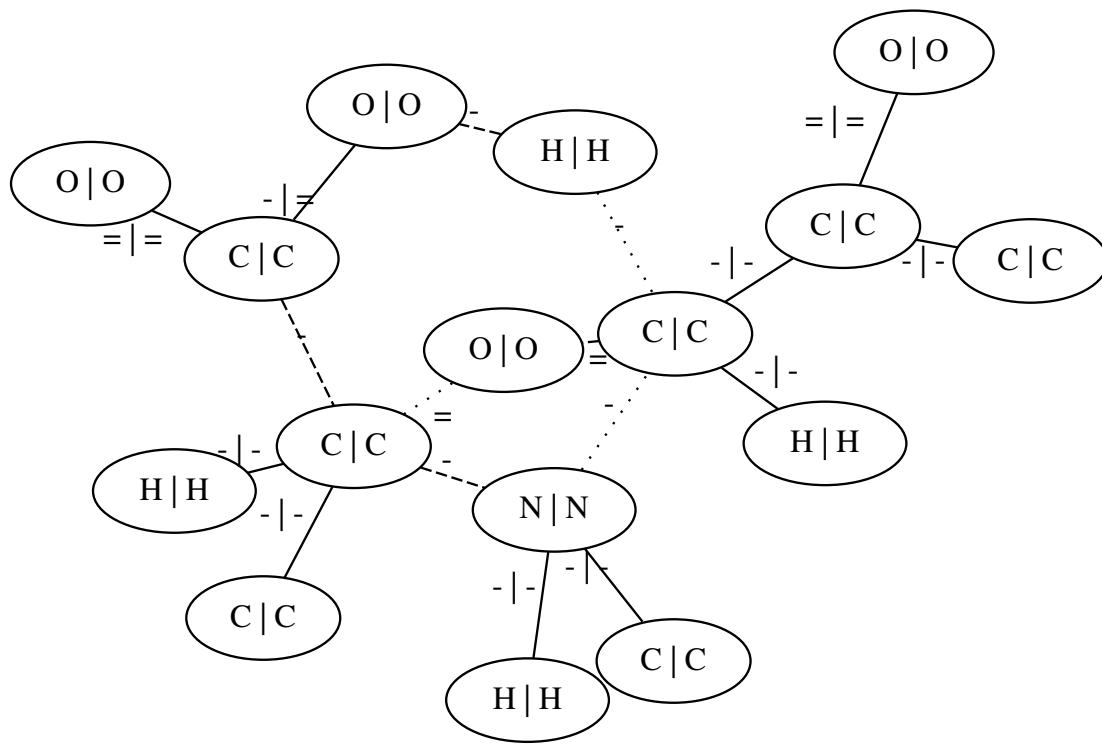
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{'=\'} \\
& \quad \}\mid = 0
\end{aligned}$$

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

1.0.53 Strecker Degradation Dicarbonyl, C, C, C, H



Files: out/209_r_52_10300110_{L, K, R}



File: out/210_r_52_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

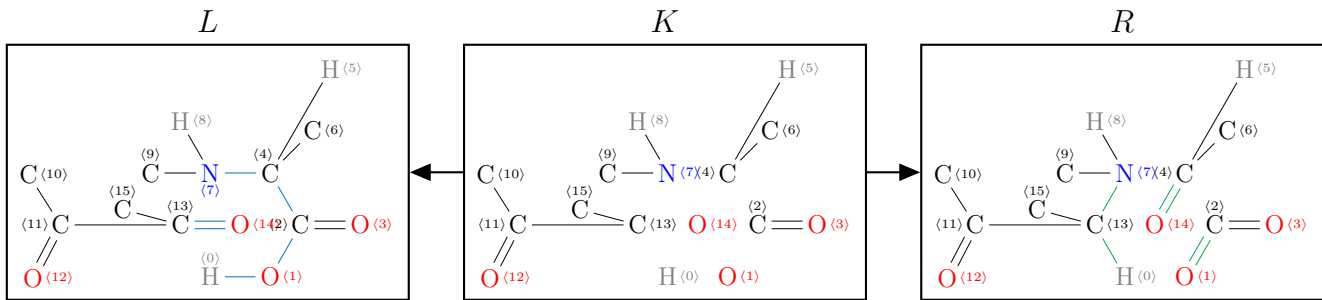
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

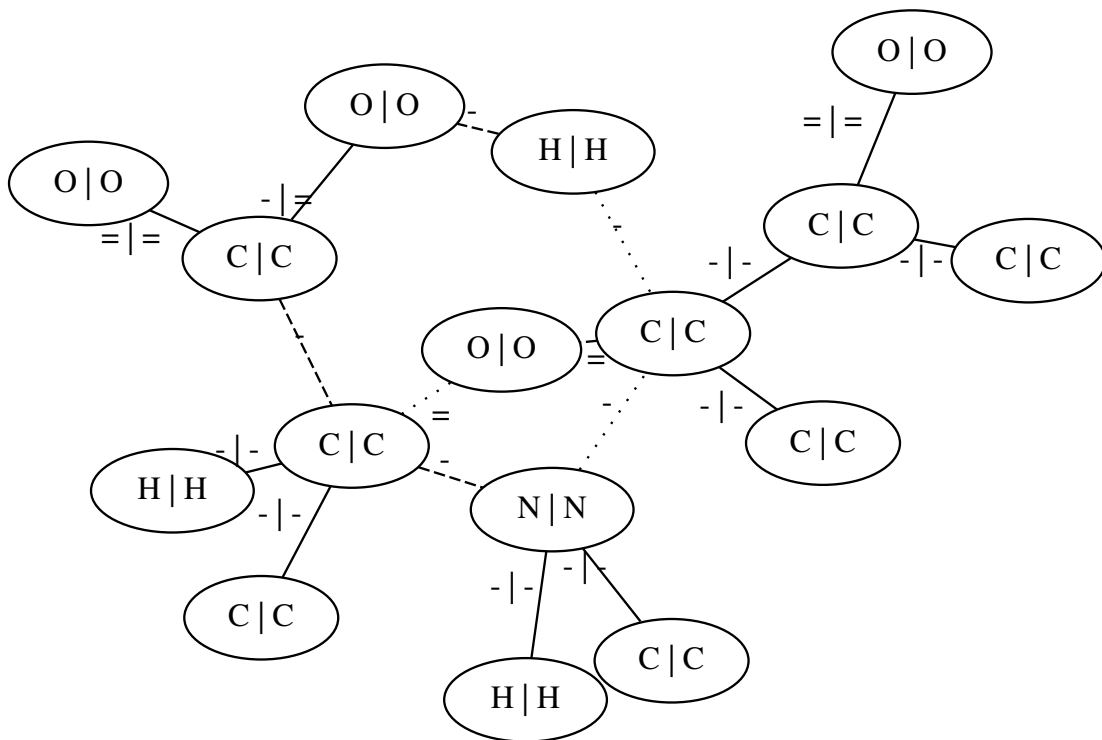
$$\text{label}(e) \in \{'=\'}\}$$

$$\}| = 0$$

1.0.54 Strecker Degradation Dicarboxyl, C, C, C, C



Files: out/213_r_53_10300110_{L, K, R}



File: out/214_r_53_combined

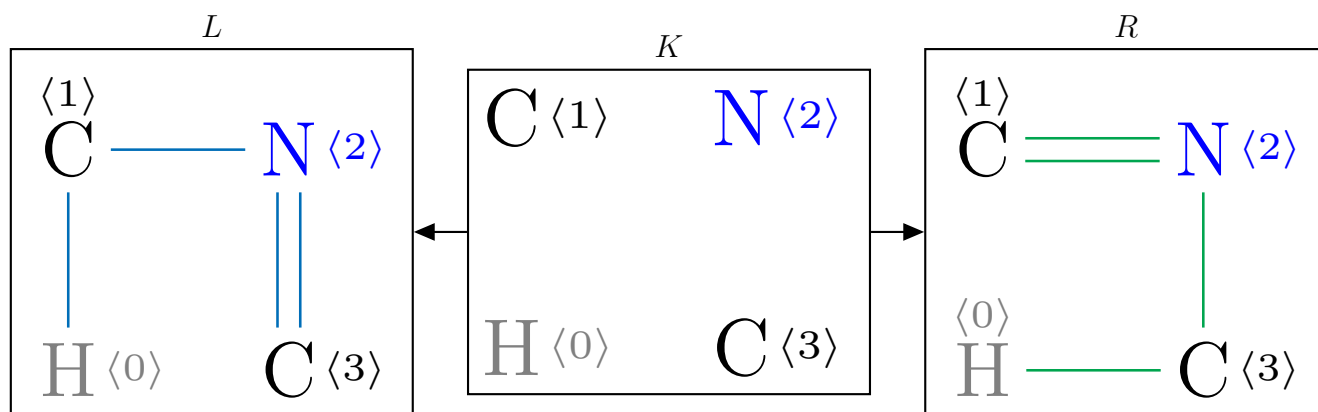
$$\begin{aligned} & |\{e \in \text{outEdges}(6) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'='}\} \\ & \quad \}| = 0 \end{aligned}$$

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

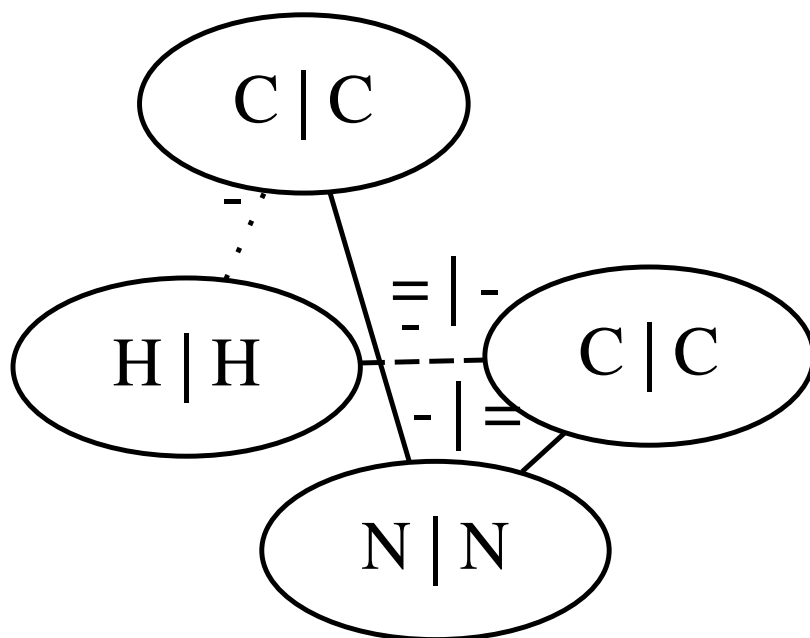
$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

1.0.55 Schiff Tautomerization

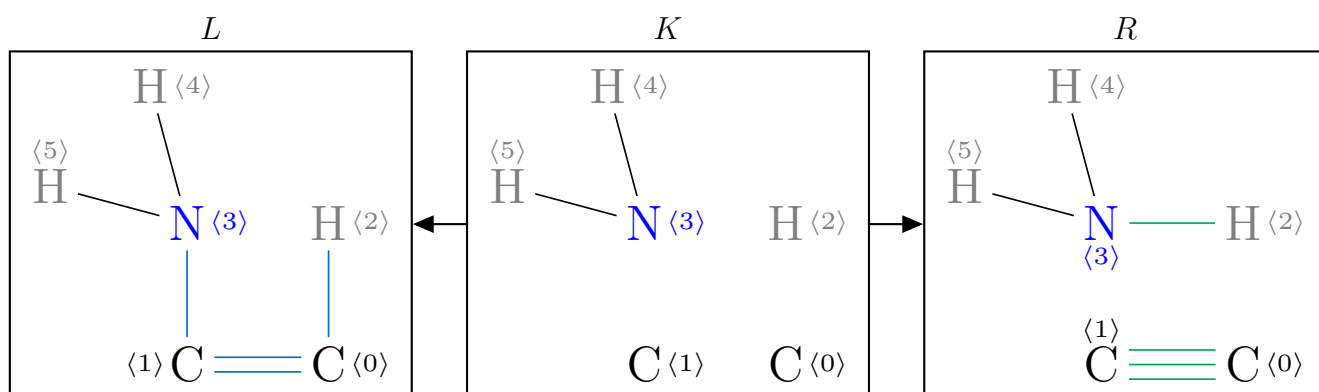


Files: out/217_r_54_10300110_{L, K, R}

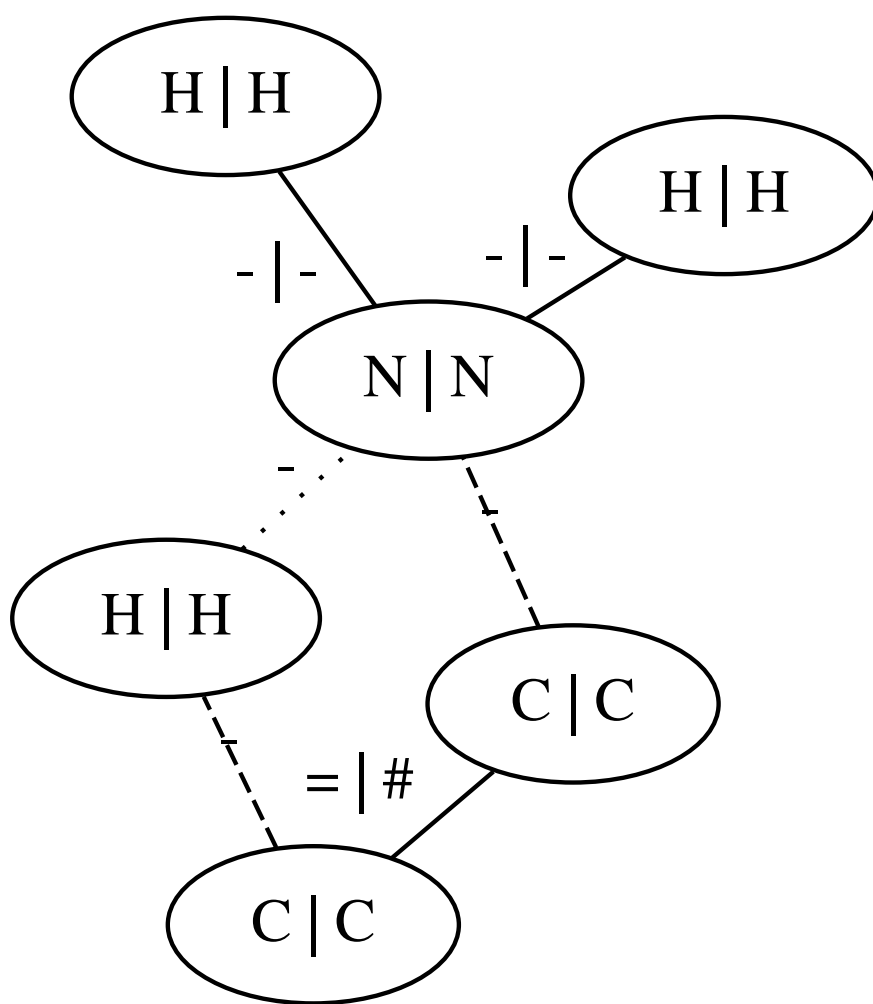


File: out/218_r_54_combined

1.0.56 Alkyne Addition, N, HH, inverse

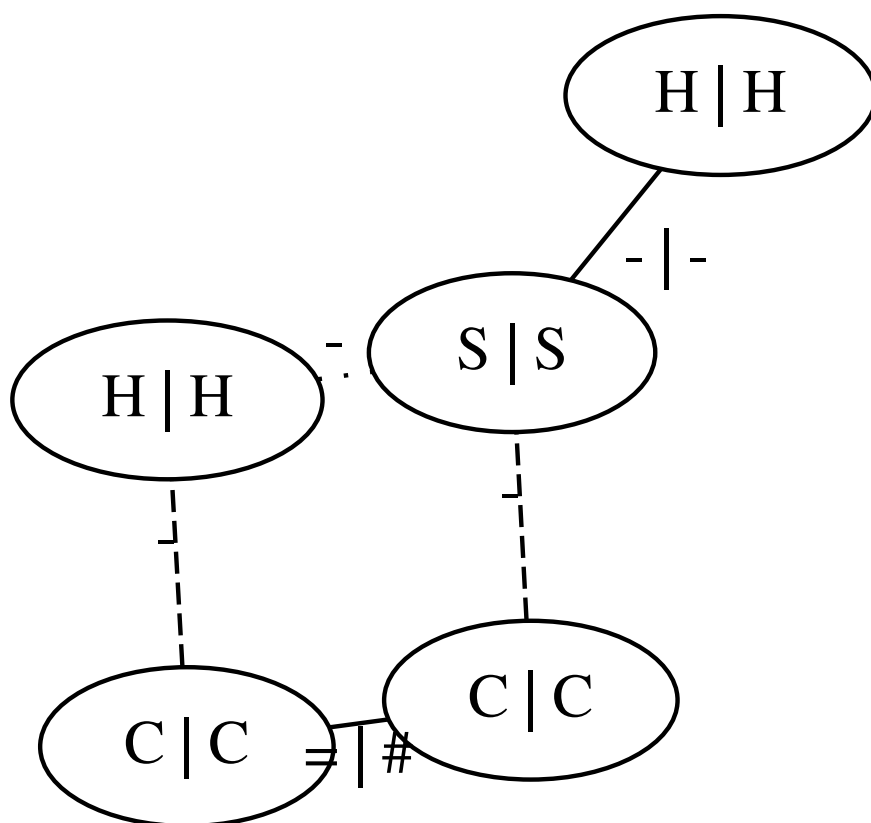
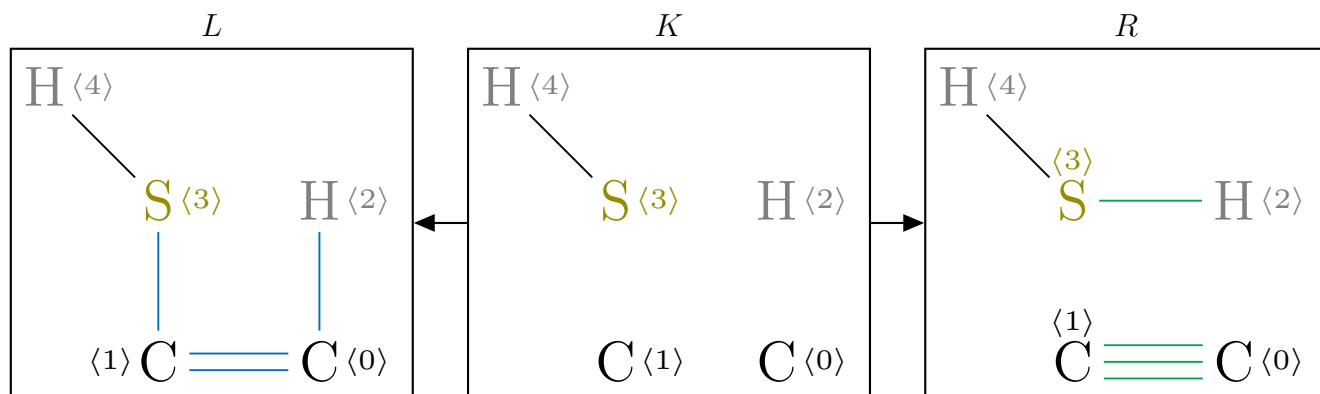


Files: out/221_r_55_10300110_{L, K, R}



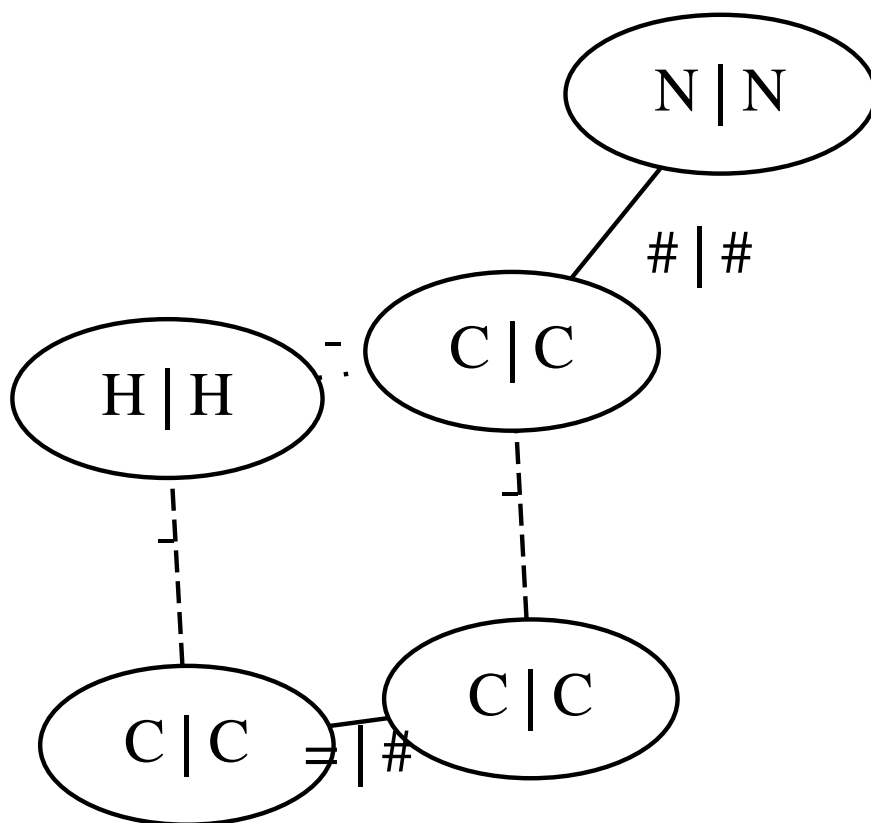
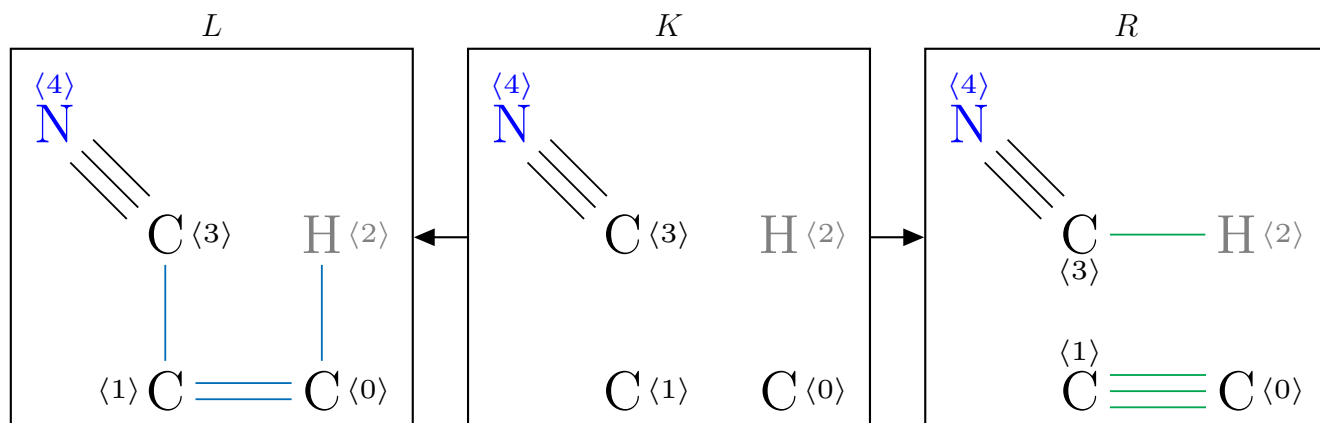
File: out/222_r_55_combined

1.0.57 Alkyne Addition, S, H, inverse

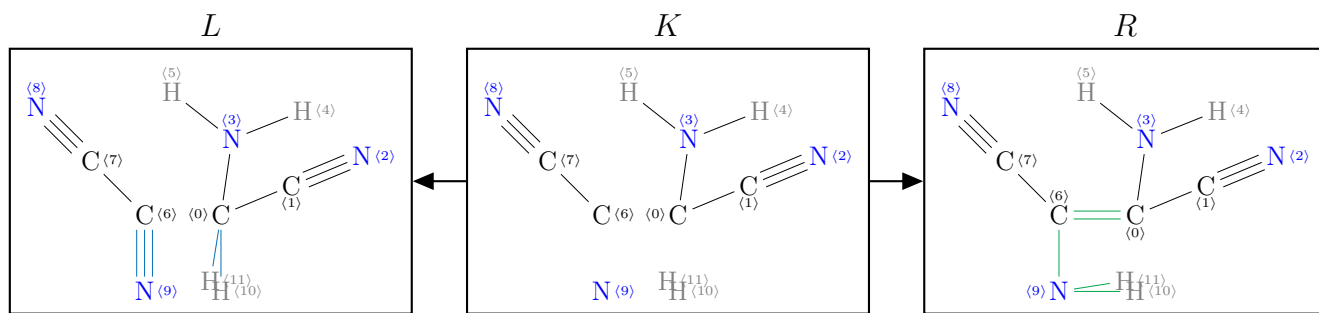


File: out/226_r_56_combined

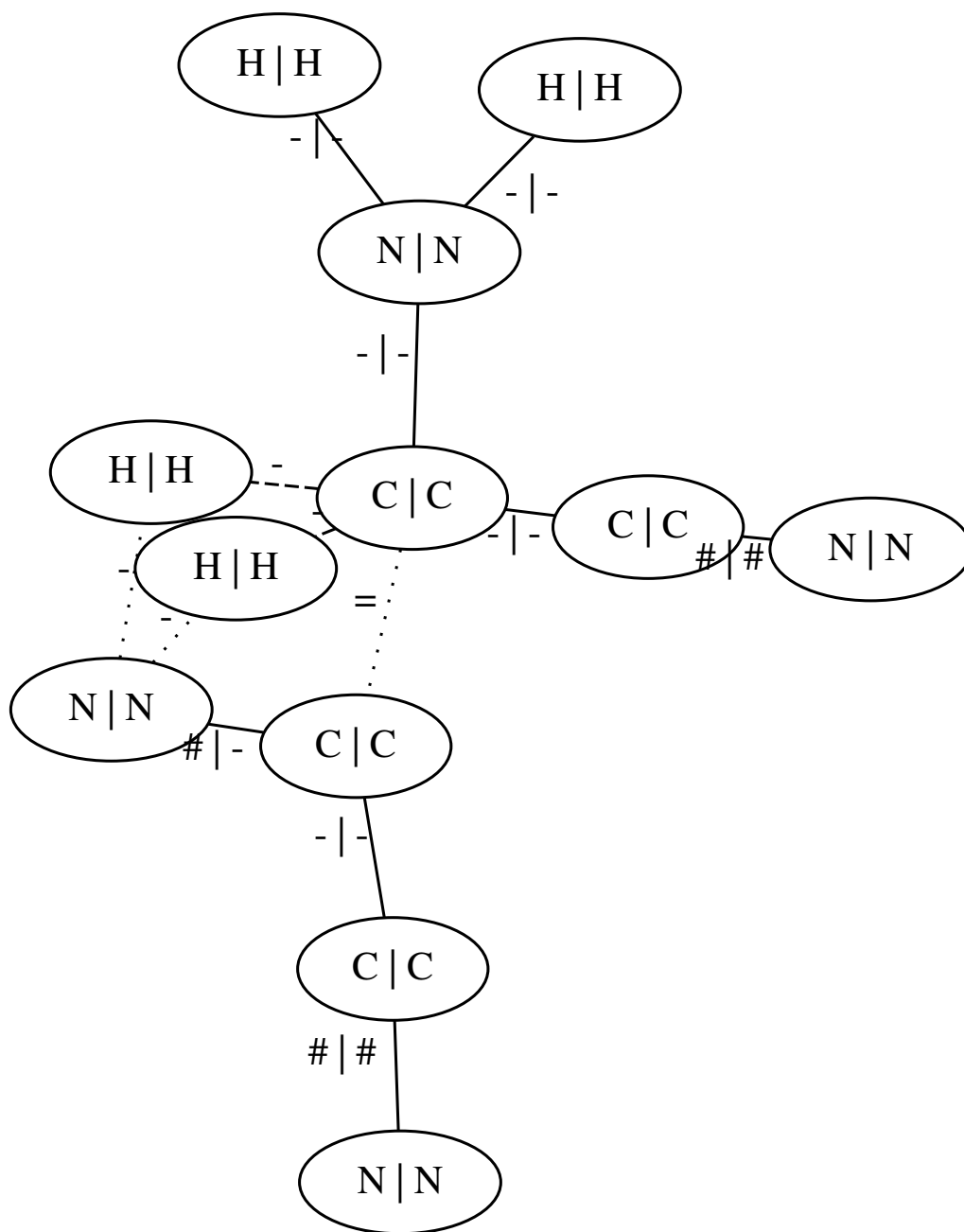
1.0.58 Alkyne Addition, C, inverse



1.0.59 DAMN Scission, inverse

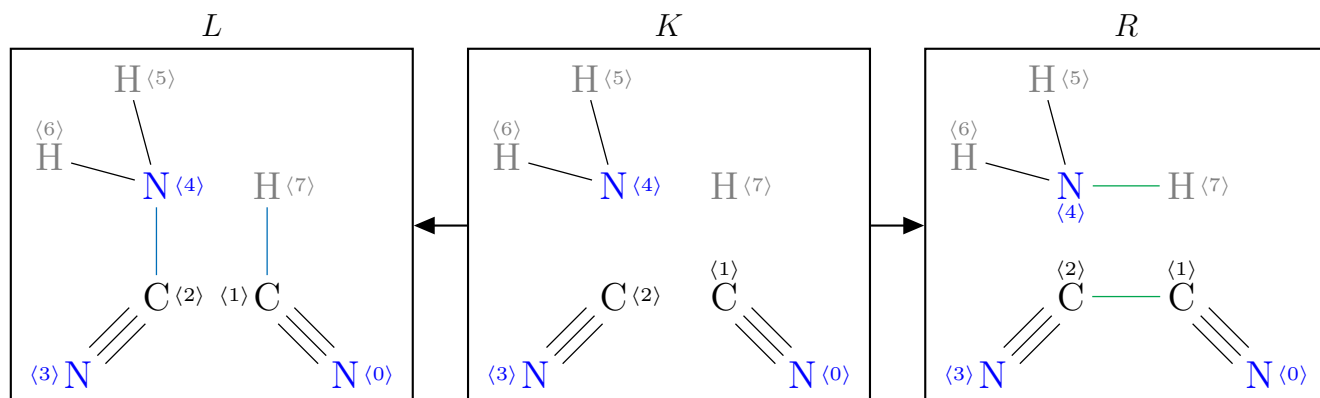


Files: out/233_r_58_10300110_{L, K, R}

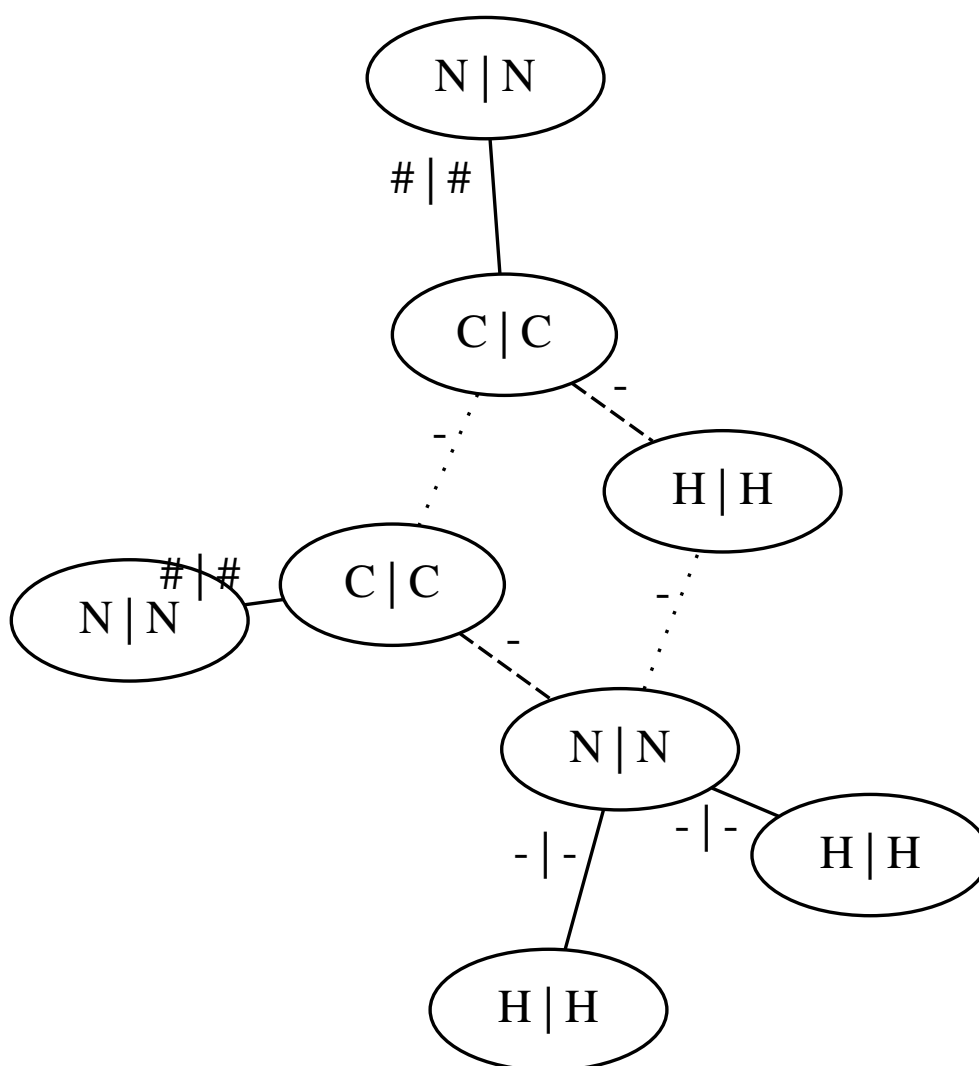


File: out/234_r_58_combined

1.0.60 Cyanogen Ammonolysis, inverse

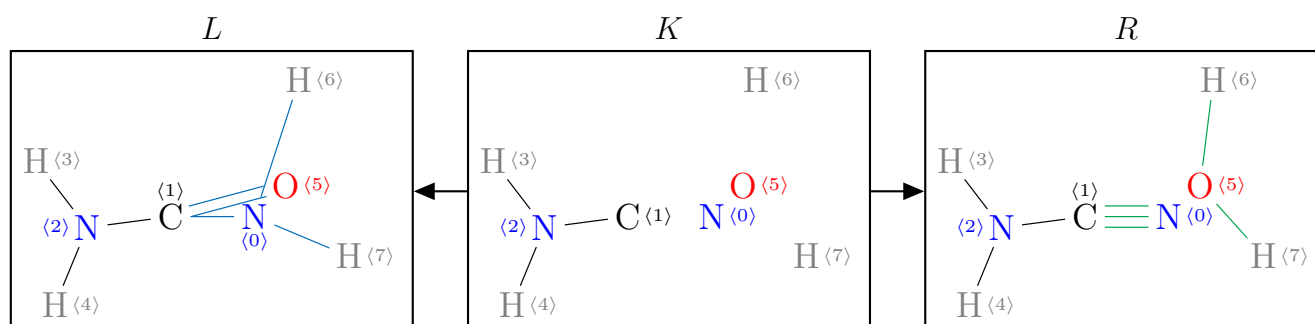


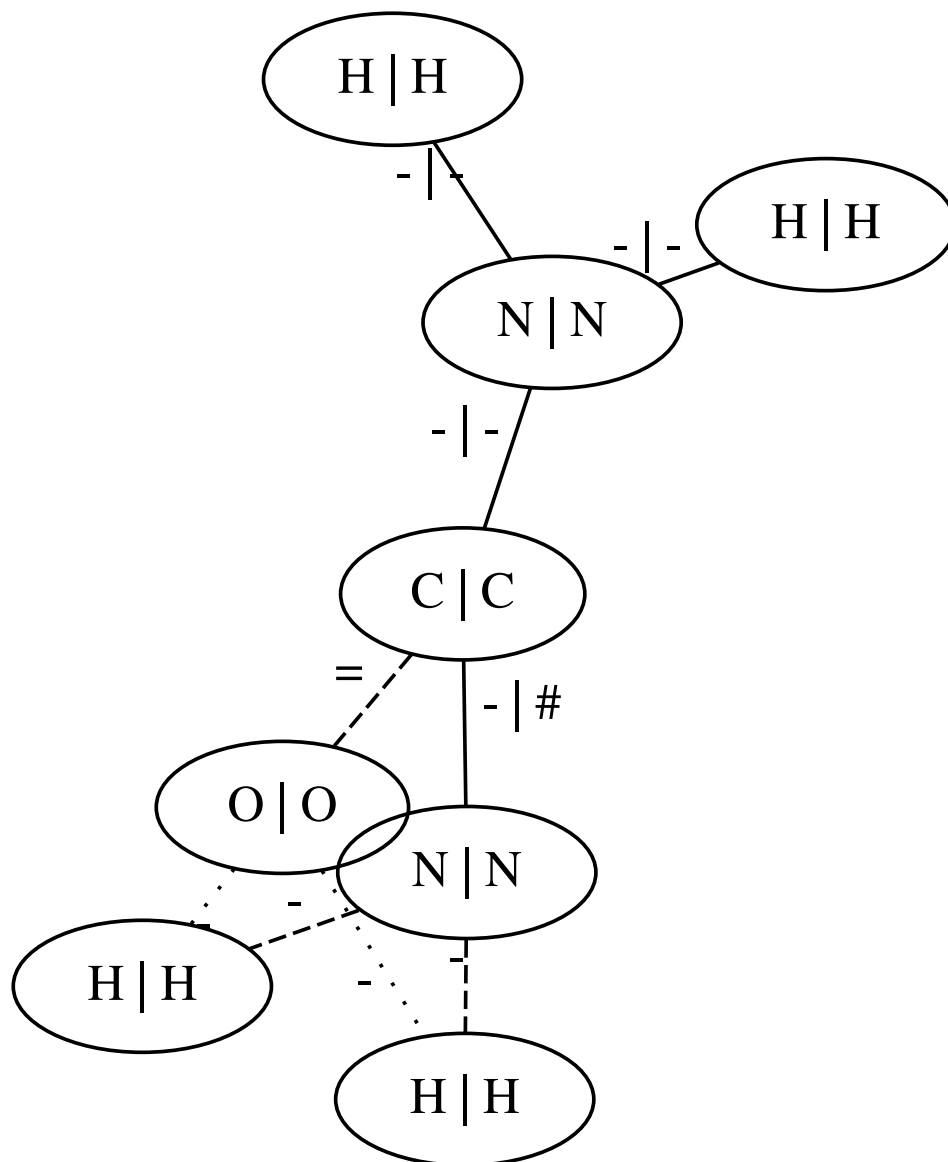
Files: out/237_r_59_10300110_{L, K, R}



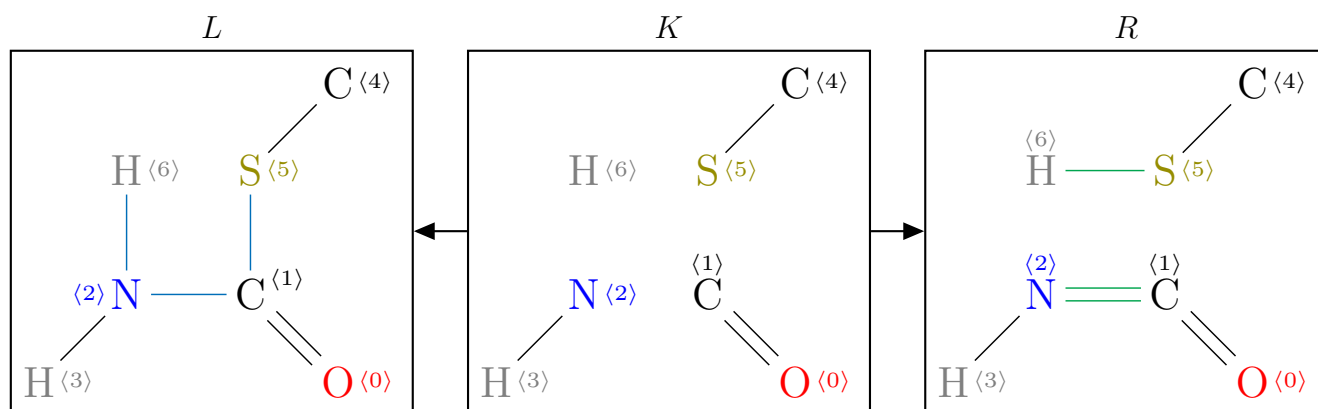
File: out/238_r_59_combined

1.0.61 Cyanamide Hydration, inverse

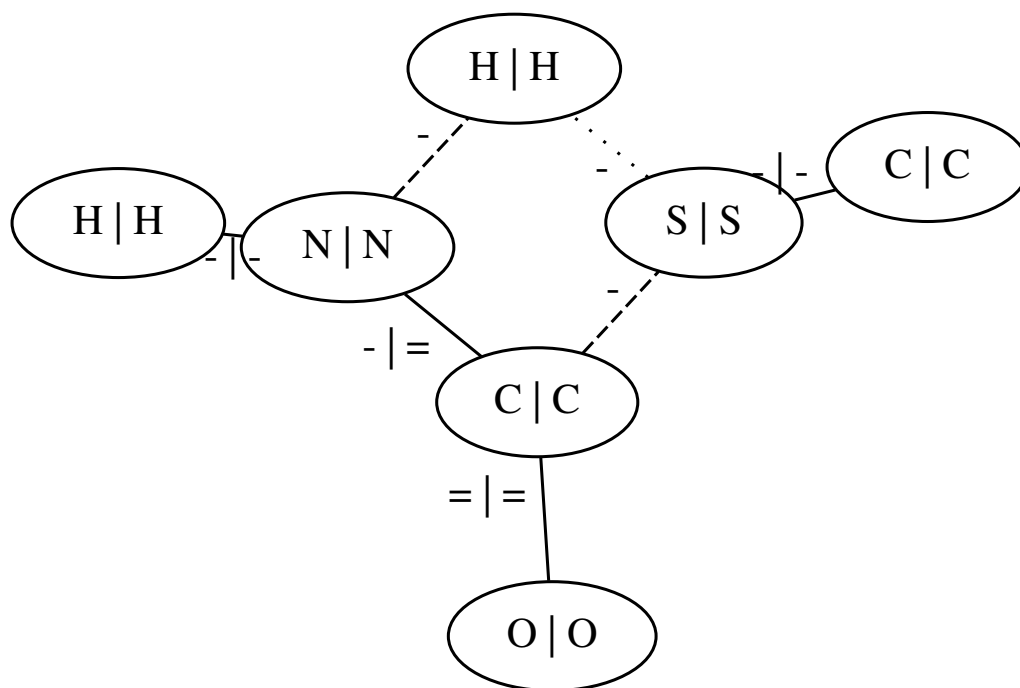




1.0.62 Carbamylation, SC, inverse

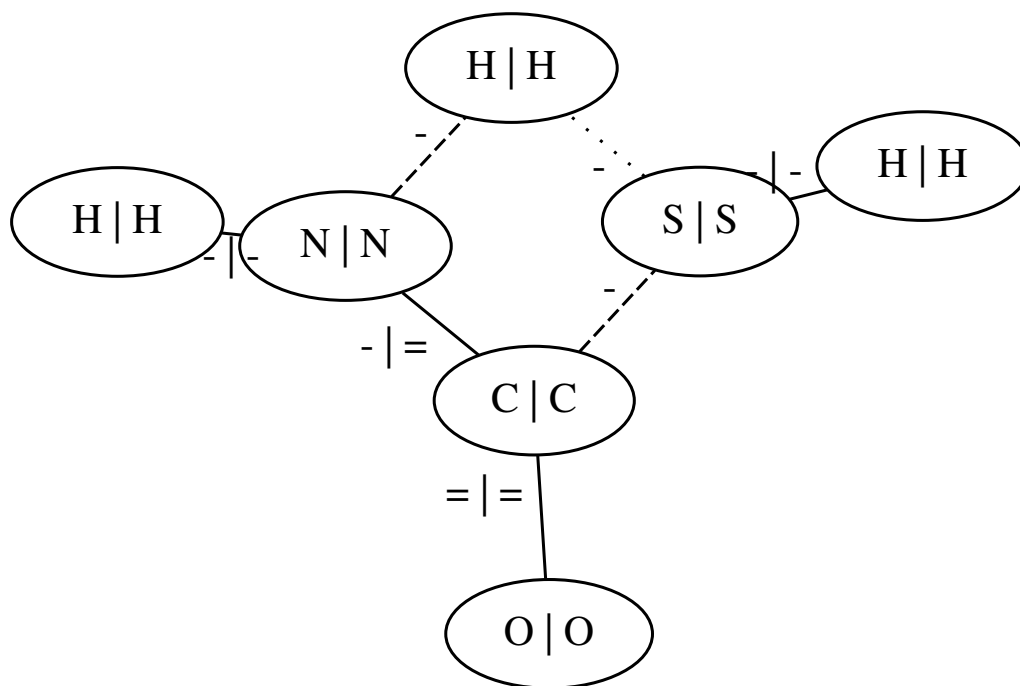
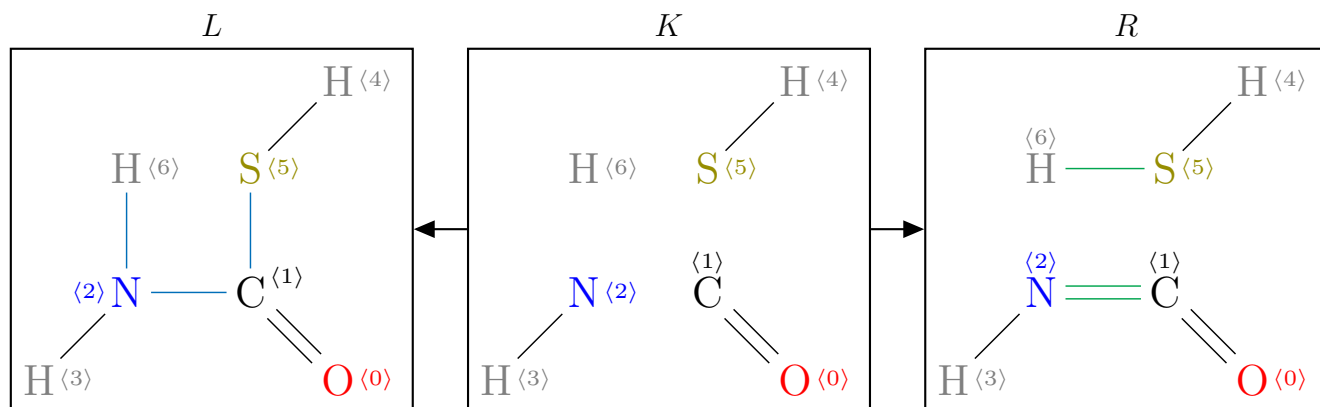


Files: out/245_r_61_10300110_{L, K, R}



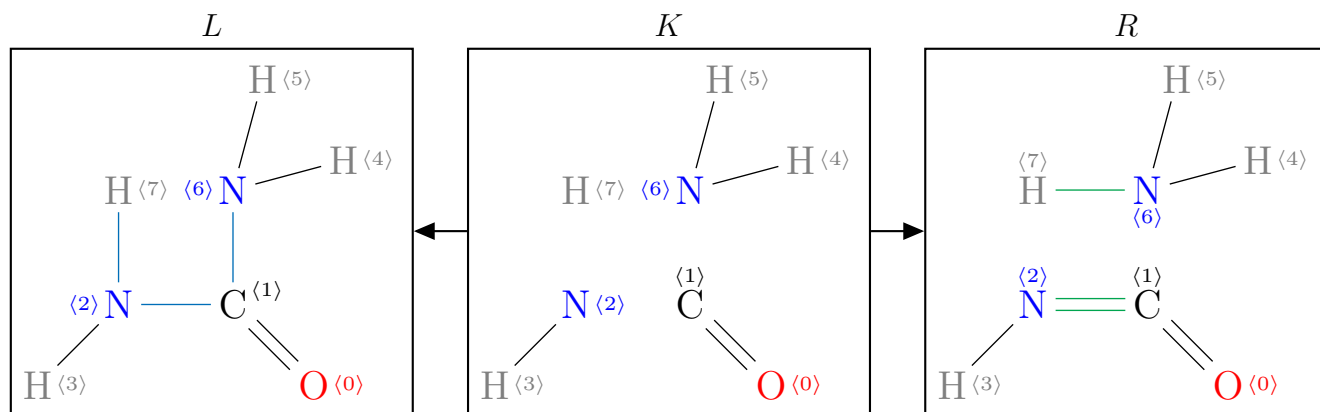
File: out/246_r_61_combined

1.0.63 Carbamylation, SH, inverse

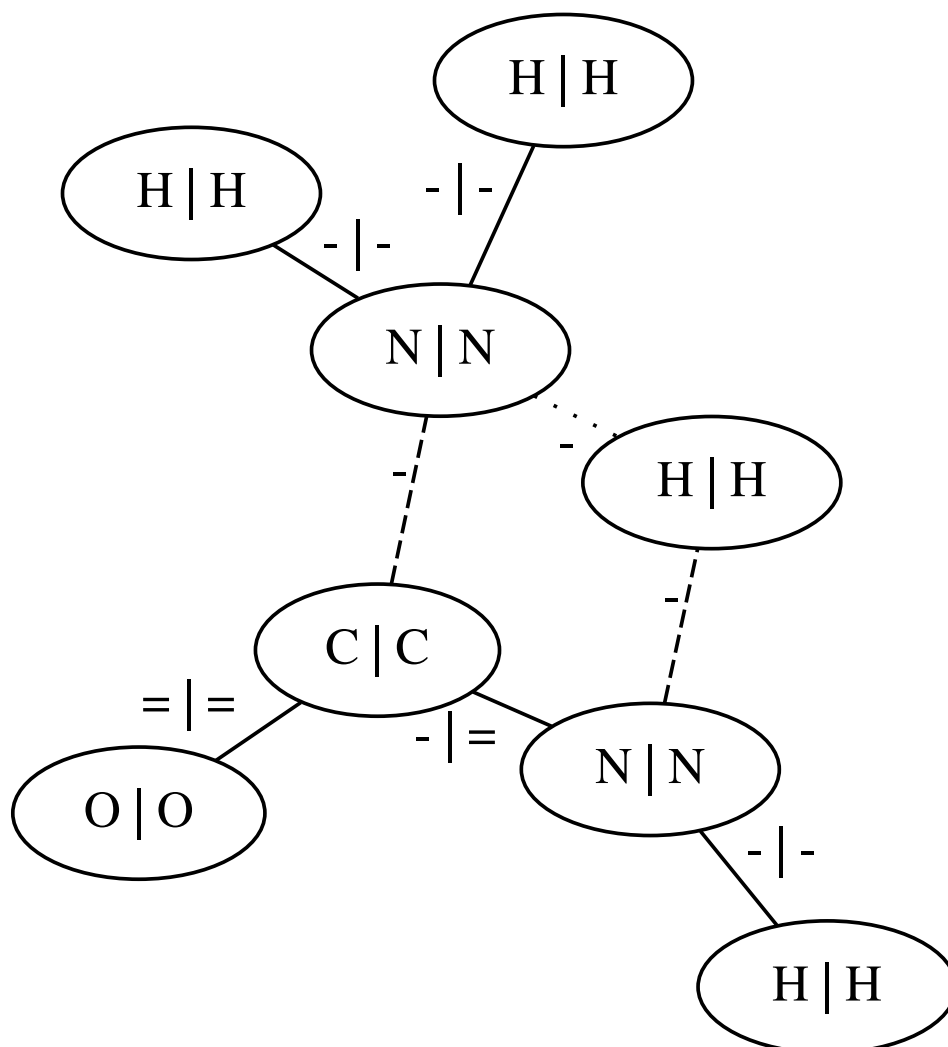


File: out/250_r_62_combined

1.0.64 Carbamylation, N, HH, inverse

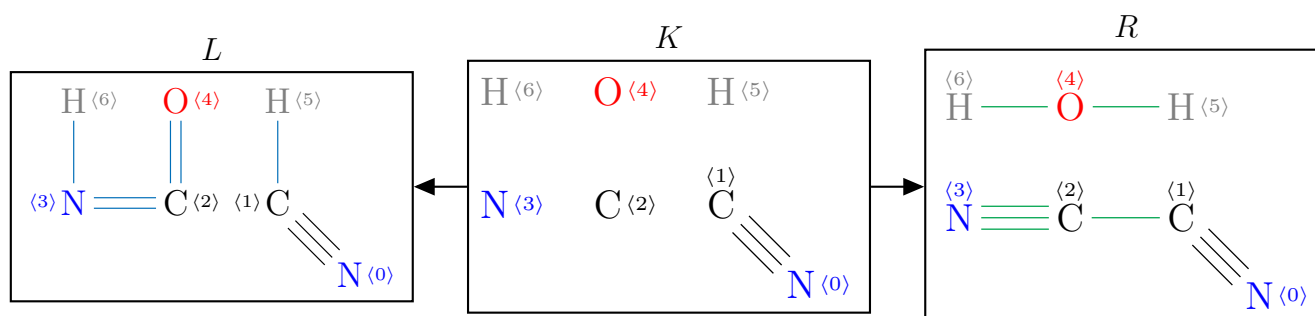


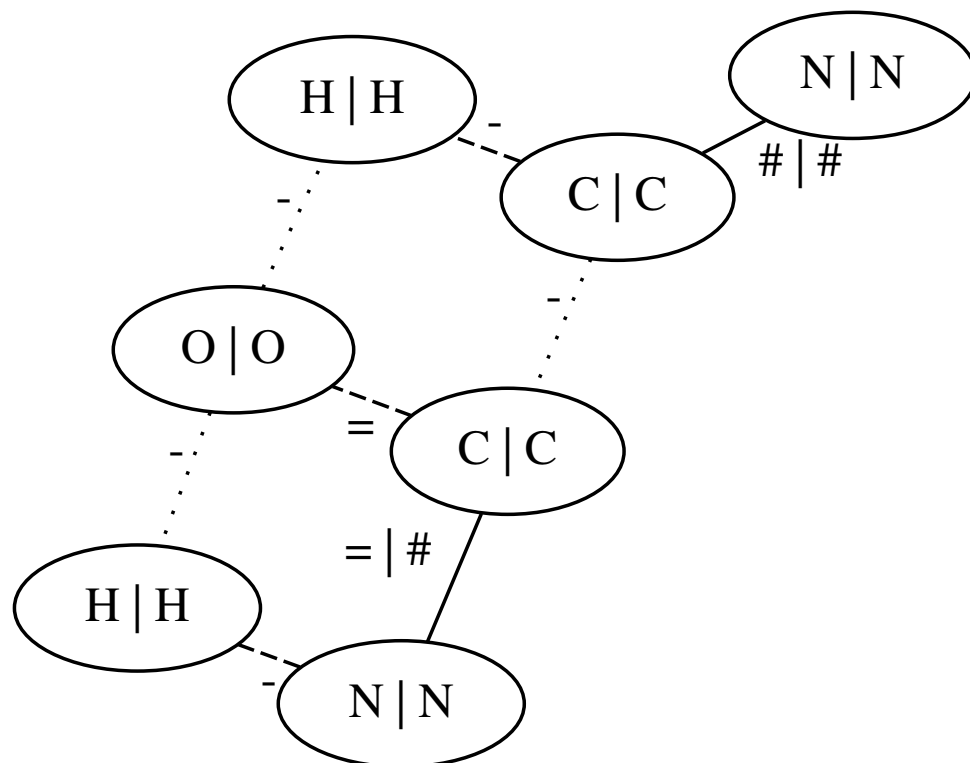
Files: out/253_r_63_10300110_{L, K, R}



File: out/254_r_63_combined

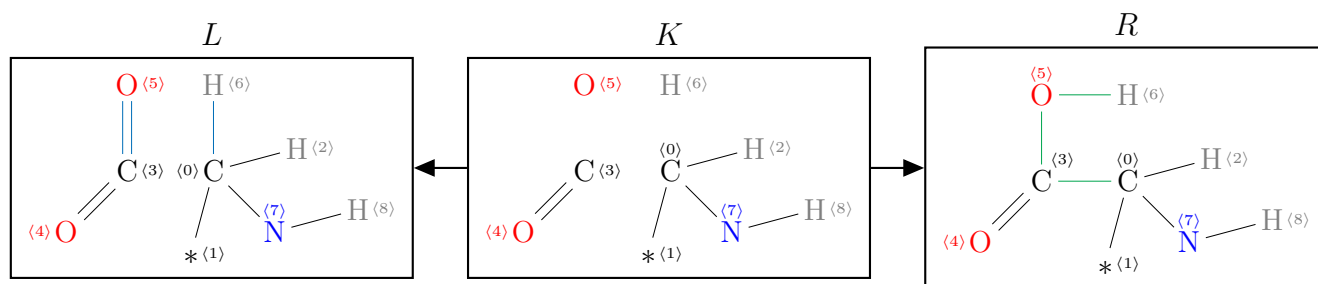
1.0.65 Cyanate from cyanogen, inverse



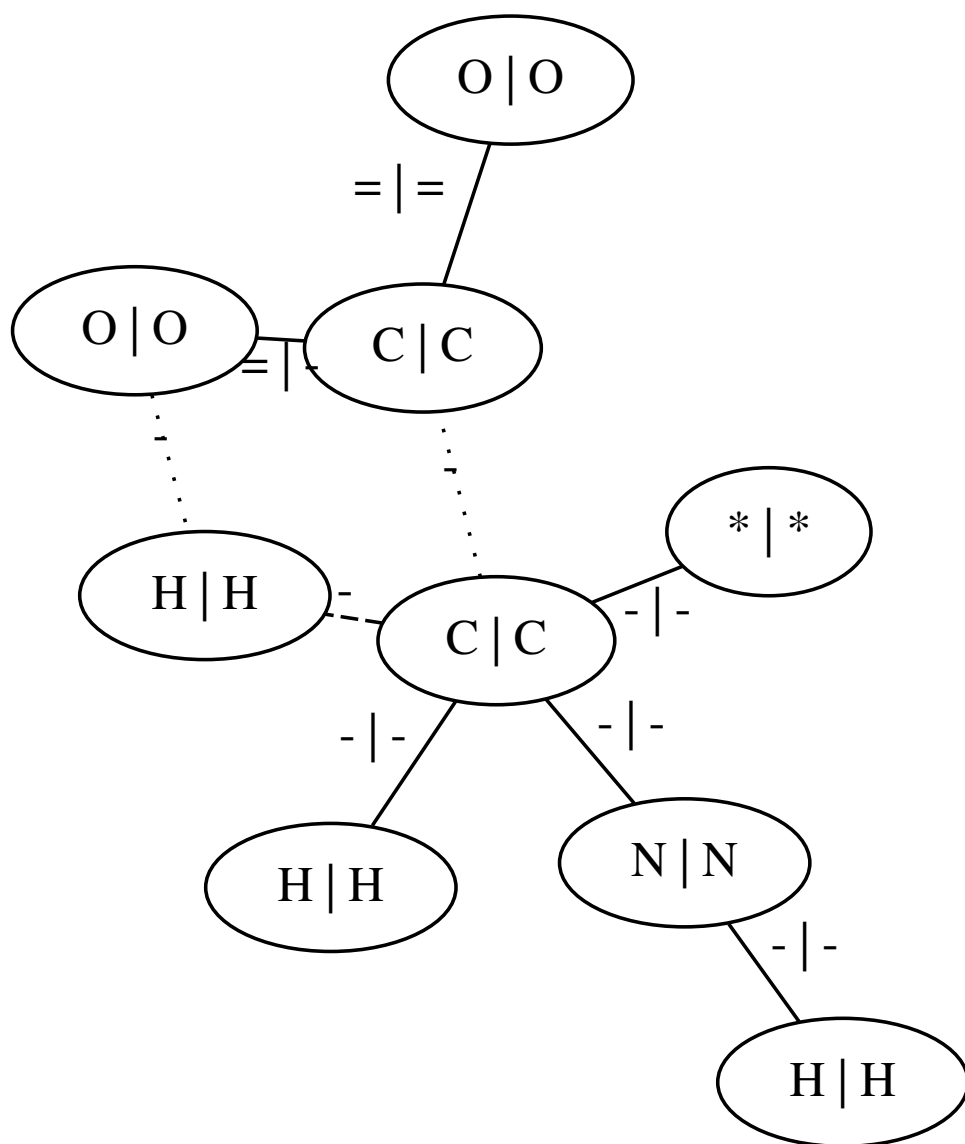


File: out/258_r_64_combined

1.0.66 Ketone-Catalyzed Decarboxylation, inverse

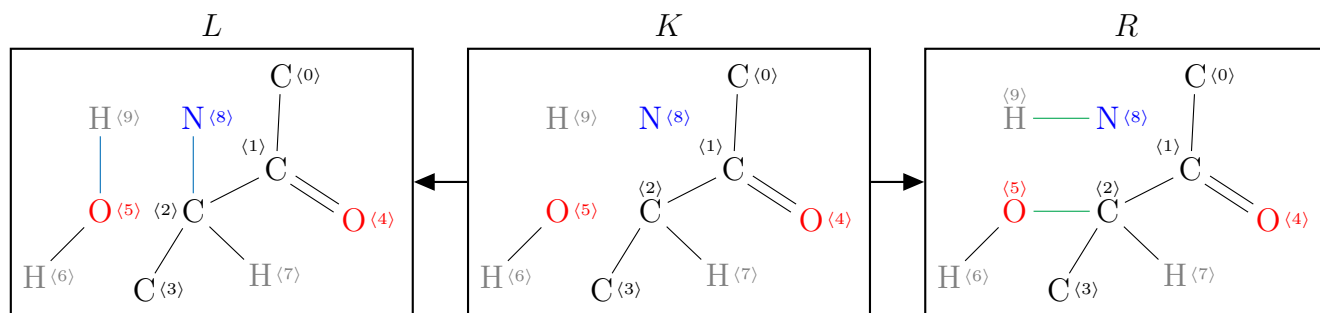


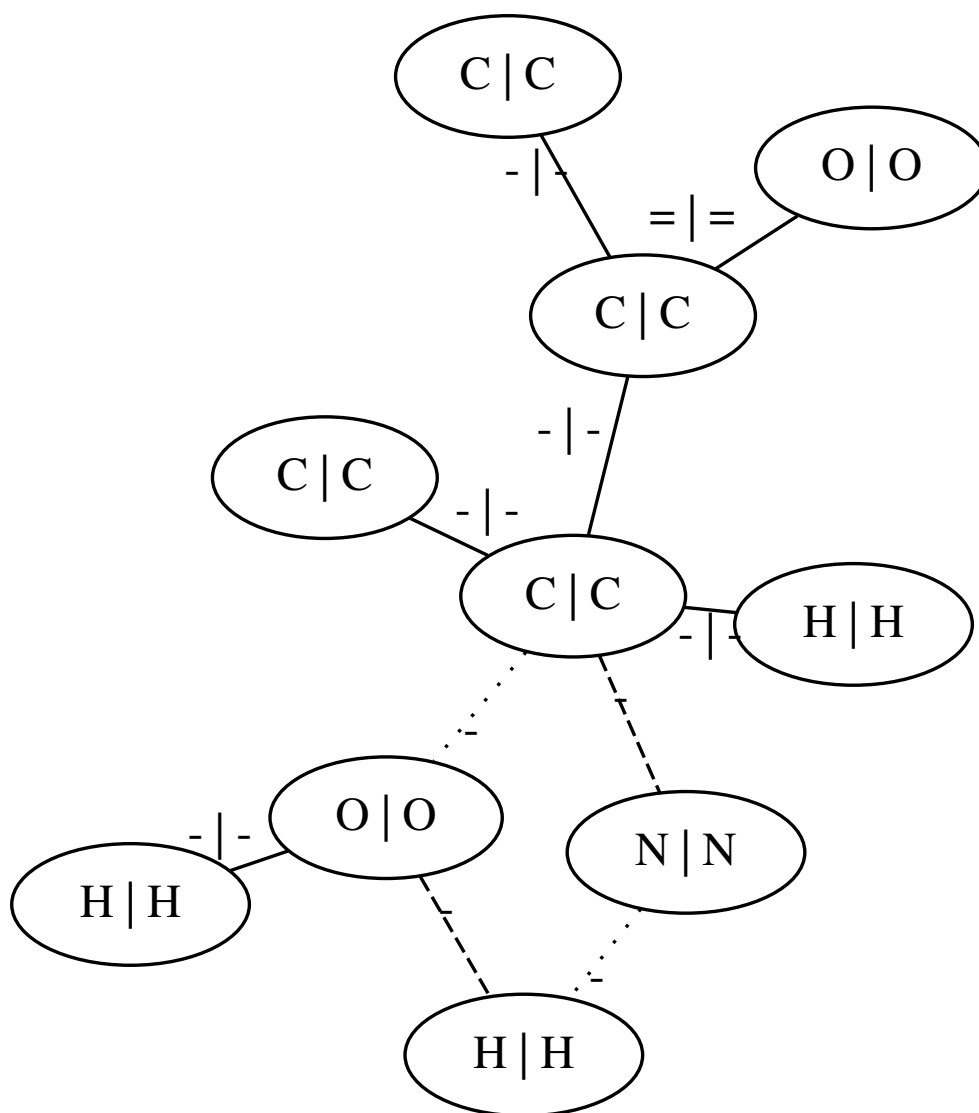
Files: out/261_r_65_10300110_{L, K, R}



File: out/262_r_65_combined

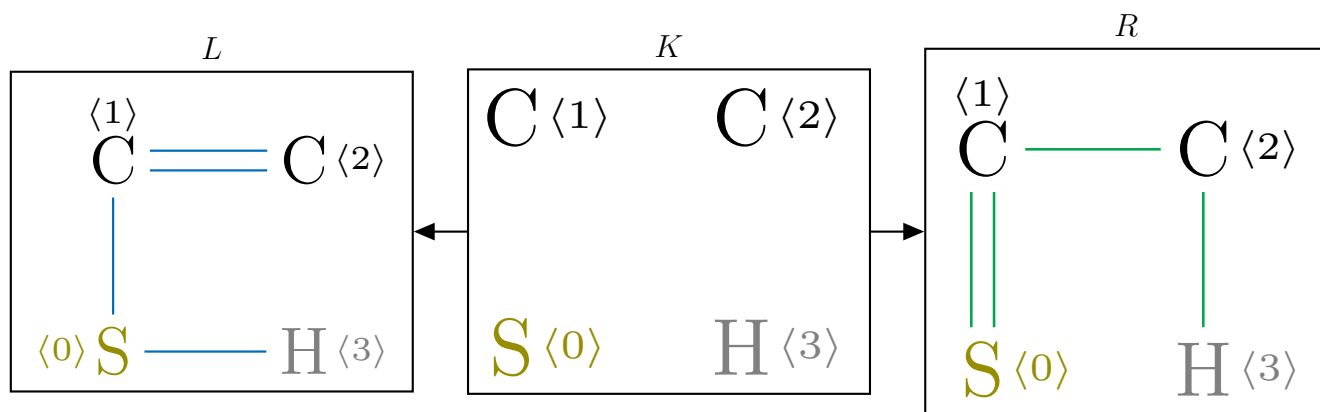
1.0.67 Amadori Rearrangement, inverse



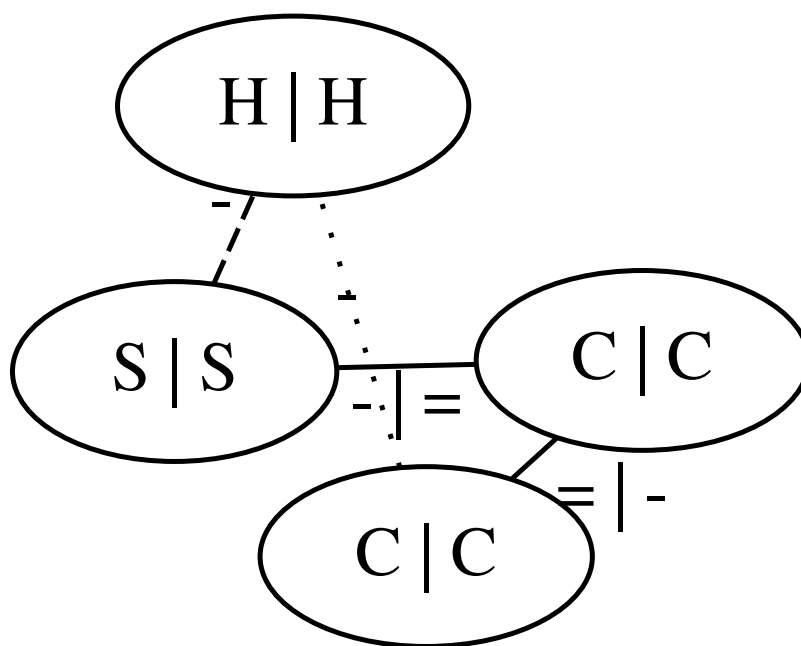


File: out/266_r_66_combined

1.0.68 Thial -> Thiene, inverse

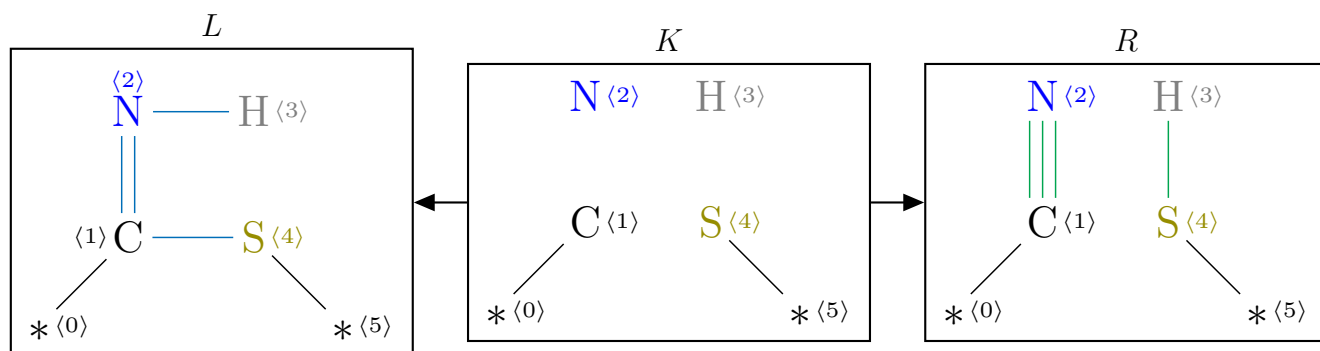


Files: out/269_r_67_10300110_{L, K, R}

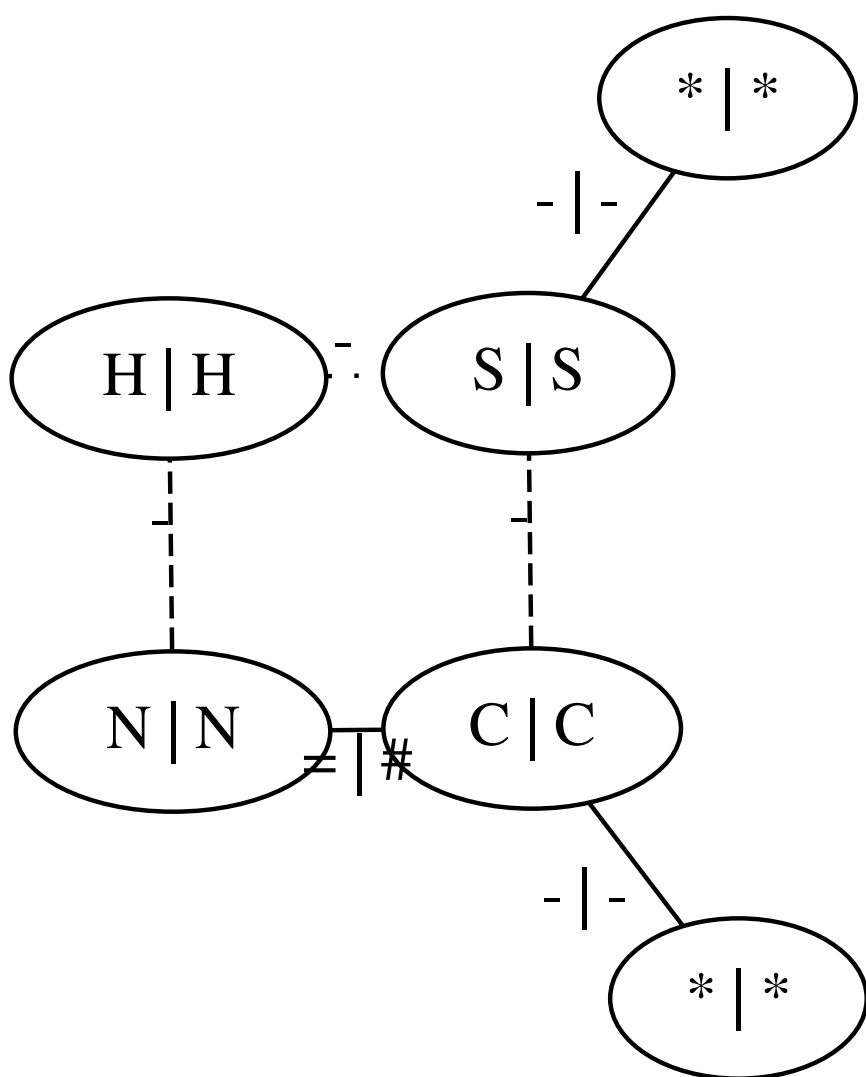


File: out/270_r_67_combined

1.0.69 Sulfide to Nitrile Addition, inverse

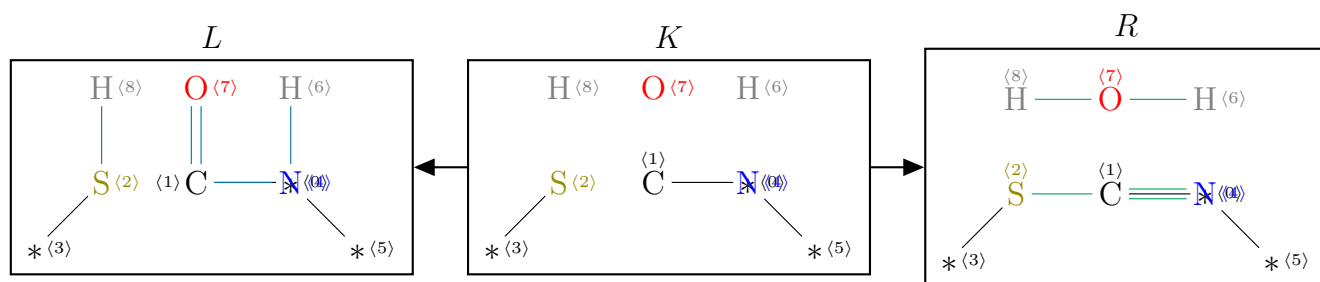


Files: out/273_r_68_10300110_{L, K, R}

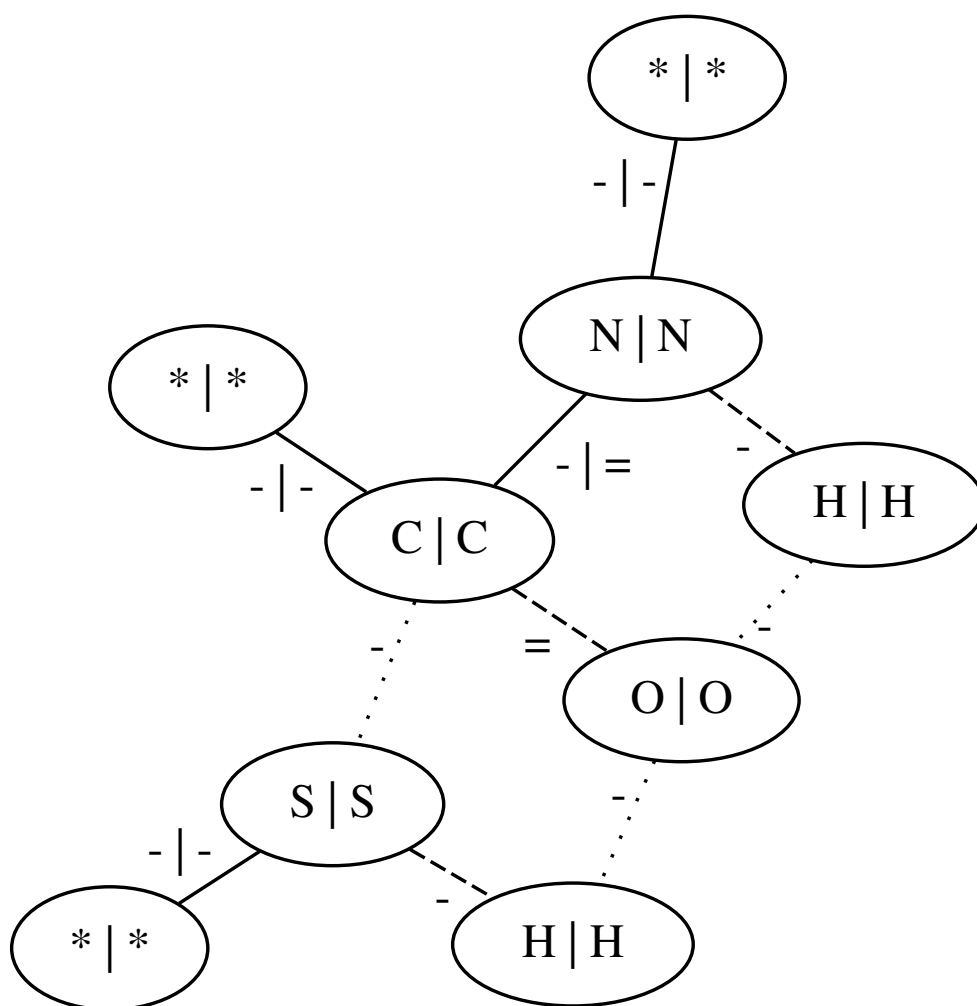


File: out/274_r_68_combined

1.0.70 Thioamidine to Amide Hydrolysis, inverse

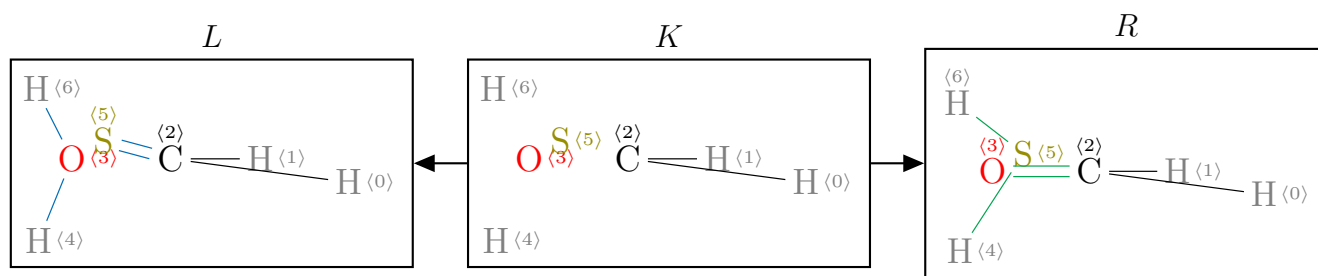


Files: out/277_r_69_10300110_{L, K, R}

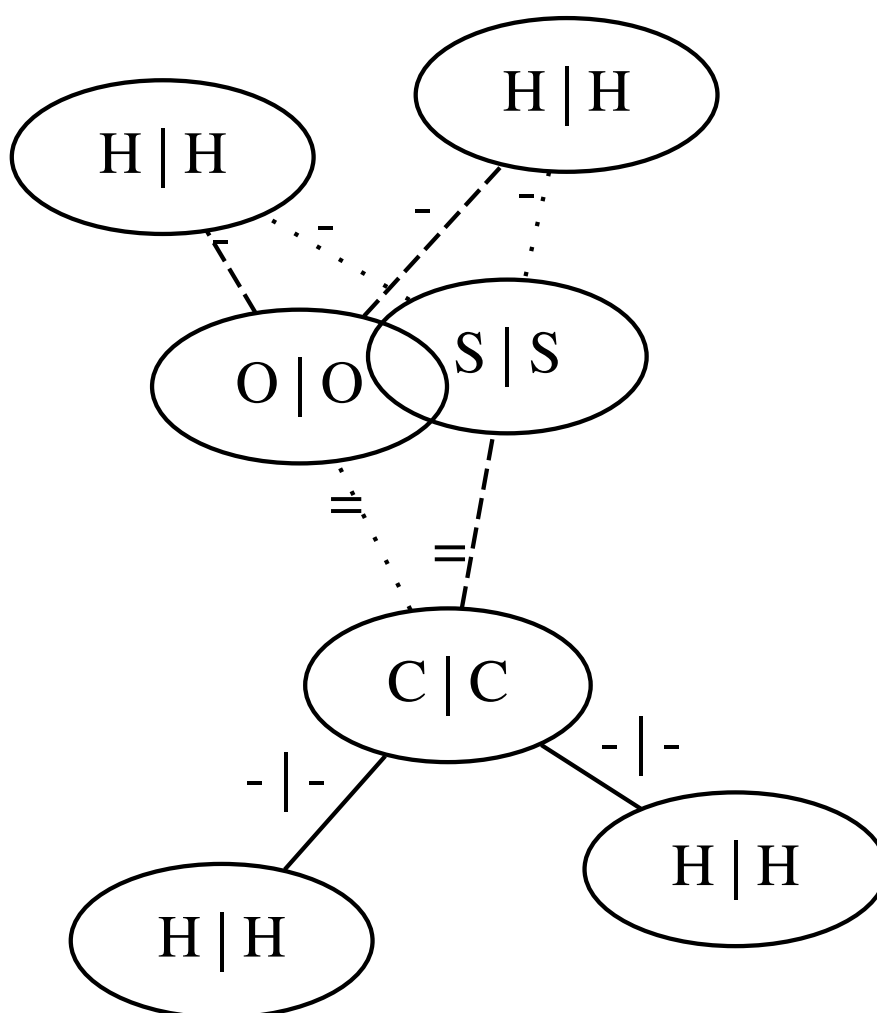


File: out/278_r_69_combined

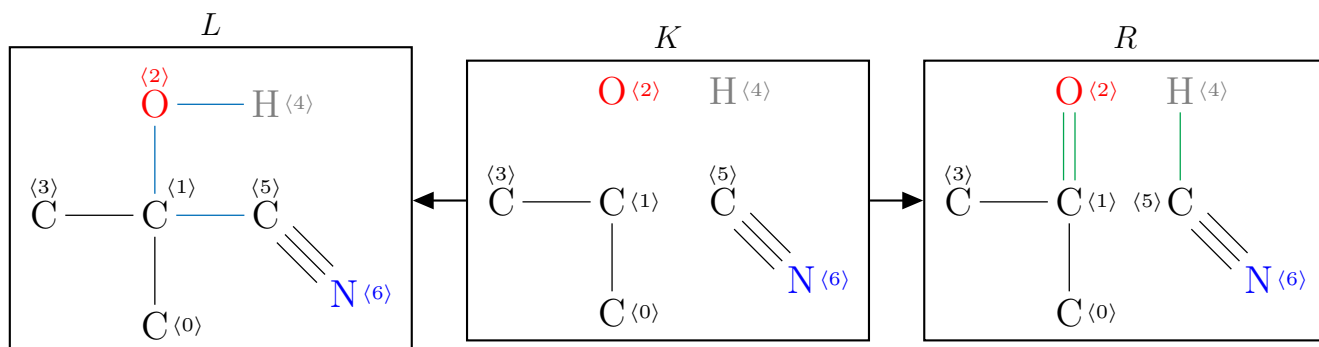
1.0.71 Ketone/Aldehyde to Thioketone/Thial, HH, inverse



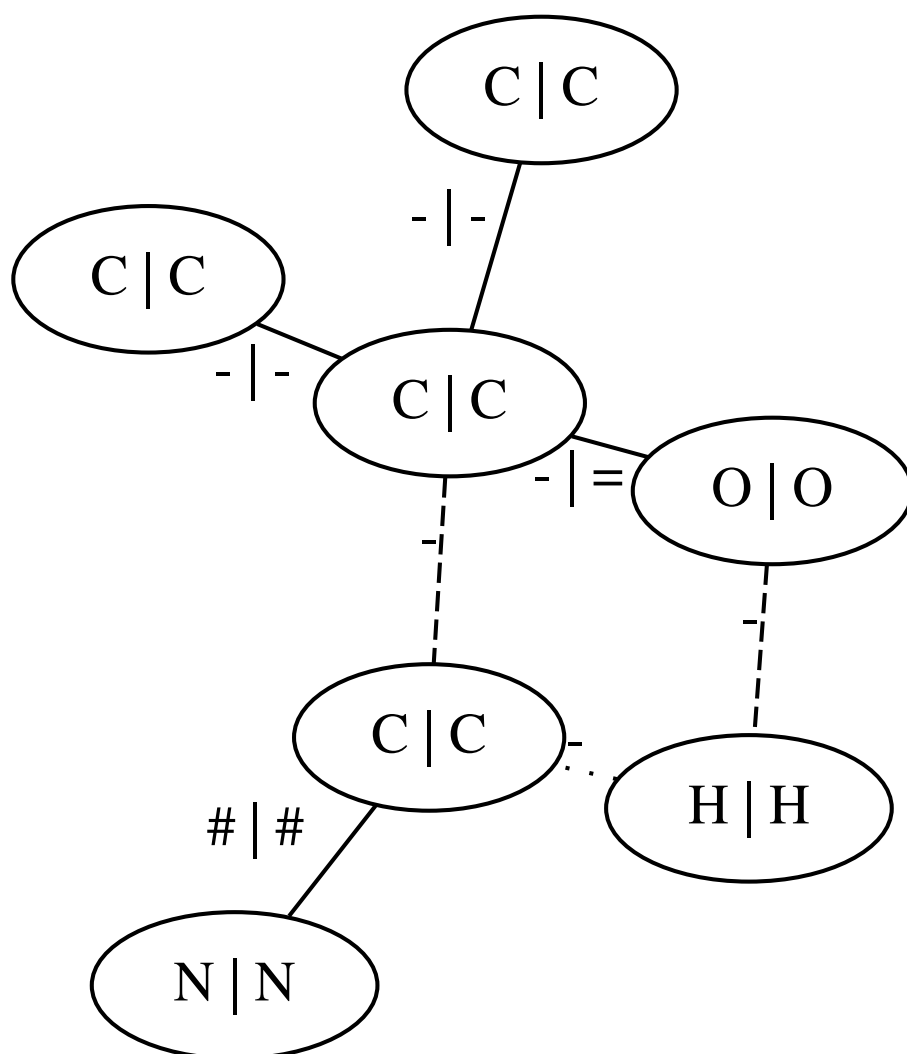
Files: out/281_r_70_10300110_{L, K, R}



1.0.72 HCN to Ketone, inverse

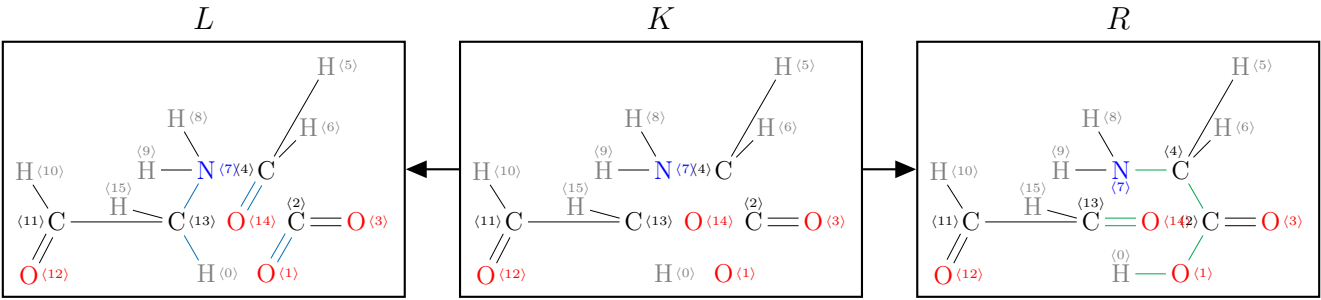


Files: out/285_r_71_10300110_{L, K, R}

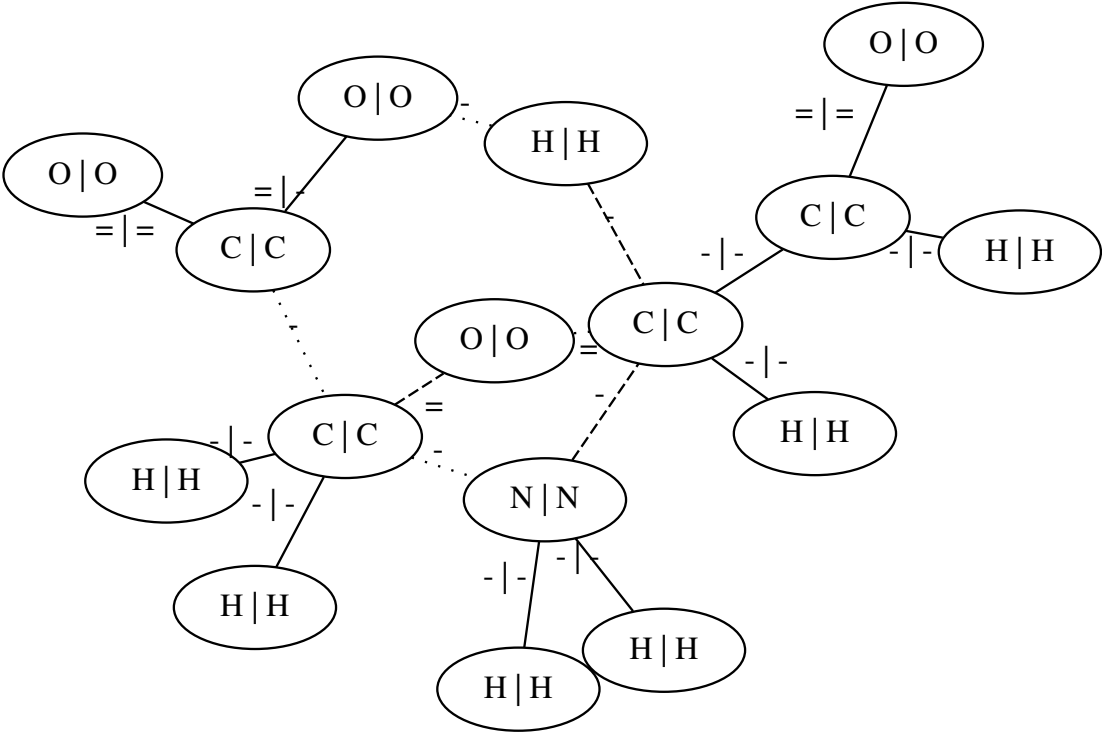


File: out/286_r_71_combined

1.0.73 Strecker Degradation Dicarbonyl, H, H, H, H, inverse

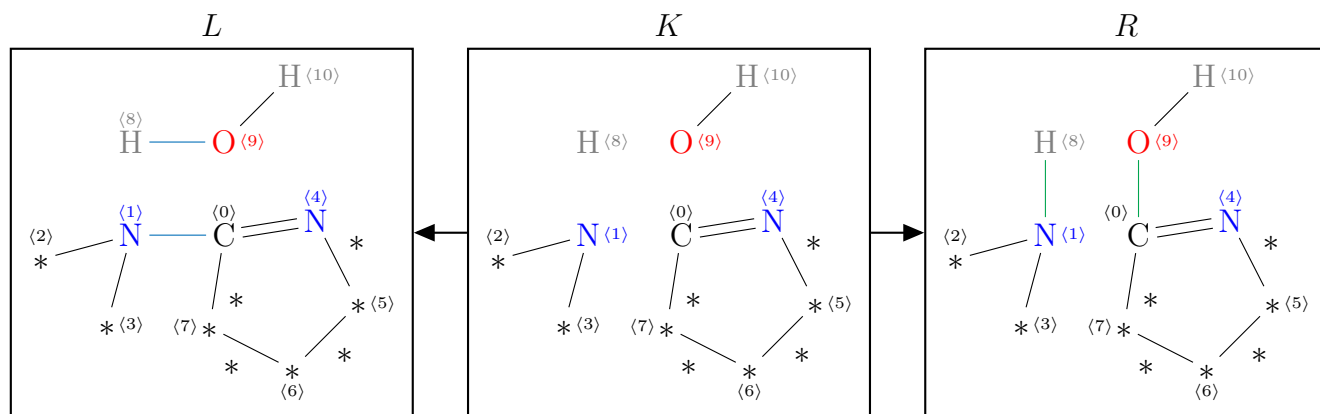


Files: out/289_r_72_10300110_{L, K, R}

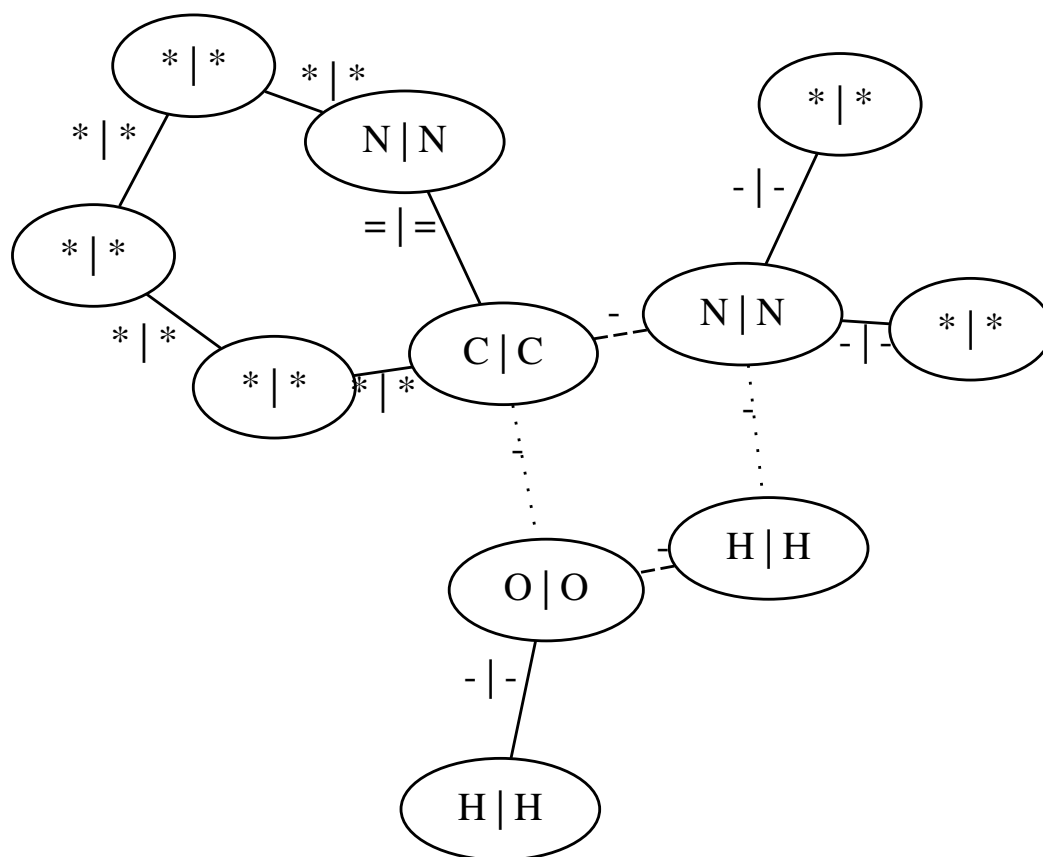


File: out/290_r_72_combined

1.0.74 5 Membered Ring Exoamine Hydrolysis

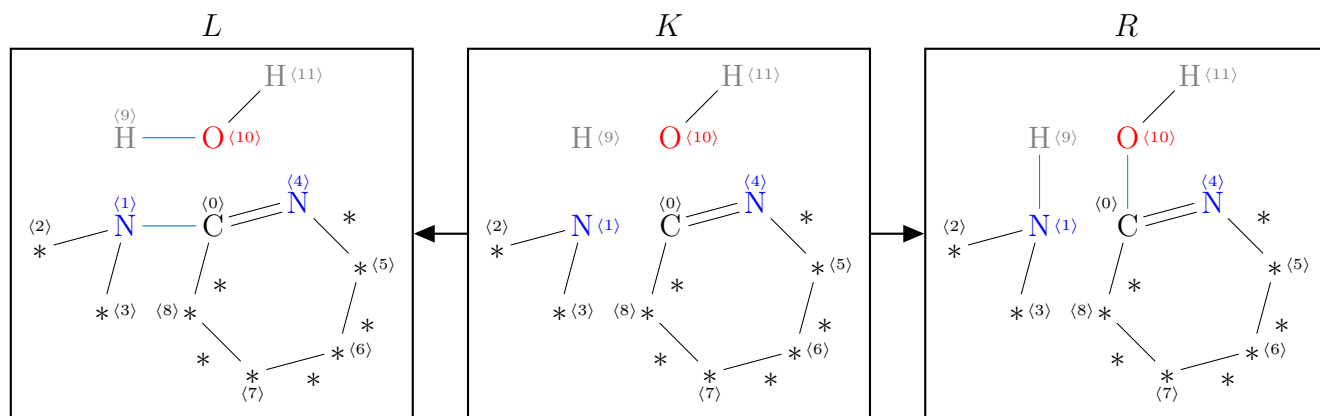


Files: out/293_r_74_10300110_{L, K, R}

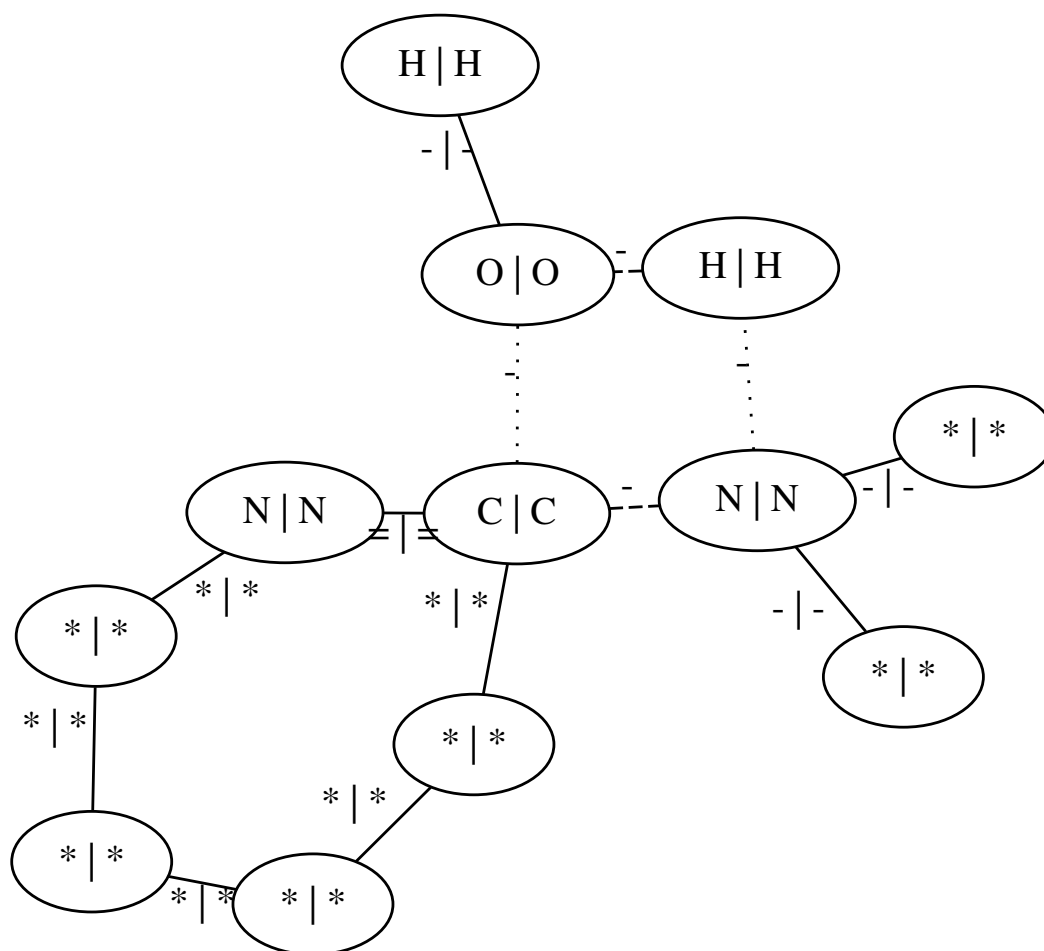


File: out/294_r_74_combined

1.0.75 6 Membered Ring Exoamine Hydrolysis

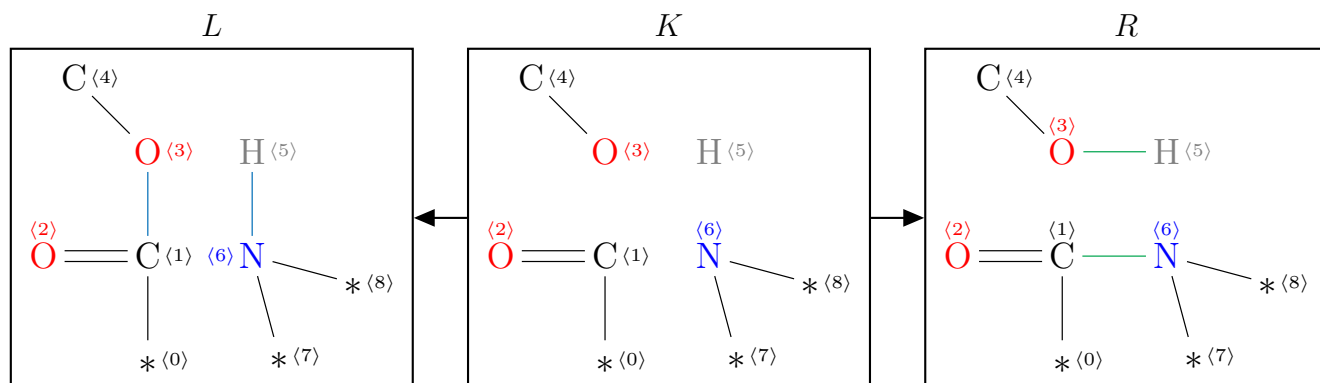


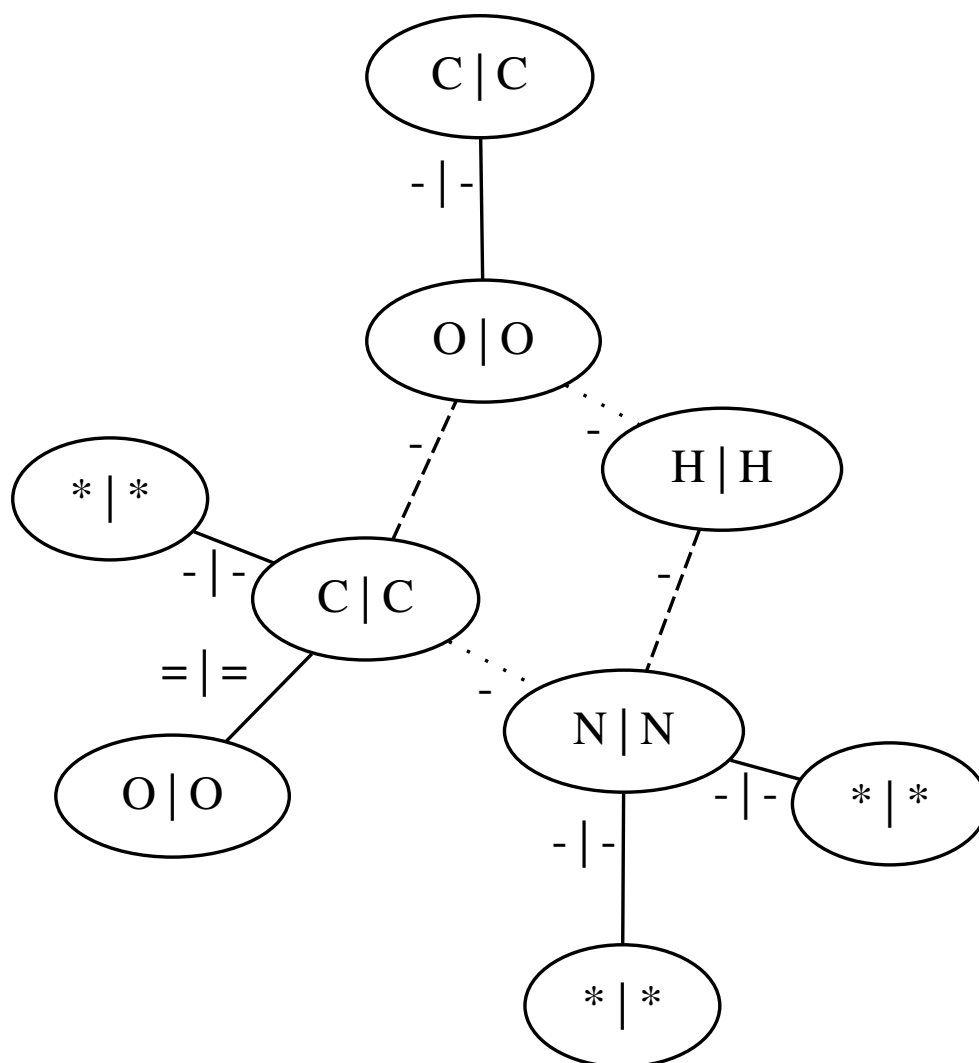
Files: out/297_r_75_10300110_{L, K, R}



File: out/298_r_75_combined

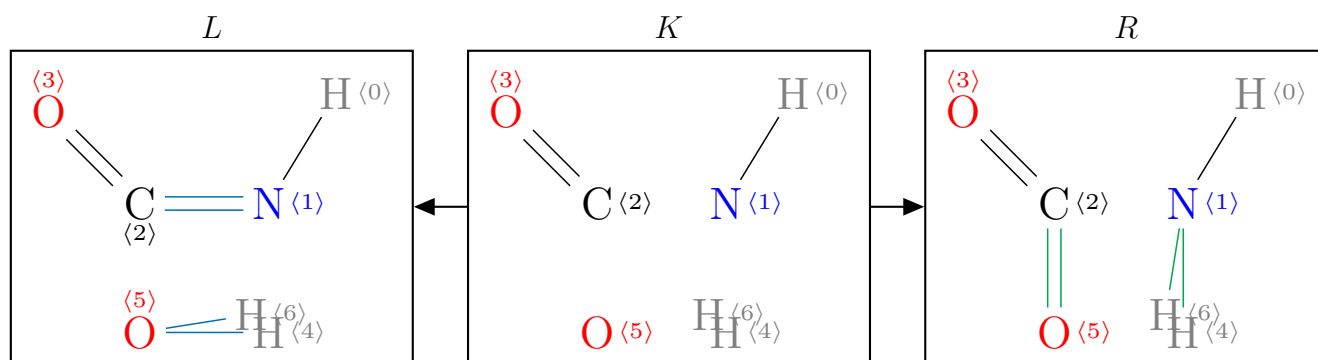
1.0.76 Ammonolysis of Esters



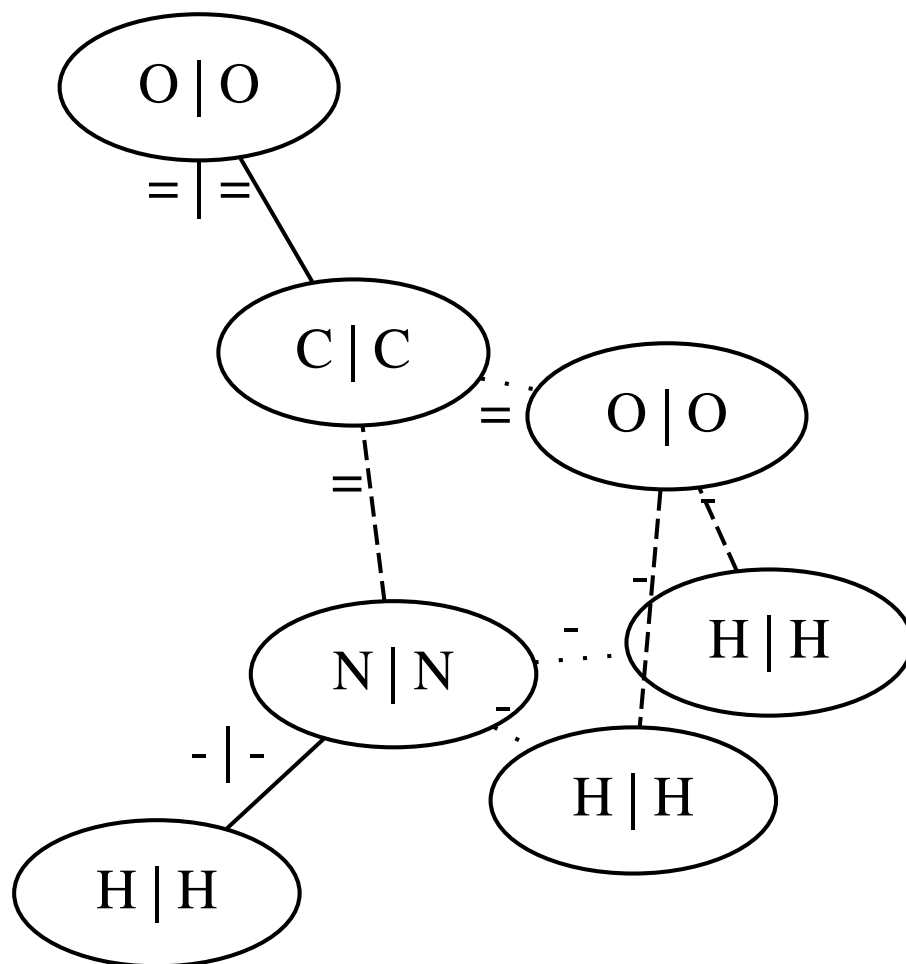


File: out/302_r_76_combined

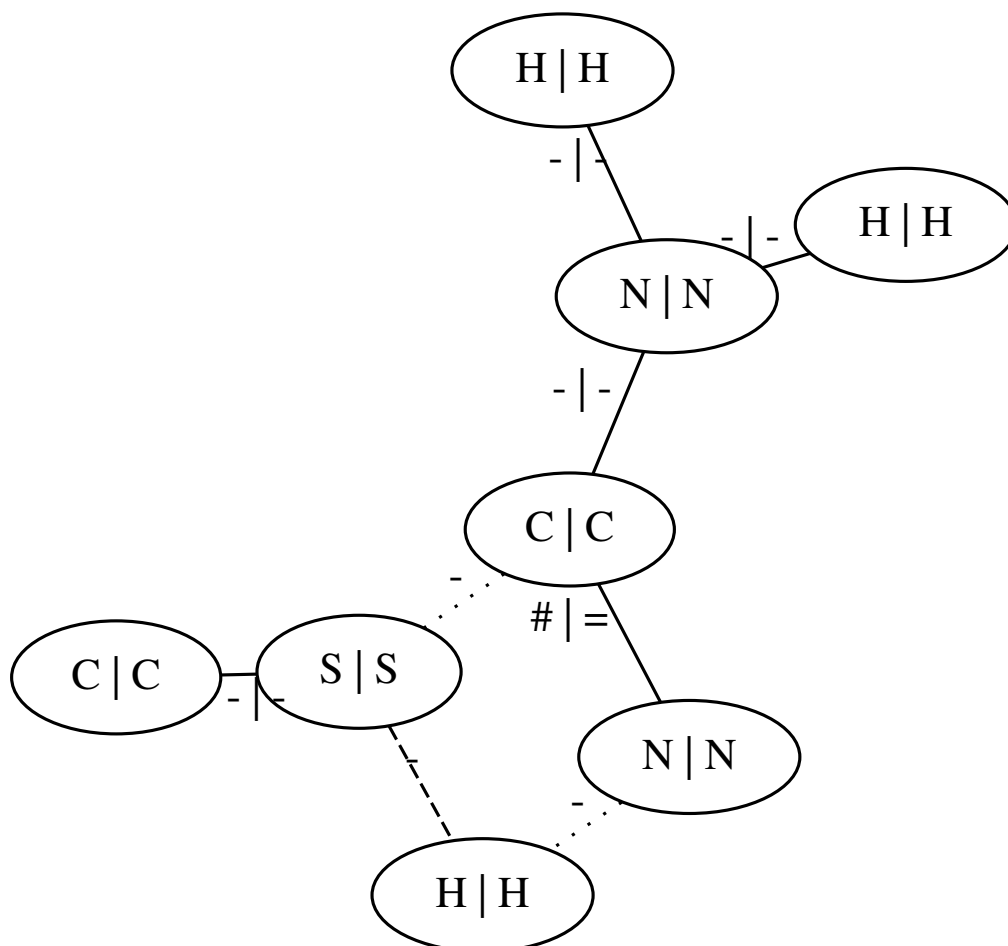
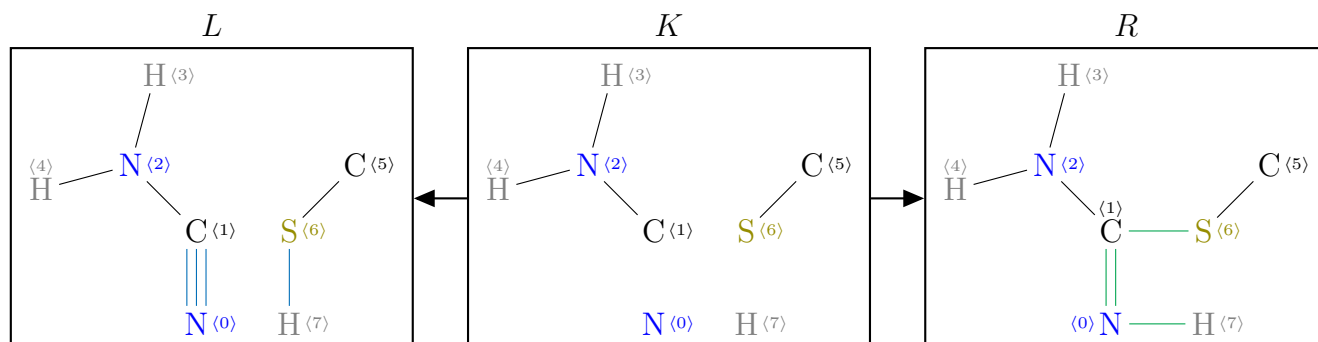
1.0.77 Isocyanate Hydrolysis



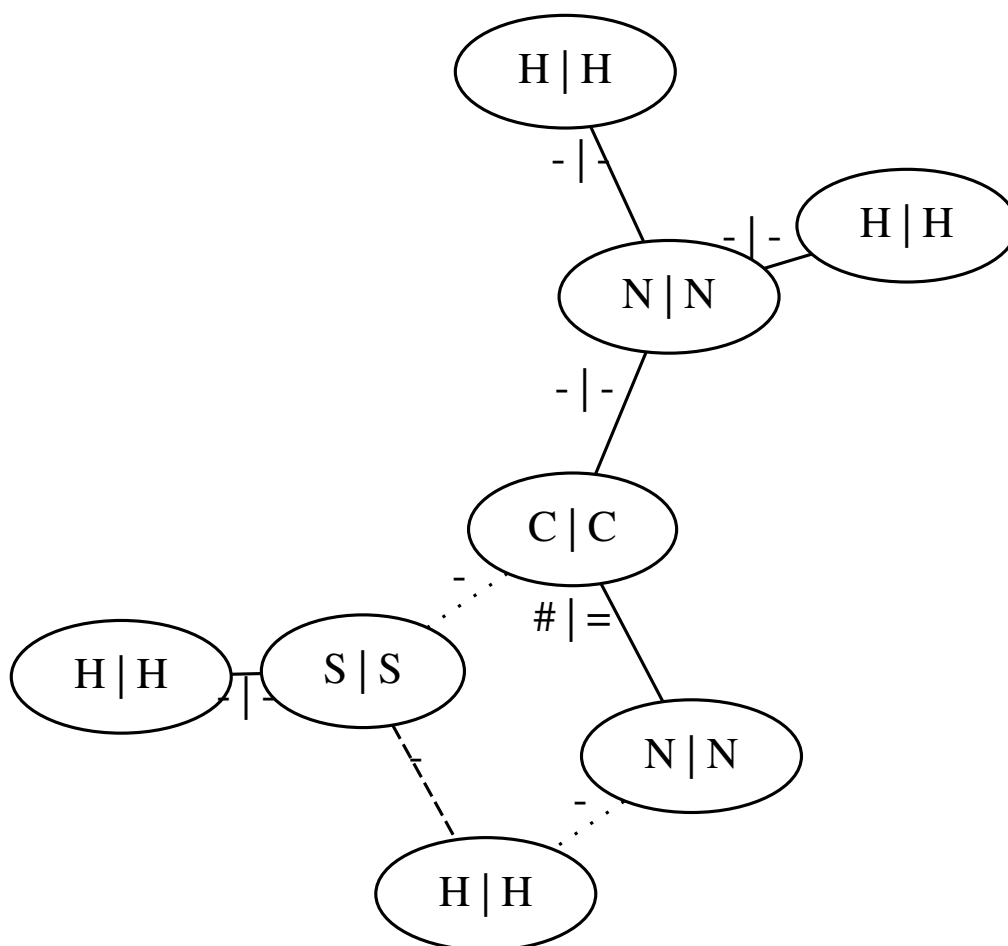
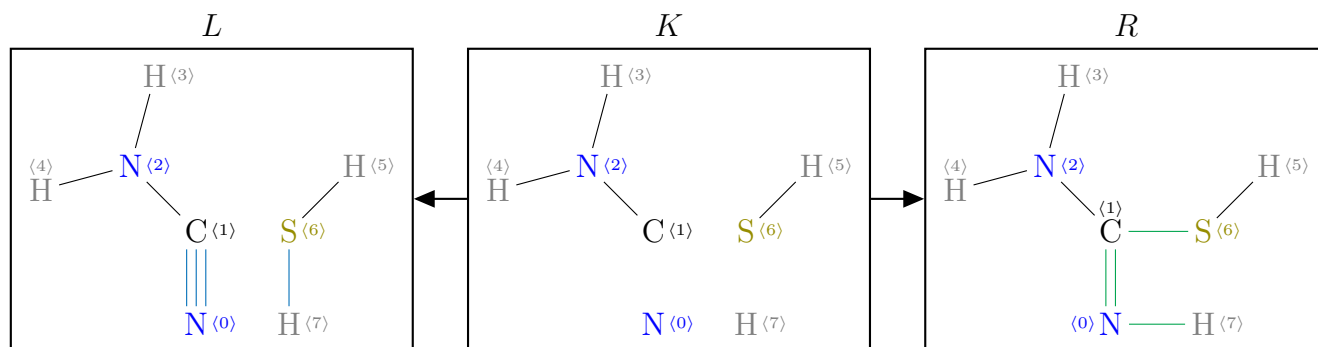
Files: out/305_r_77_10300110_{L, K, R}



1.0.78 Cyanamidation, SC

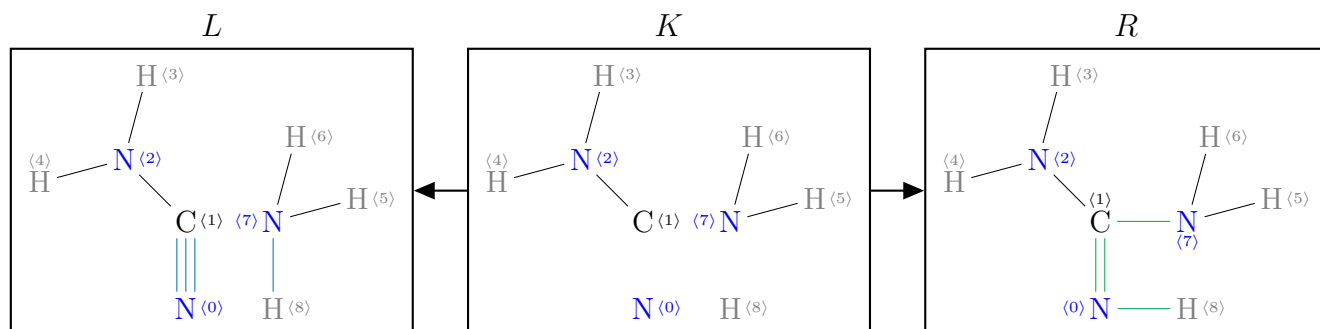


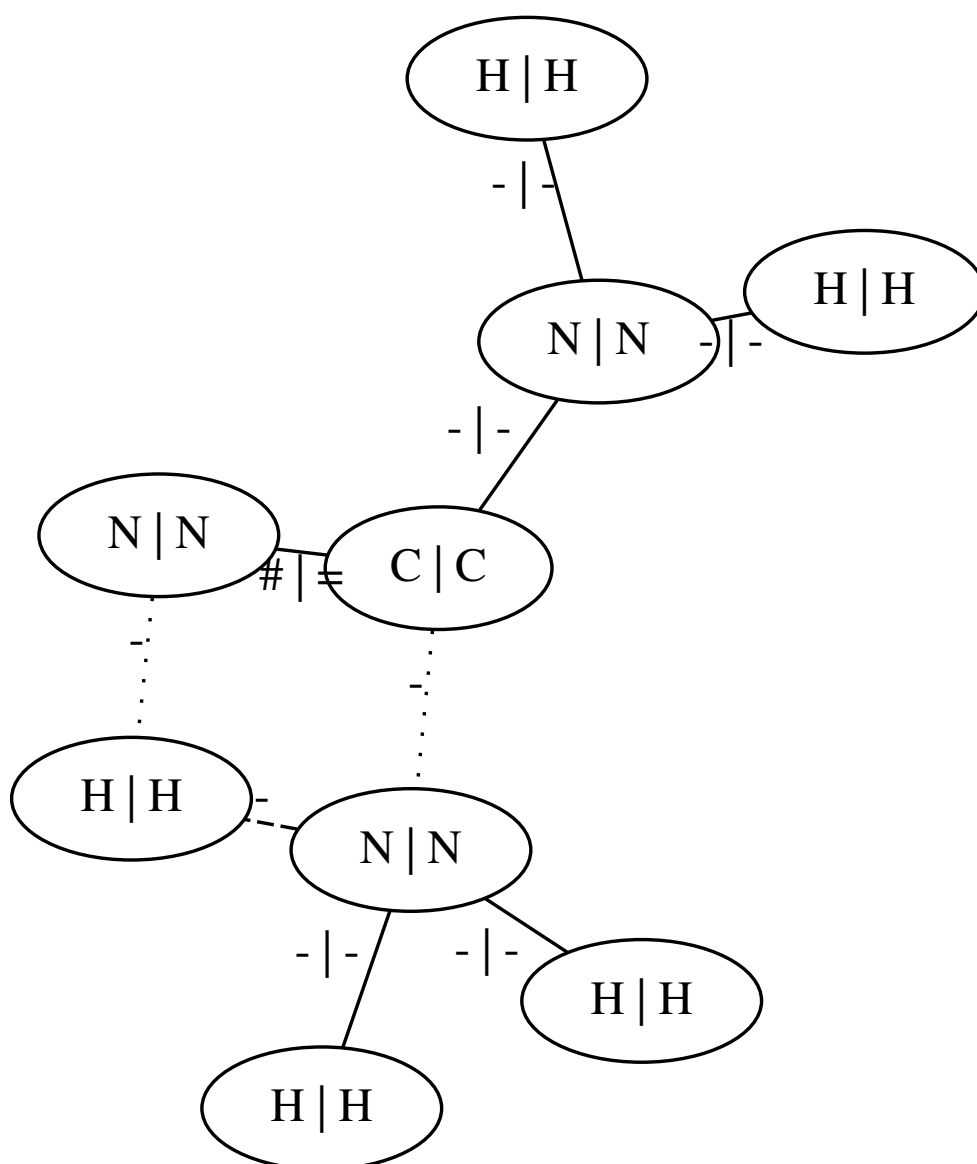
1.0.79 Cyanamidation, SH



File: out/314_r_79_combined

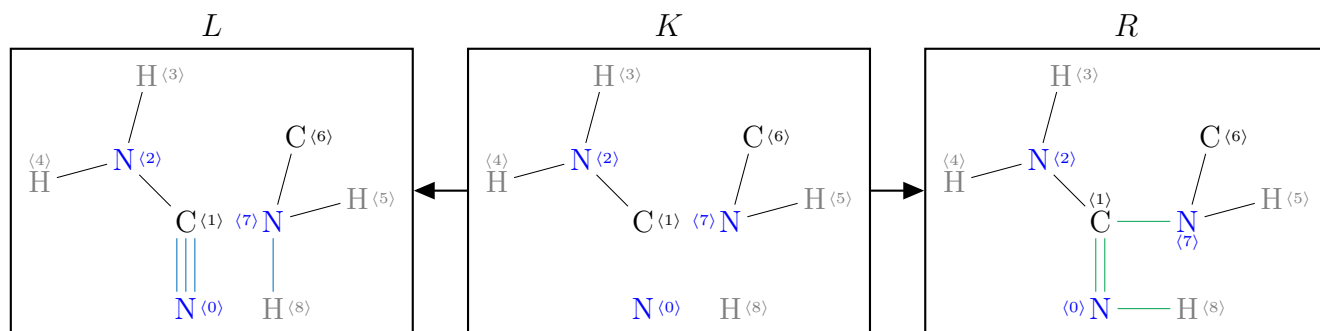
1.0.80 Cyanamidation, N, HH



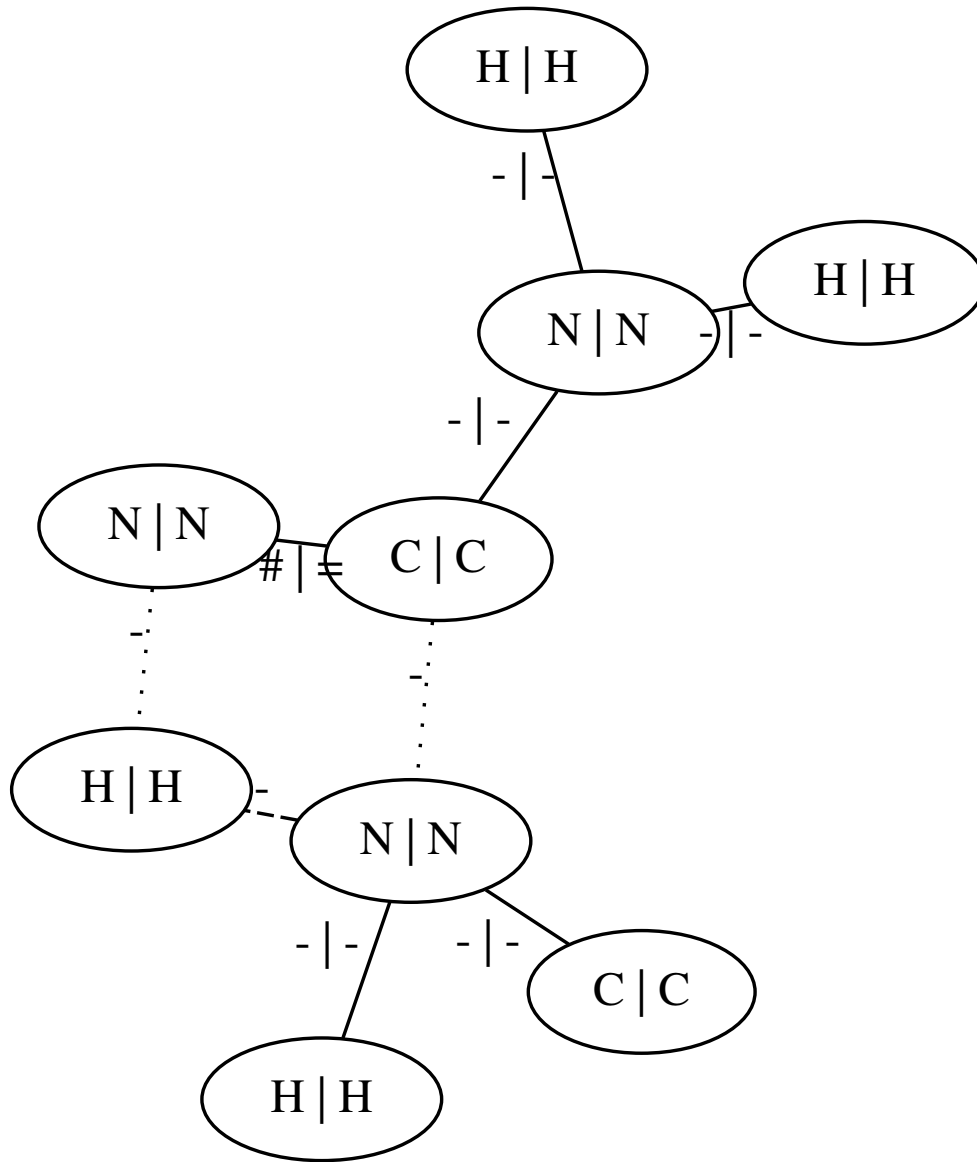


File: out/318_r_80_combined

1.0.81 Cyanamidation, N, HC



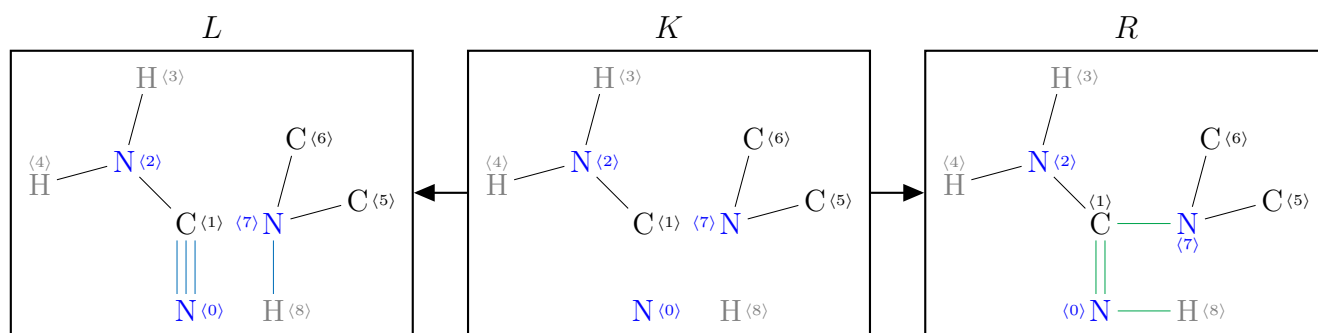
Files: out/321_r_81_10300110_{L, K, R}



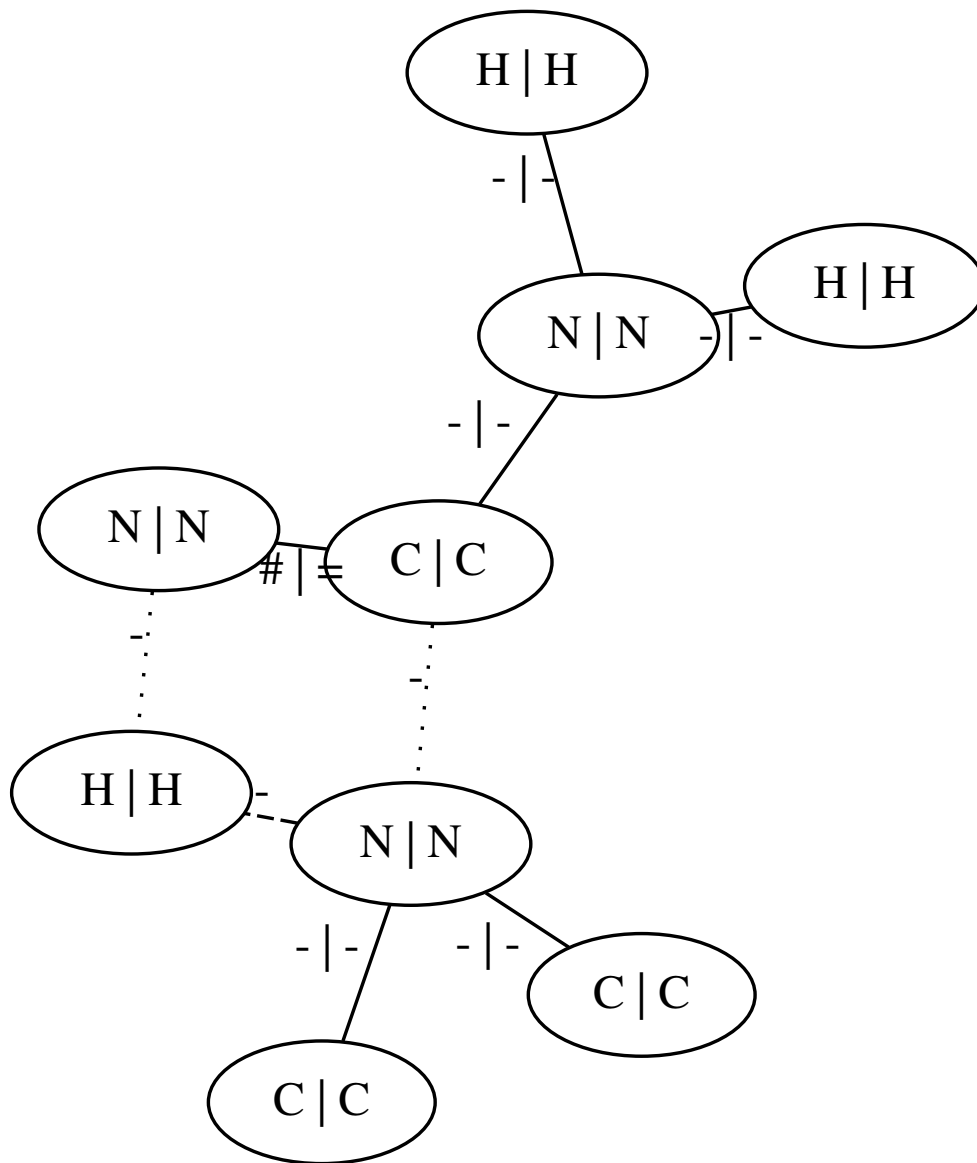
File: out/322_r_81_combined

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

1.0.82 Cyanamidation, N, CC



Files: out/325_r_82_10300110_{L, K, R}

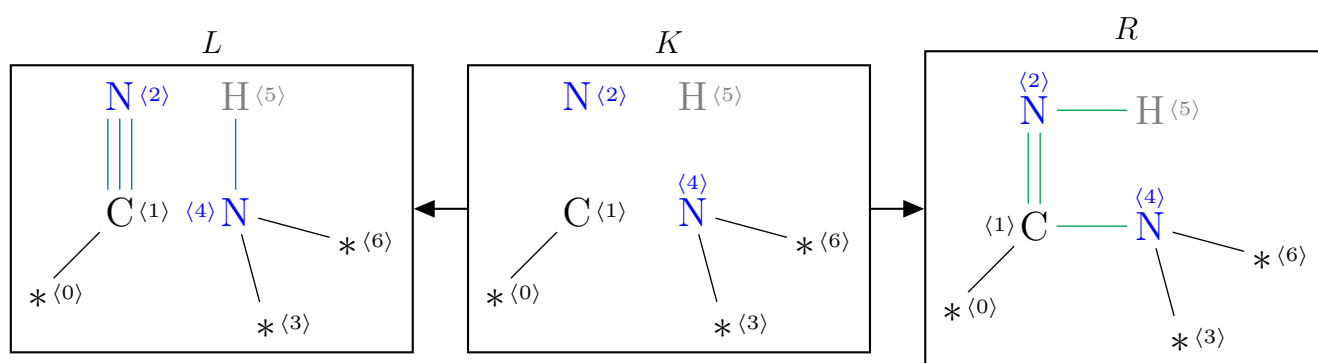


File: out/326_r_82_combined

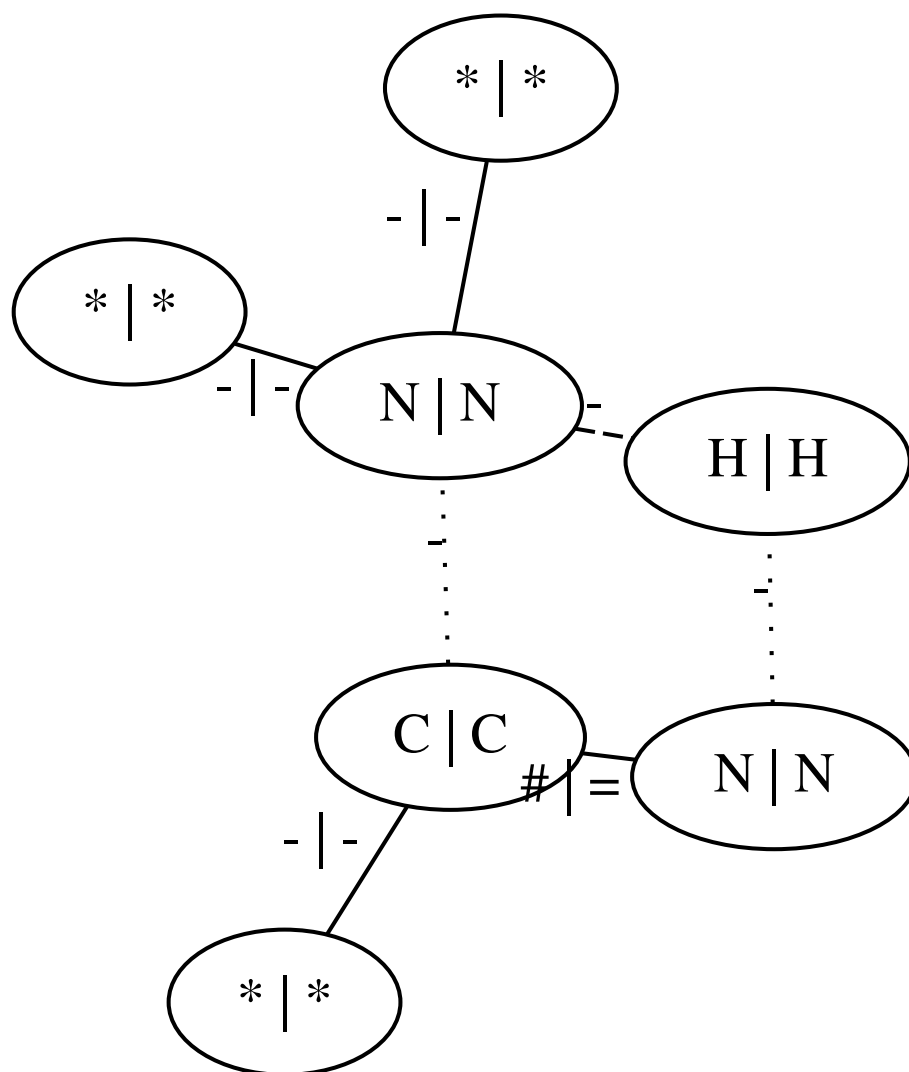
$$\begin{aligned}
 &|\{e \in \text{outEdges}(5) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{ '0' \} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{ '=' \} \\
 &\} | = 0
 \end{aligned}$$

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

1.0.83 Nitrile Amination

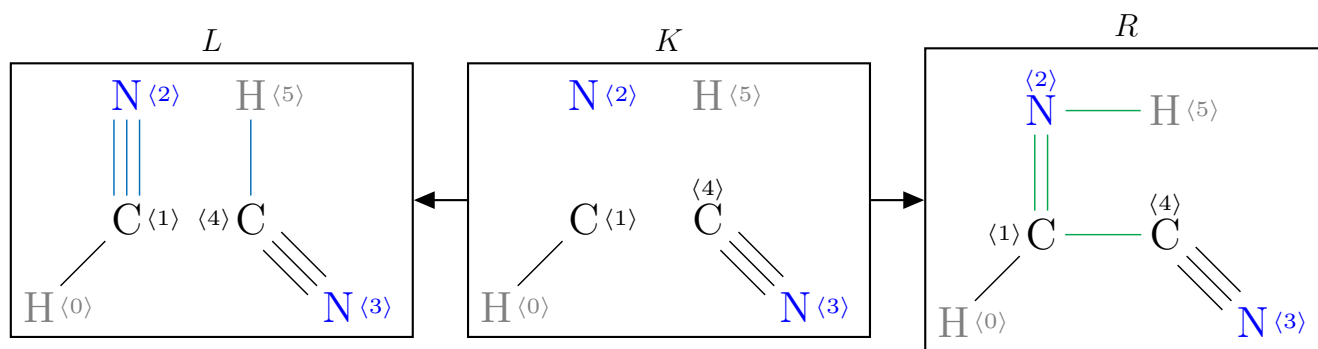


Files: out/329_r_83_10300110_{L, K, R}

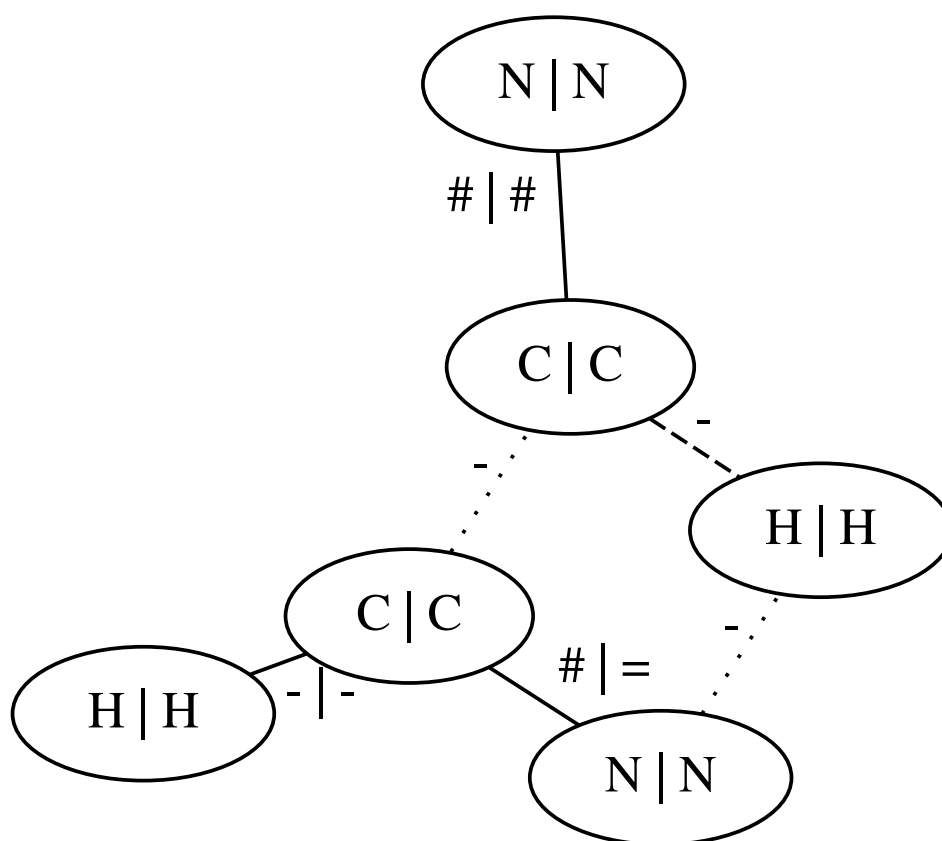


File: out/330_r_83_combined

1.0.84 HCN Addition to Nitriles

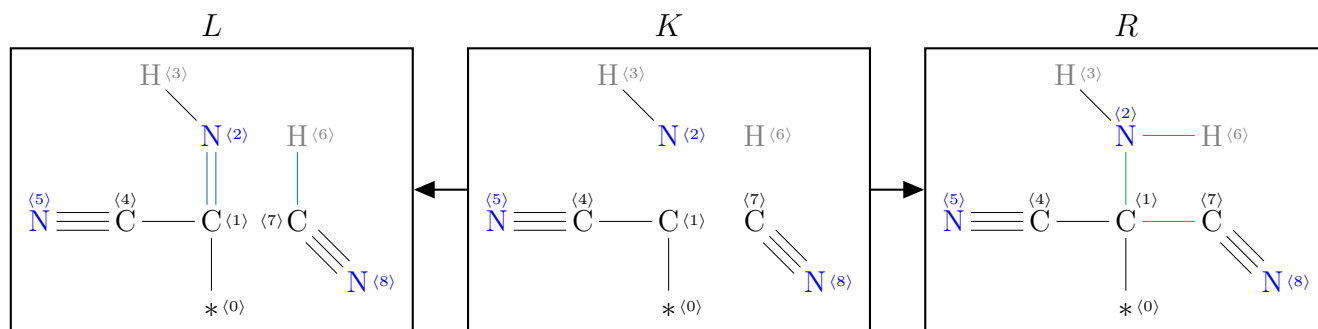


Files: out/333_r_84_10300110_{L, K, R}

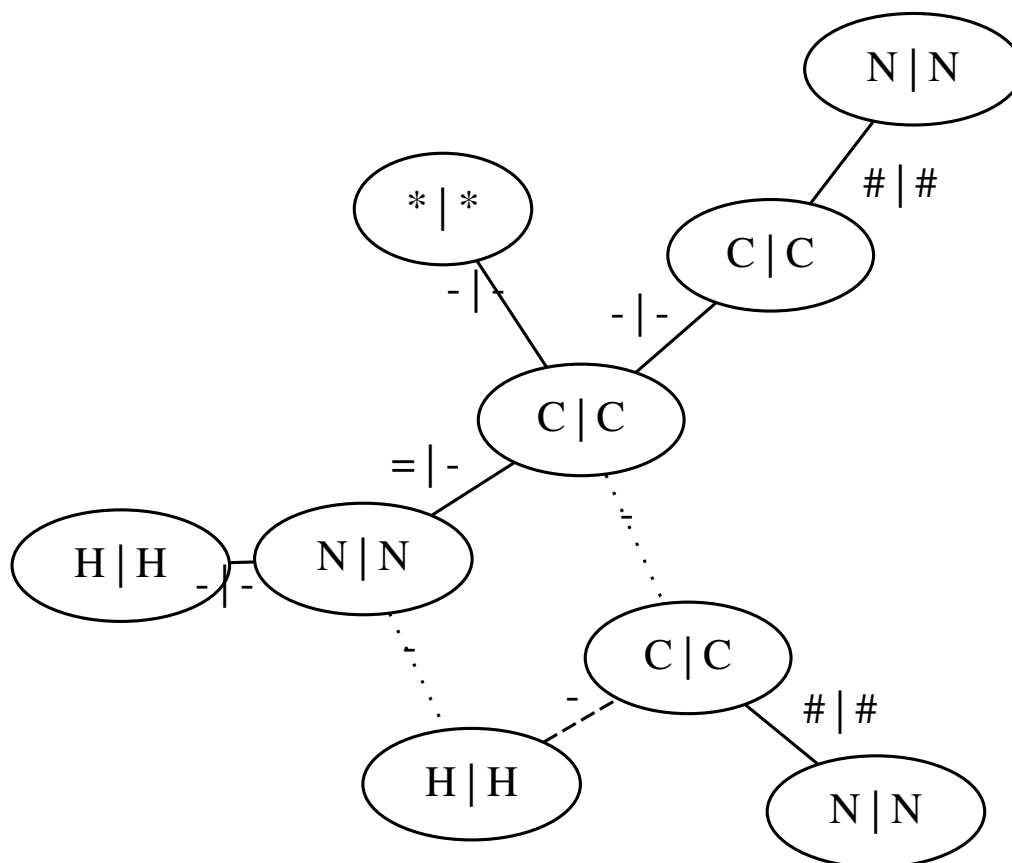


File: out/334_r_84_combined

1.0.85 CN addition to iminonitriles

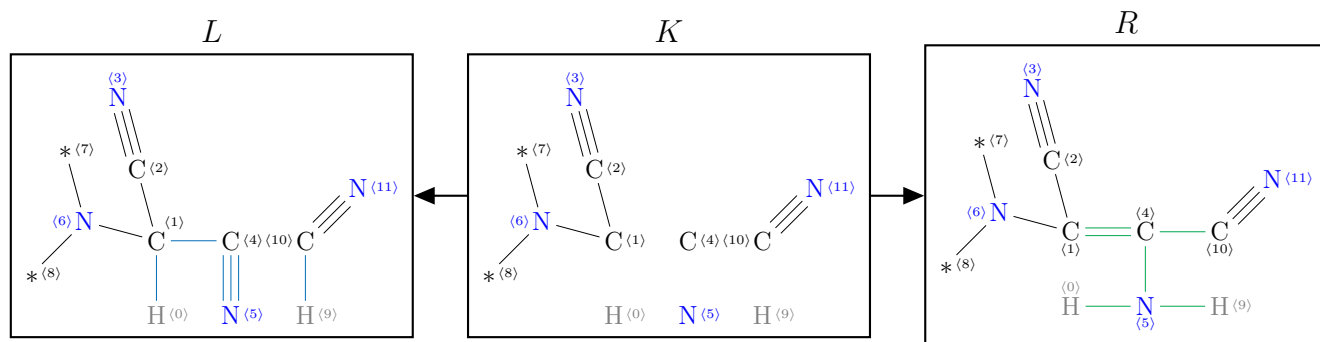


Files: out/337_r_86_10300110_{L, K, R}

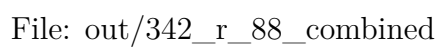


File: out/338_r_86_combined

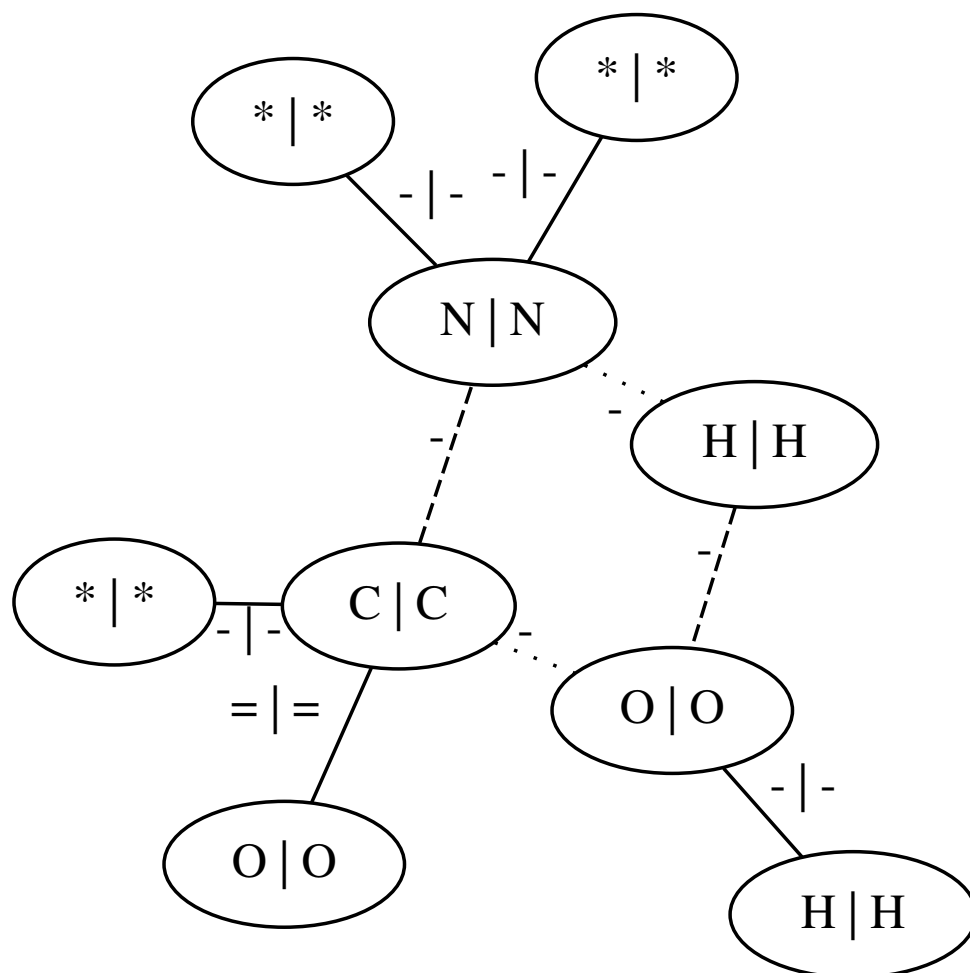
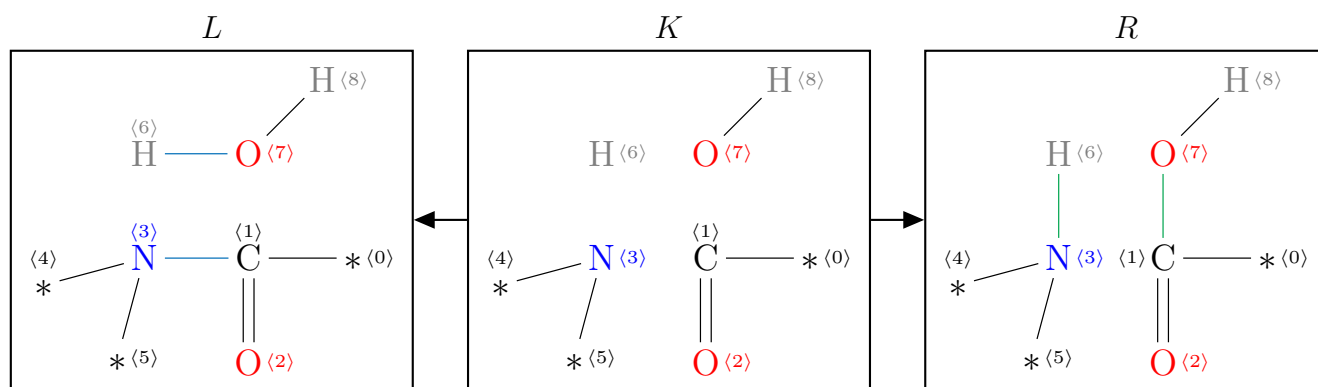
1.0.86 CN addition to aminodinitriles



Files: out/341_r_88_10300110_{L, K, R}



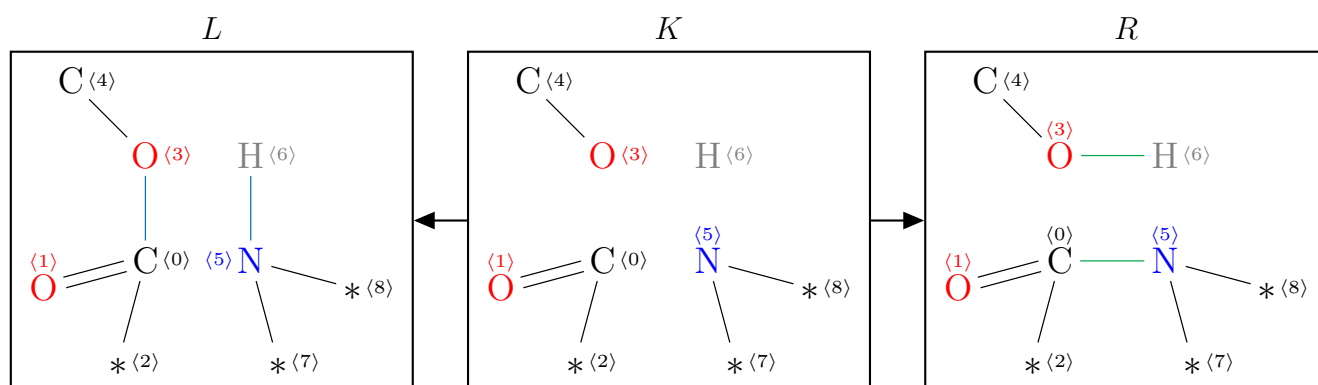
1.0.87 Amide Hydrolysis



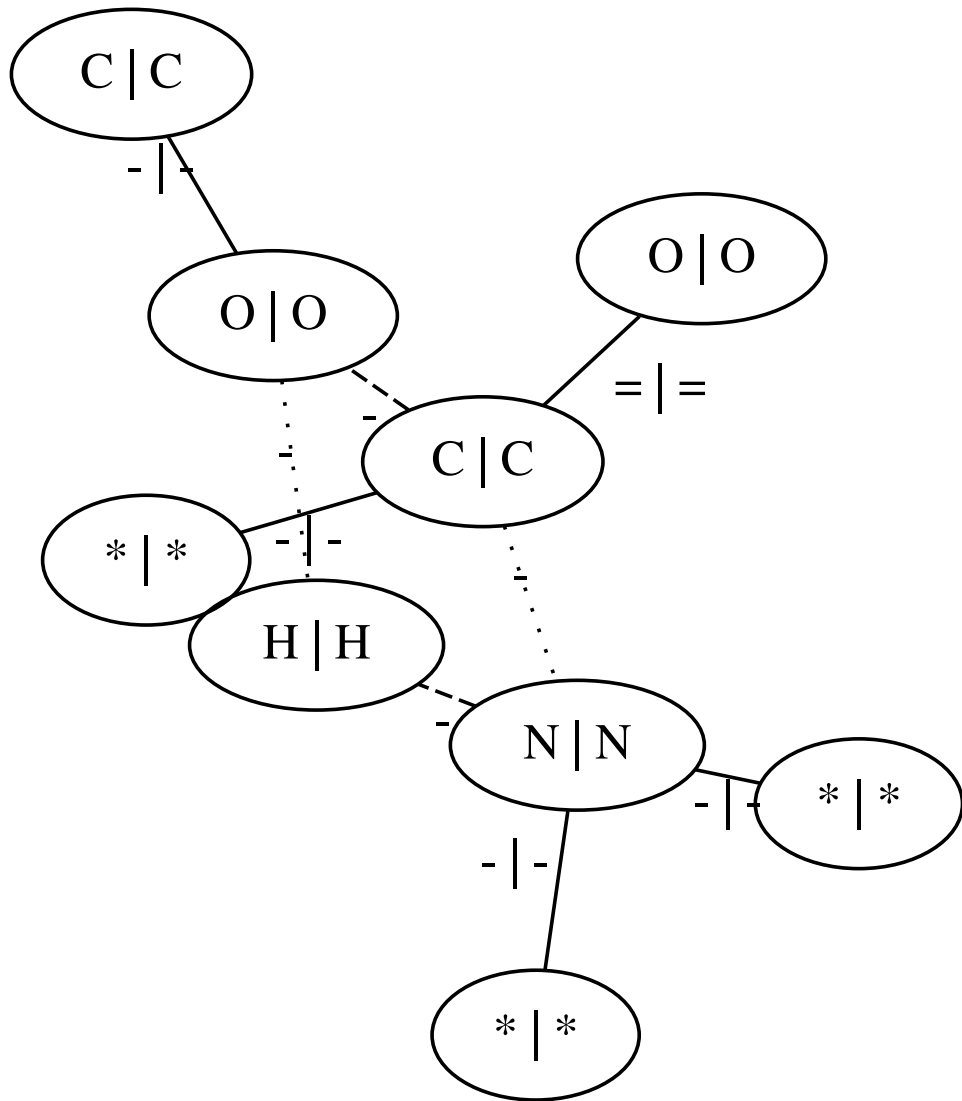
$$\begin{aligned}
 &|\{e \in \text{outEdges}(4) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\quad \}| = 1
 \end{aligned}$$

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

1.0.88 Amide Formation Hydrolysis, C



Files: out/349_r_91_10300110_{L, K, R}

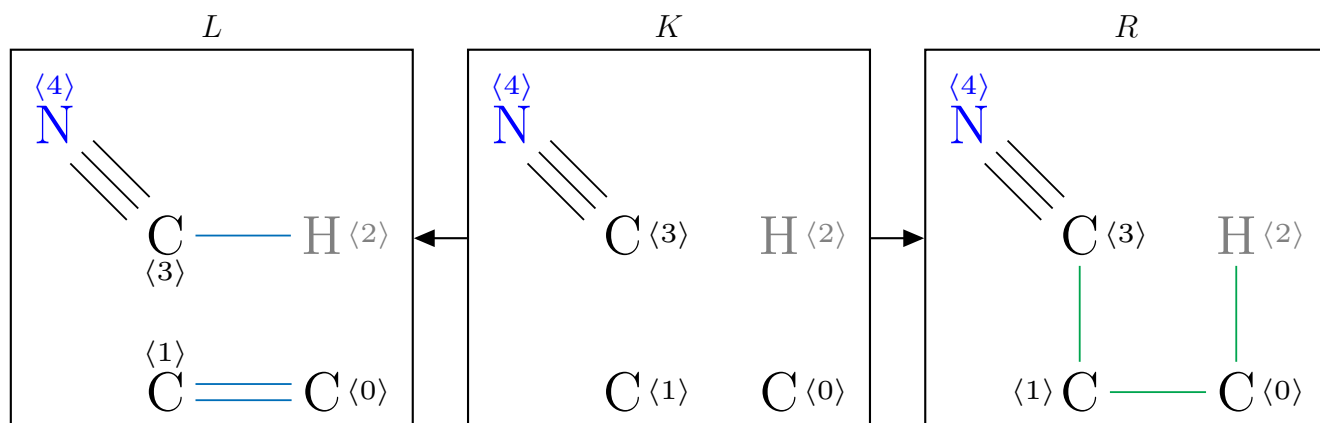


File: out/350_r_91_combined

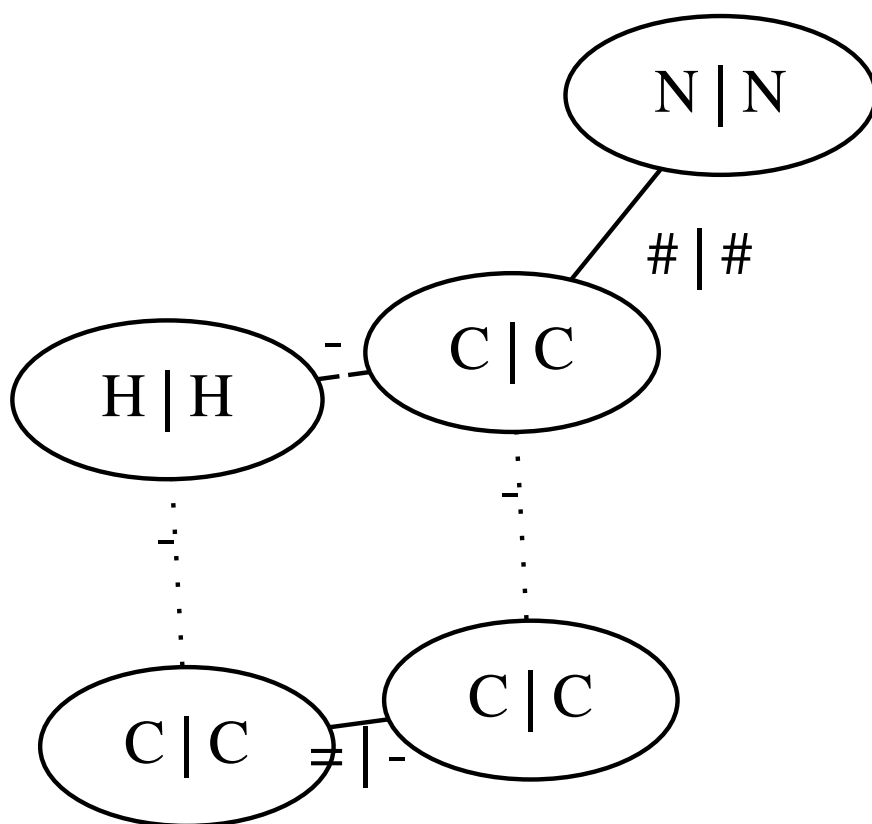
$$\begin{aligned}
 & |\{e \in \text{outEdges}(7) \mid \\
 & \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
 & \quad \wedge \\
 & \quad \text{label}(e) \in \{'=\'} \\
 & \quad \}| = 0
 \end{aligned}$$

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

1.0.89 Alkene Addition, CN

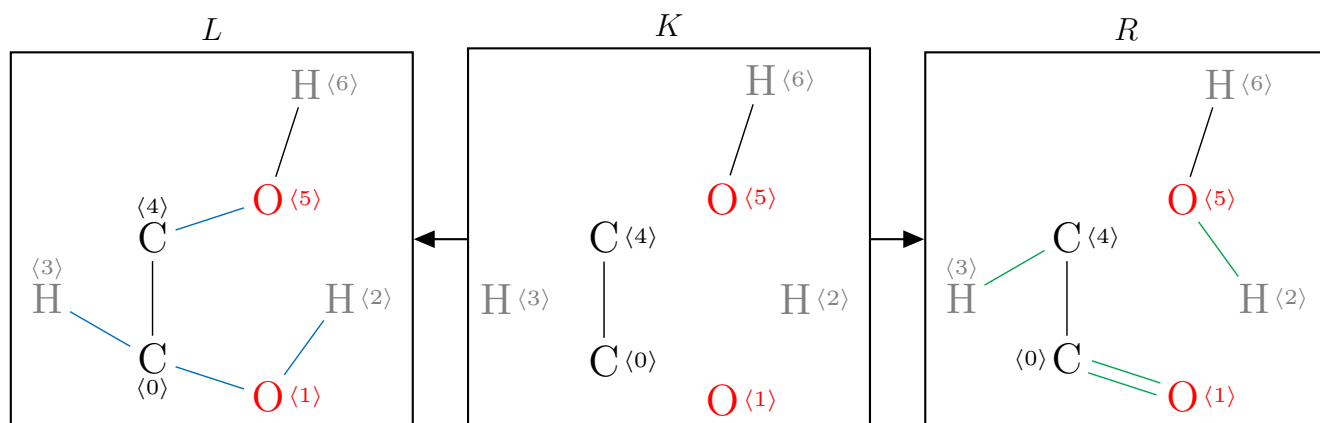


Files: out/353_r_92_10300110_{L, K, R}

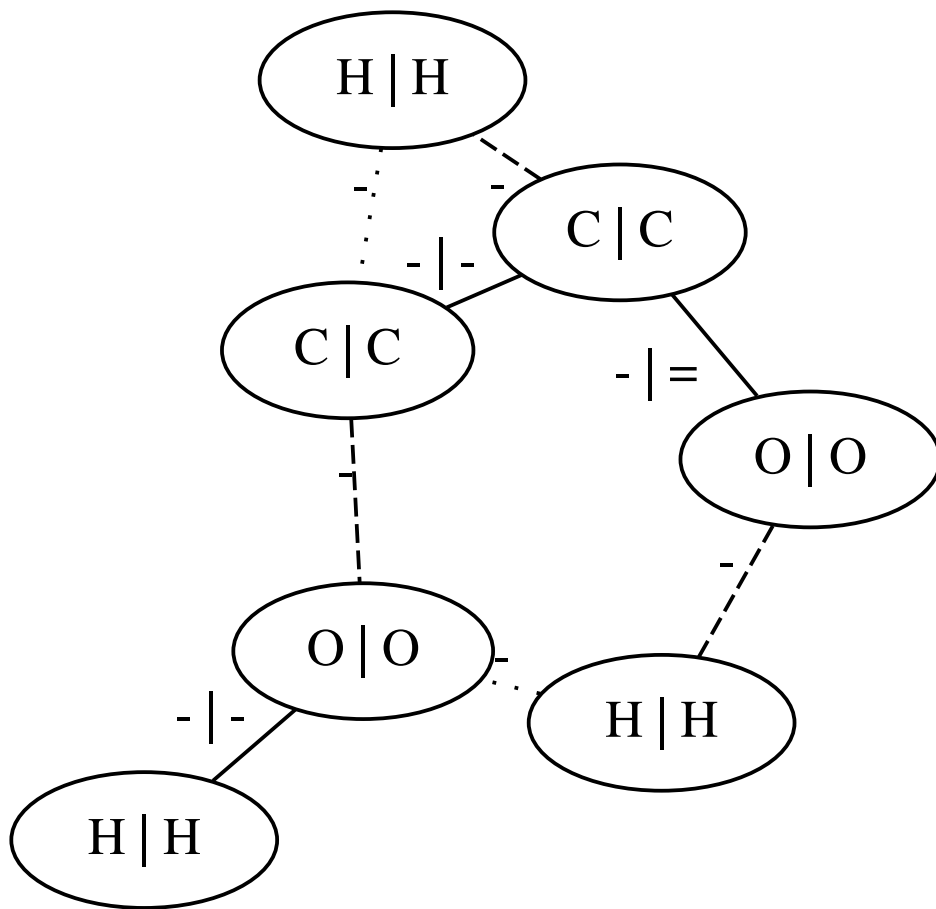


File: out/354_r_92_combined

1.0.90 Elimination + enol to keto



Files: out/357_r_93_10300110_{L, K, R}



File: out/358_r_93_combined

```

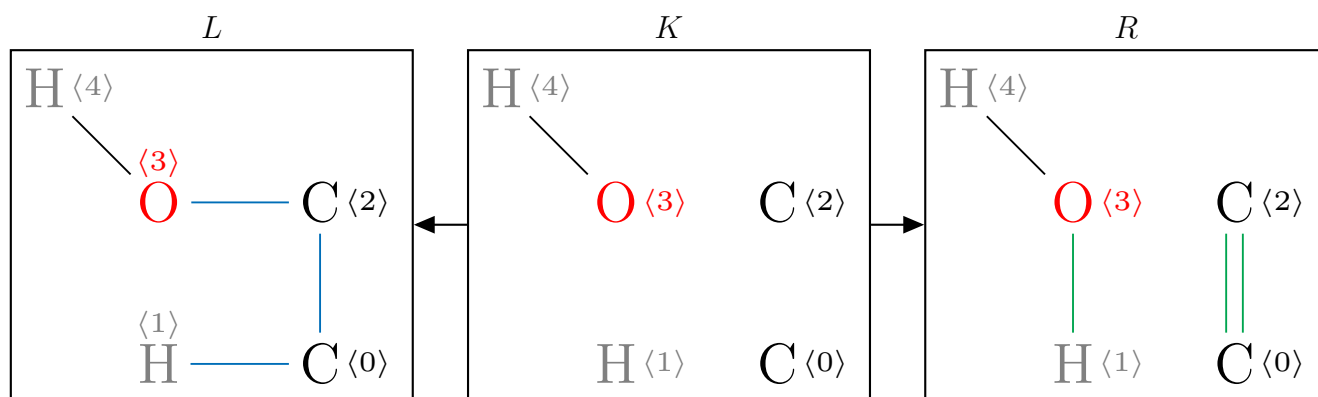
|{e ∈ outEdges(0) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'='}
}| = 0

```

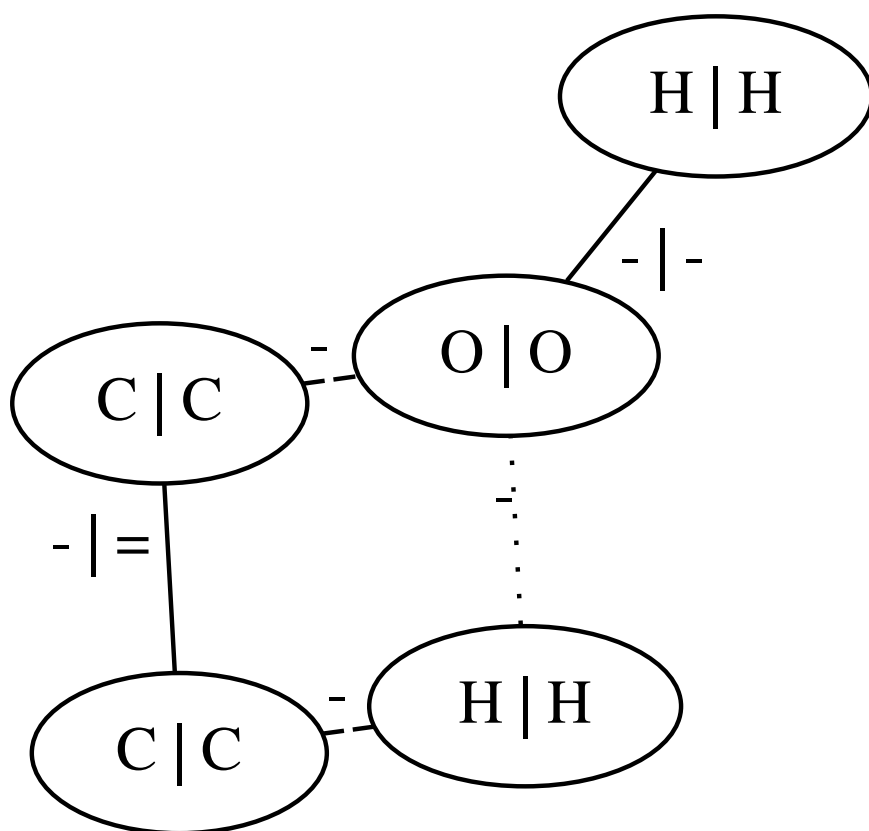
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

1.0.91 Elimination2



Files: out/361_r_94_10300110_{L, K, R}



File: out/362_r_94_combined

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

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

$$\wedge$$

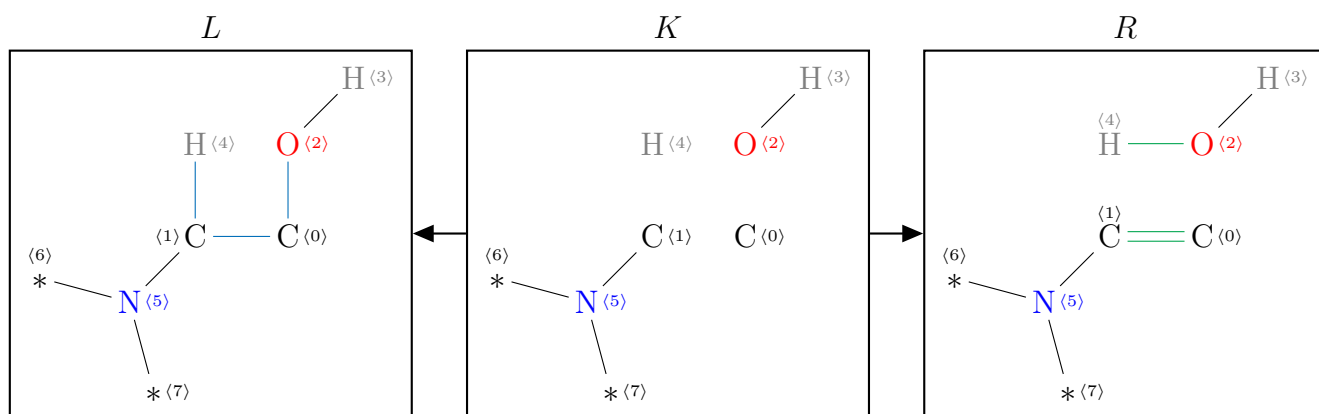
$$\text{label}(e) \in \{ '-' \}$$

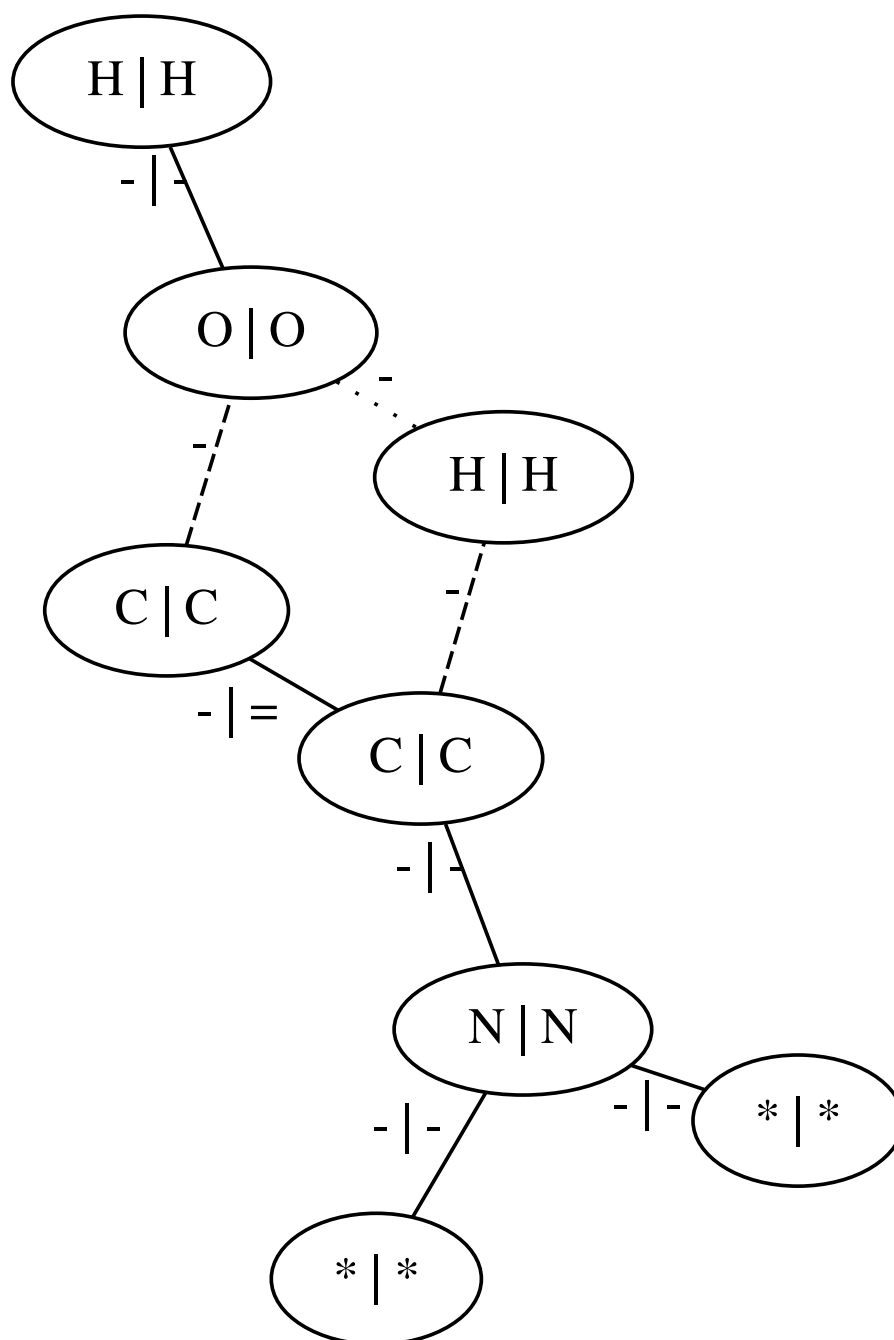
$$\}| = 0$$

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

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

1.0.92 Dehydration of Amines



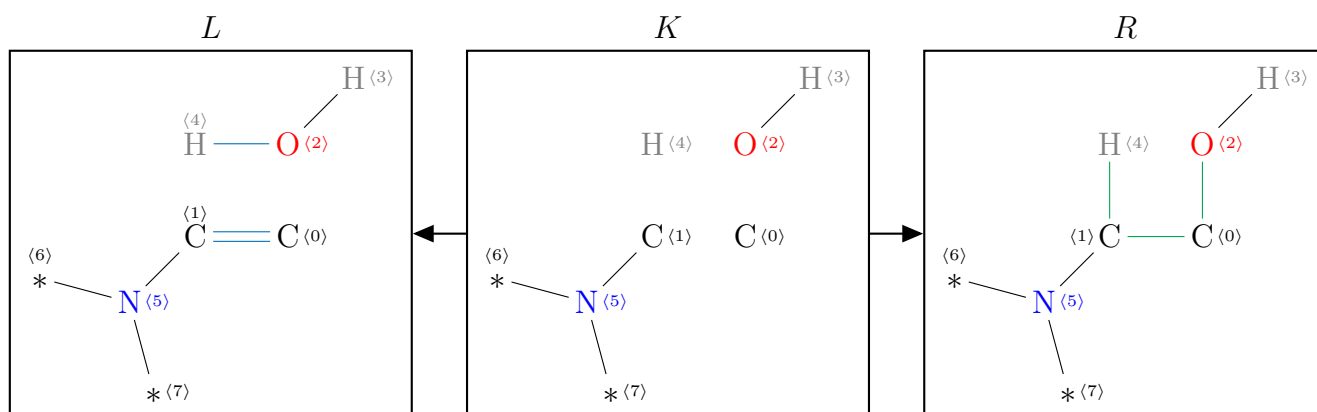


File: out/366_r_95_combined

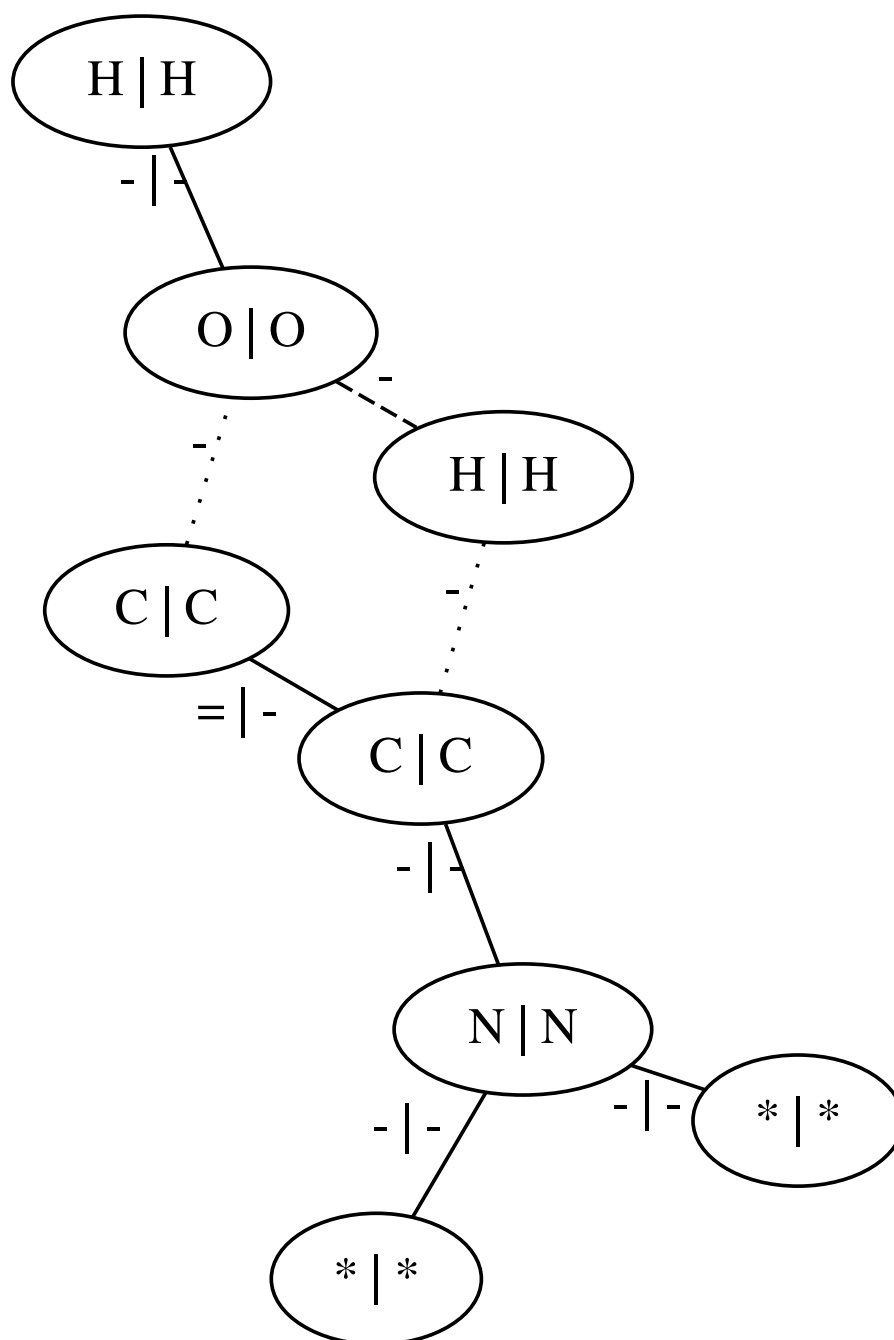
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \}\} = 0
\end{aligned}$$

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

1.0.93 Deydration of Amines (inverse)



Files: out/369_r_96_10300110_{L, K, R}



File: out/370_r_96_combined

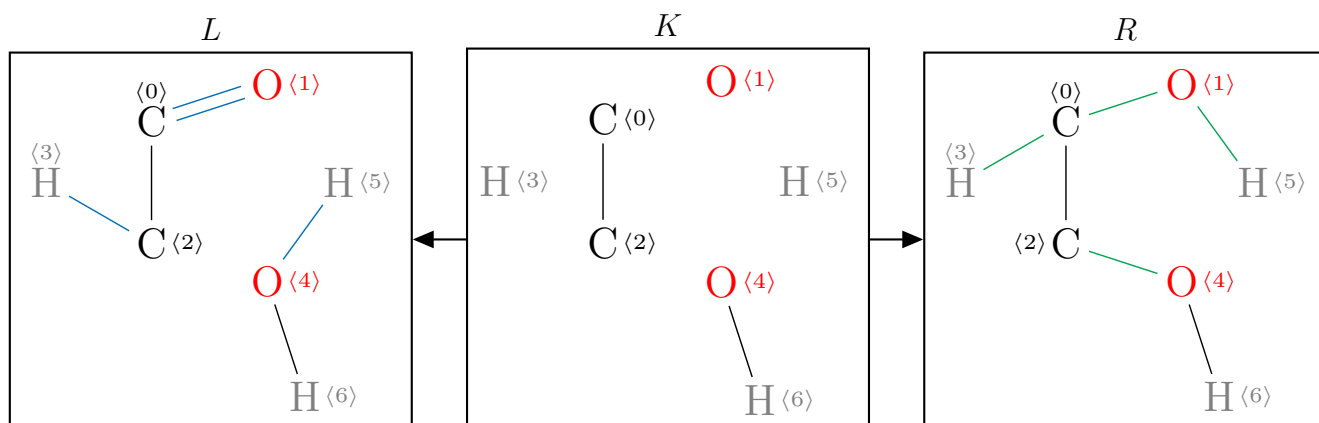
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

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

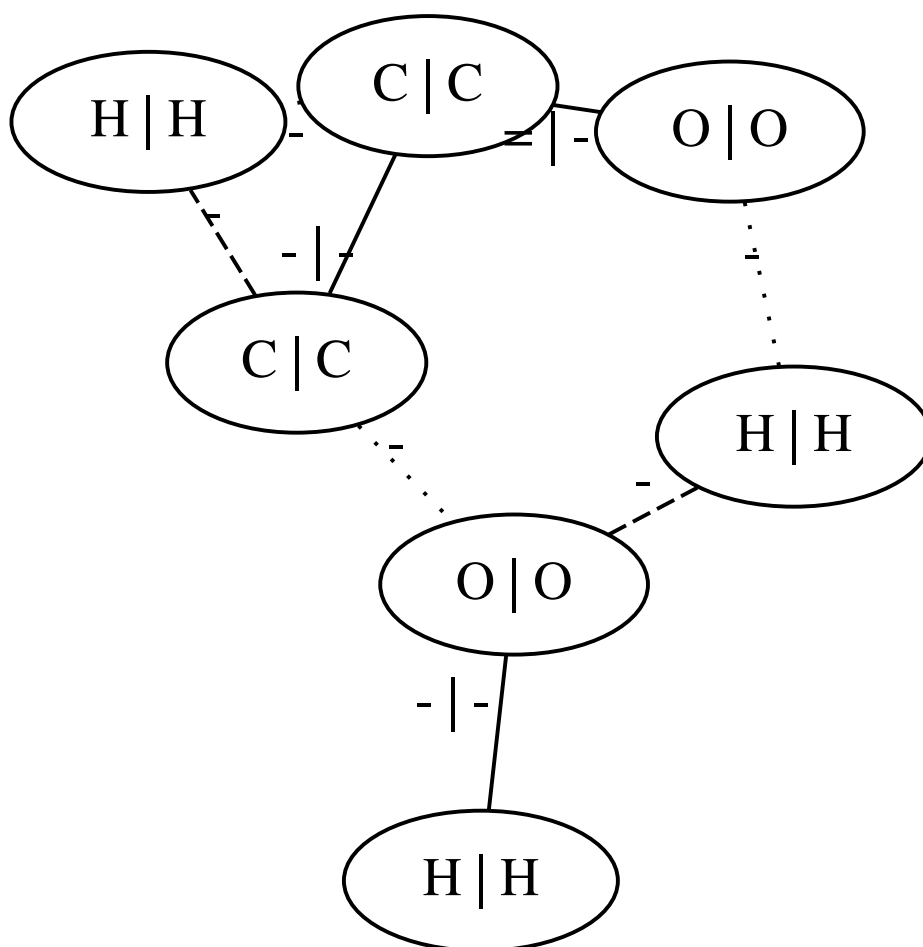
$$\begin{aligned}
& |\{e \in \text{outEdges}(6) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.94 Hydration of C(=O)C



Files: out/373_r_97_10300110_{L, K, R}



File: out/374_r_97_combined

```

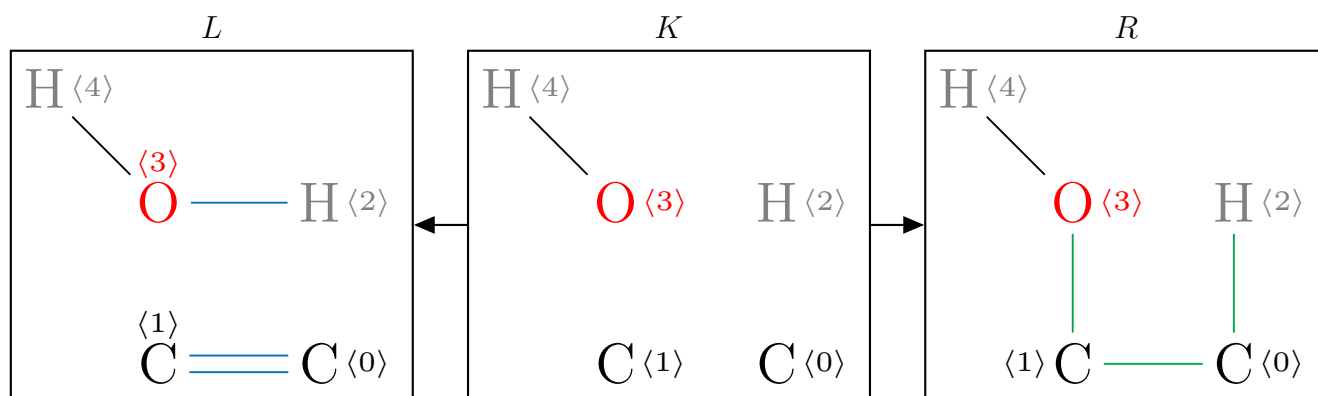
|{e ∈ outEdges(0) |
  label(target(e)) ∈ {'O', 'N', 'S'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```

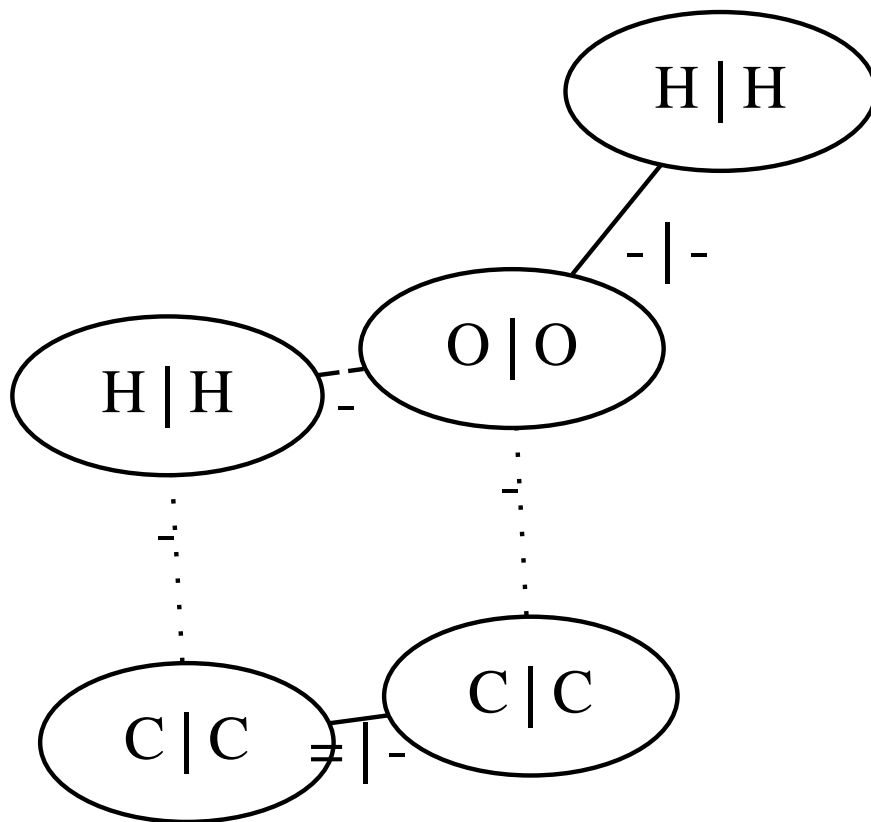
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}, \text{'='}\} \\
& \quad \}\mid = 0
\end{aligned}$$

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

1.0.95 Hydration of C=C(O)



Files: out/377_r_98_10300110_{L, K, R}



File: out/378_r_98_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

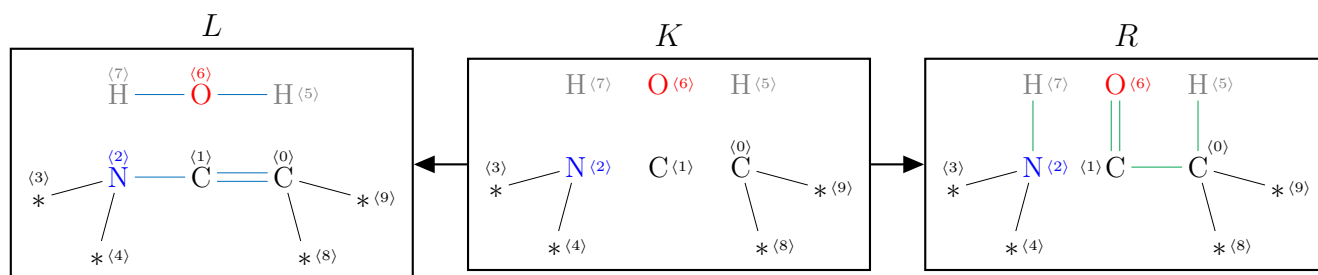
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

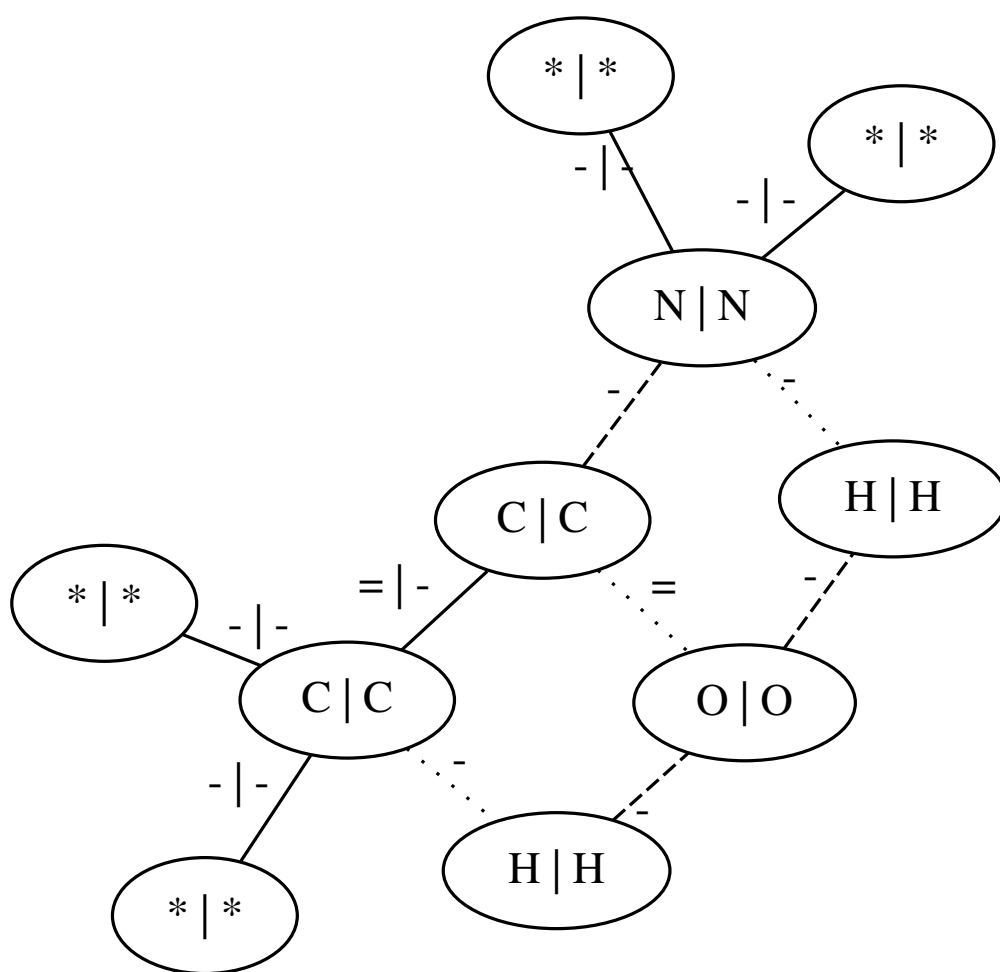
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

1.0.96 Enamine Hydration and Elimination



Files: out/381_r_99_10300110_{L, K, R}



File: out/382_r_99_combined

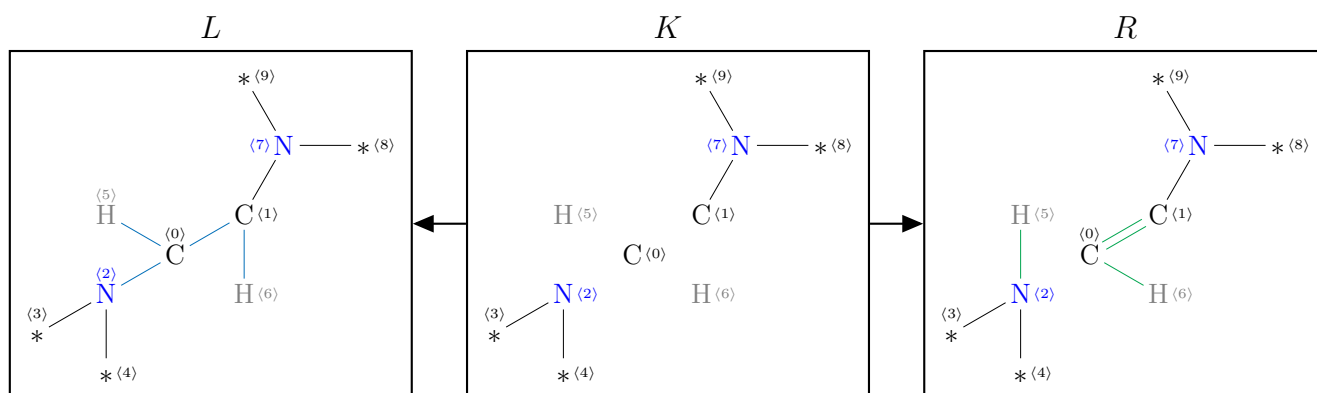
$$\begin{aligned}
& |\{e \in \text{outEdges}(3) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \} | = 0
\end{aligned}$$

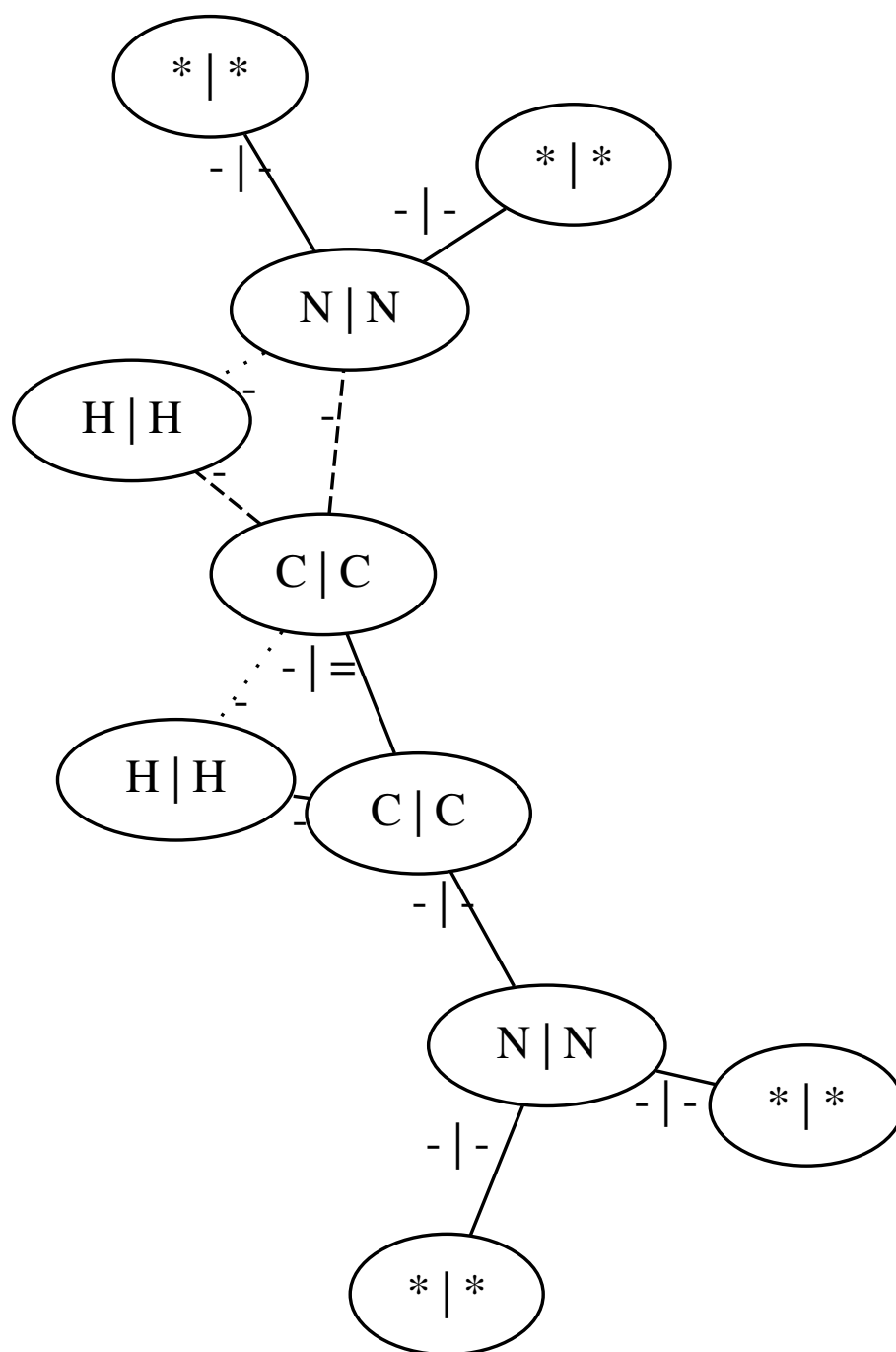
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \} | = 0
\end{aligned}$$

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

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

1.0.97 Deamination of Vicinal Diamine





File: out/386_r_100_combined

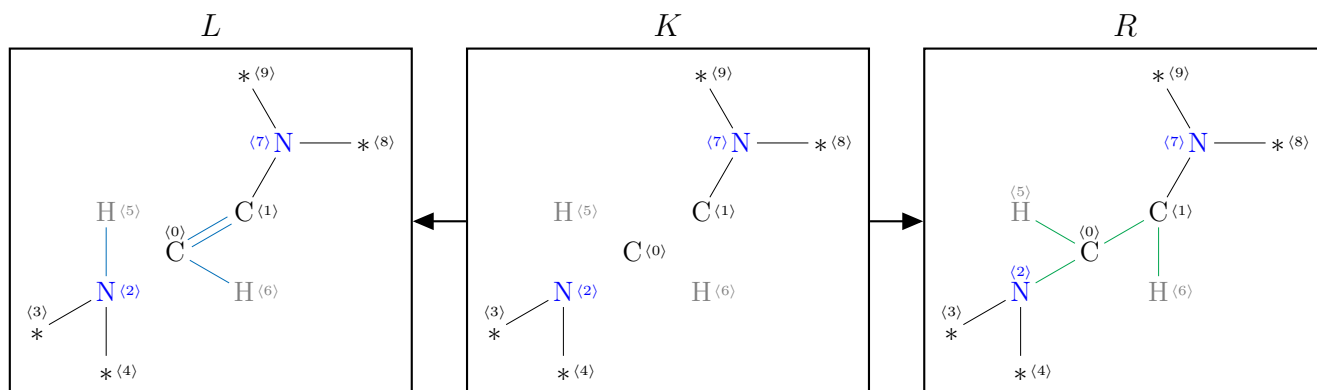
$$\begin{aligned}
&|\{e \in \text{outEdges}(3) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{'='}\} \\
&\}| = 0
\end{aligned}$$

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

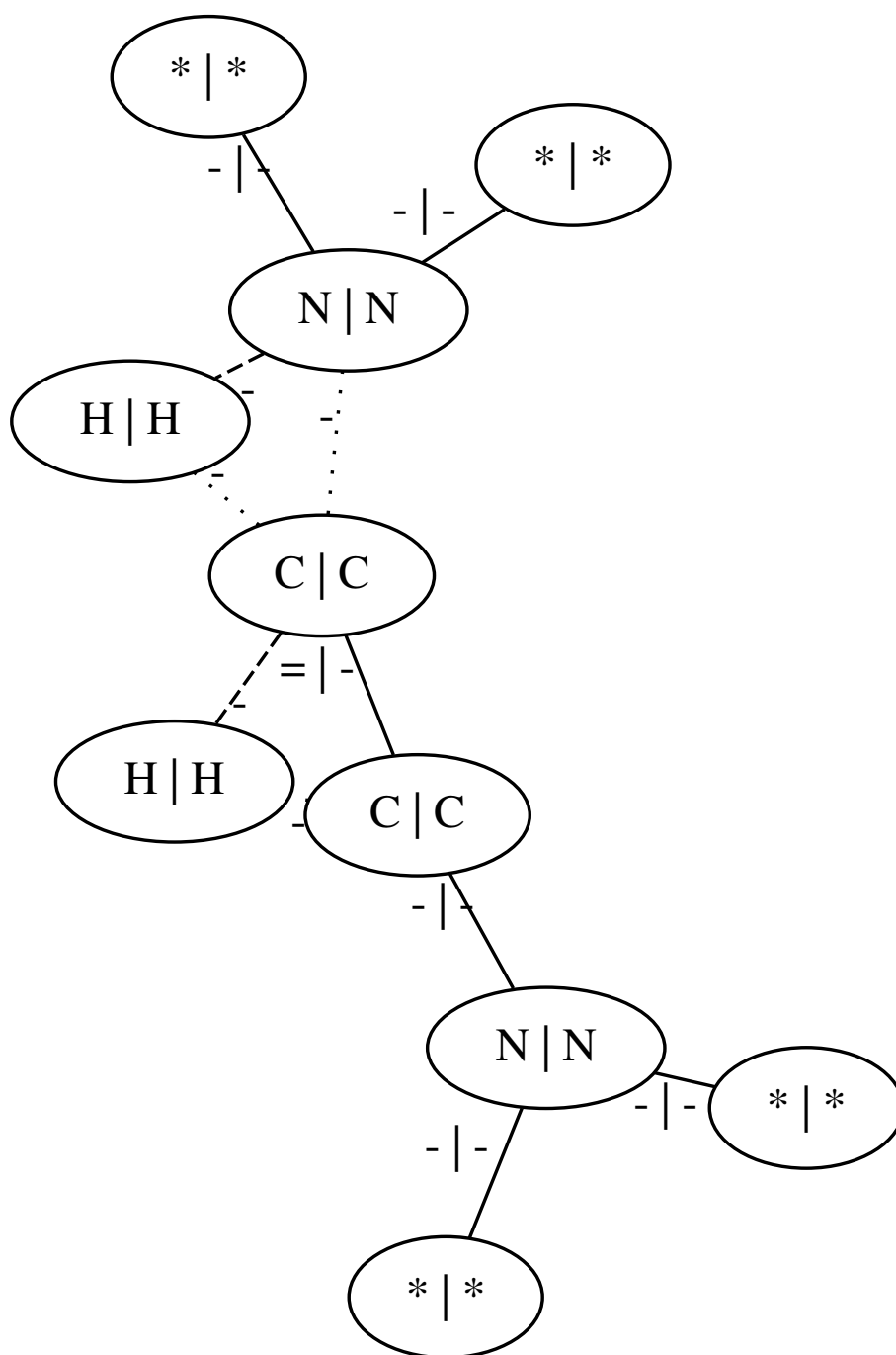
$$\begin{aligned}
&|\{e \in \text{outEdges}(8) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{'='}\} \\
&\}| = 0
\end{aligned}$$

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

1.0.98 Deamination of Vicinal Diamine, (inverse)



Files: out/389_r_101_10300110_{L, K, R}



File: out/390_r_101_combined

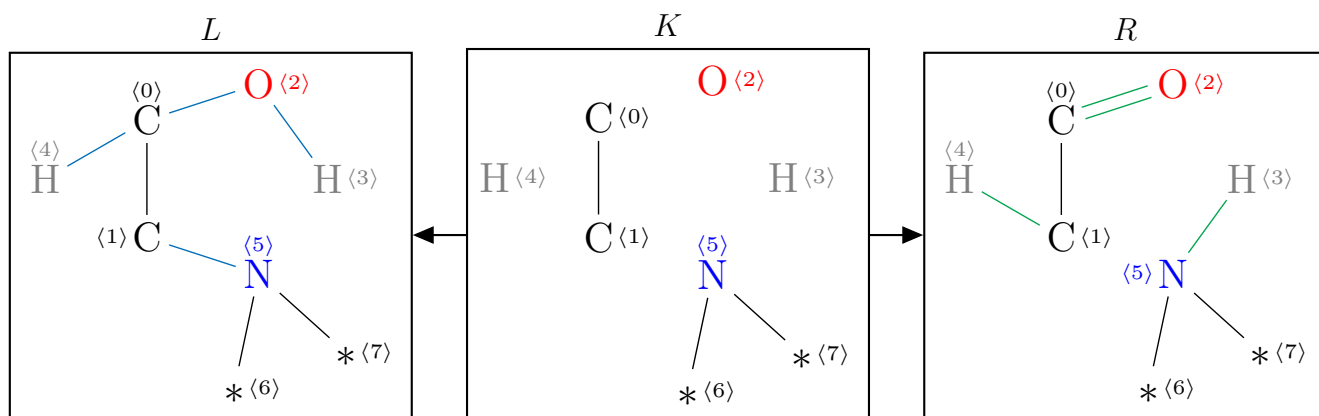
$$\begin{aligned}
& |\{e \in \text{outEdges}(3) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \}\} = 0
\end{aligned}$$

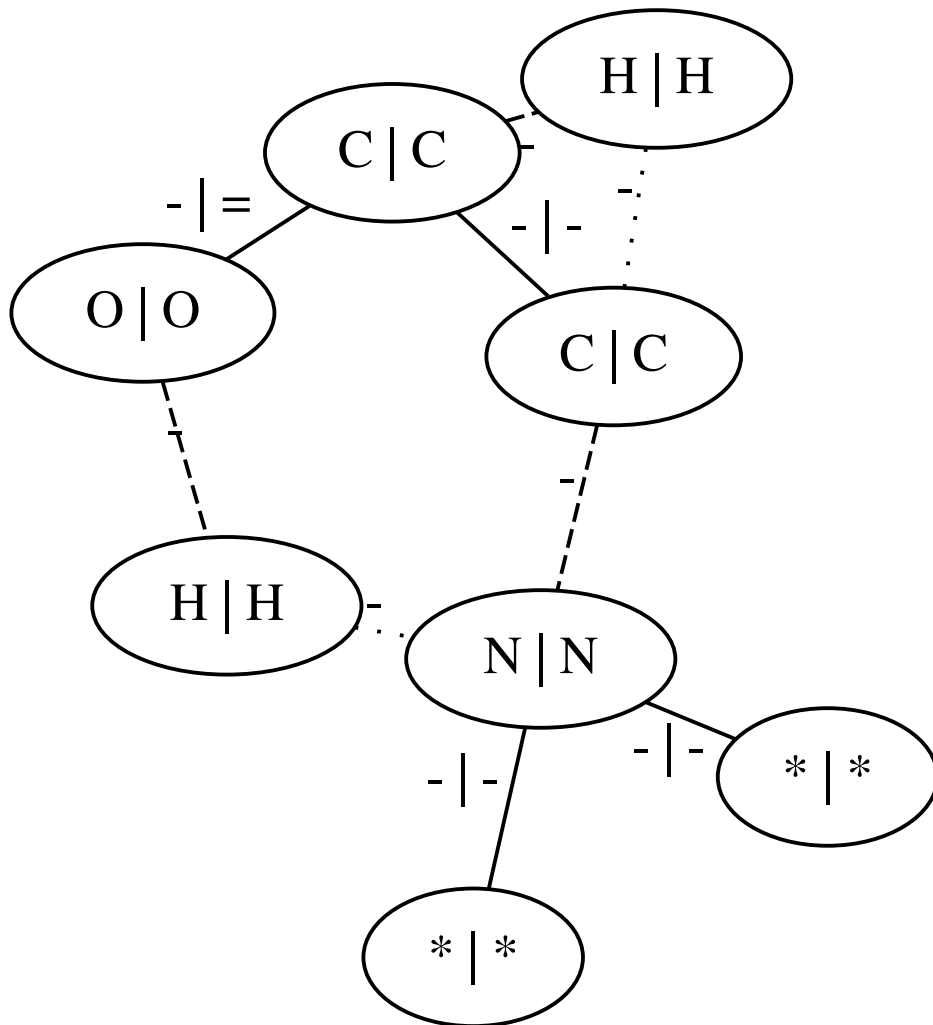
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \}\} = 0
\end{aligned}$$

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

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

1.0.99 Deamination 2



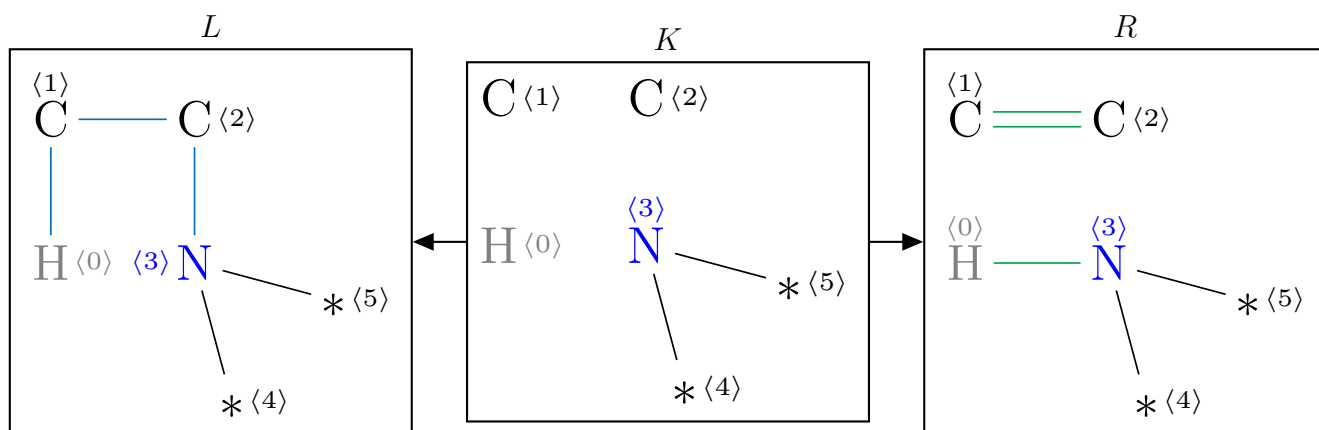


File: out/394_r_102_combined

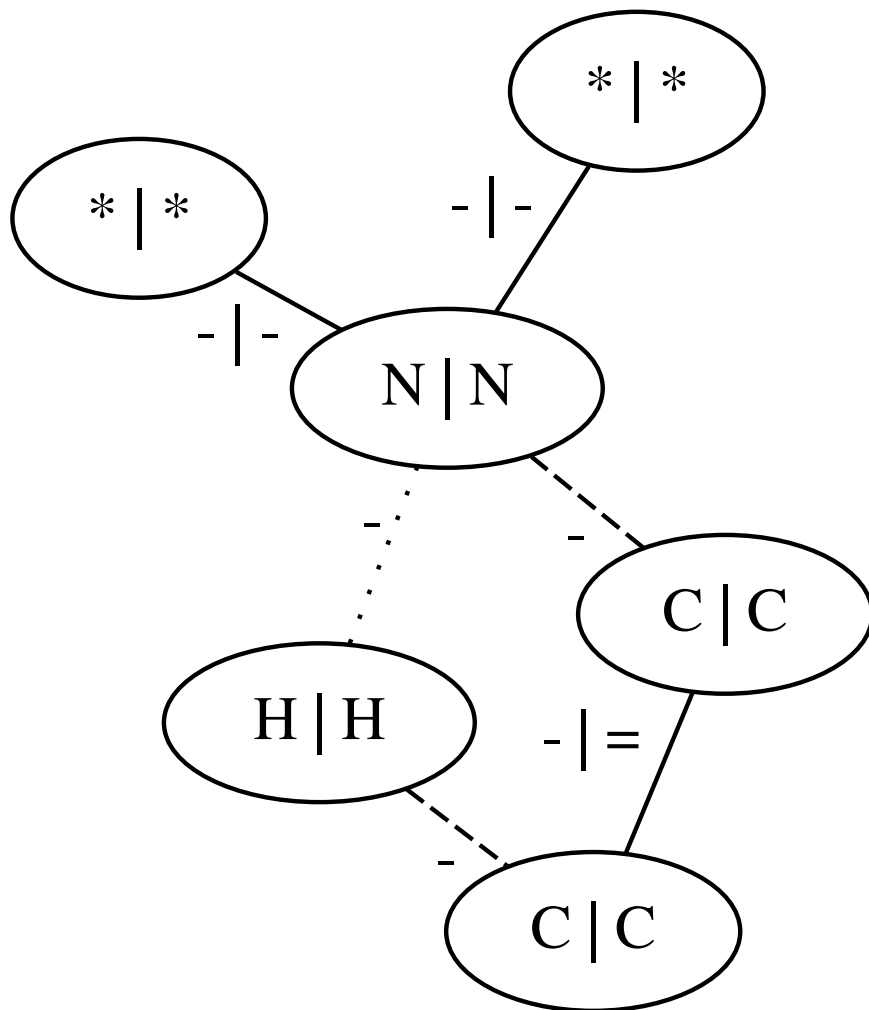
$$\begin{aligned}
 &|\{e \in \text{outEdges}(6) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}\} \\
 &\}\} = 0
 \end{aligned}$$

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

1.0.100 Deamination 3



Files: out/397_r_103_10300110_{L, K, R}



File: out/398_r_103_combined

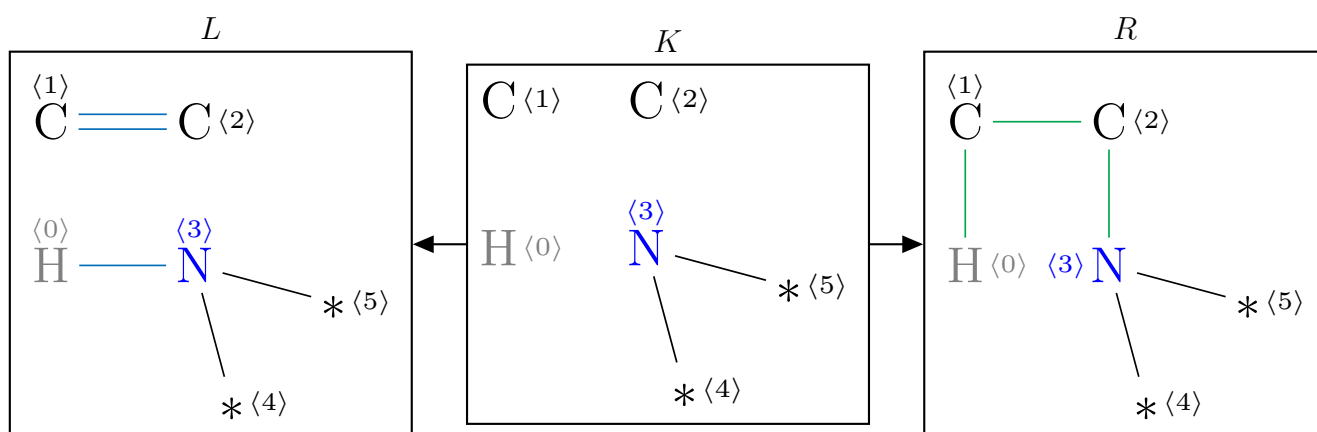
$$\begin{aligned}
 &|\{e \in \text{outEdges}(1) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
 &\quad \}| = 0
 \end{aligned}$$

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

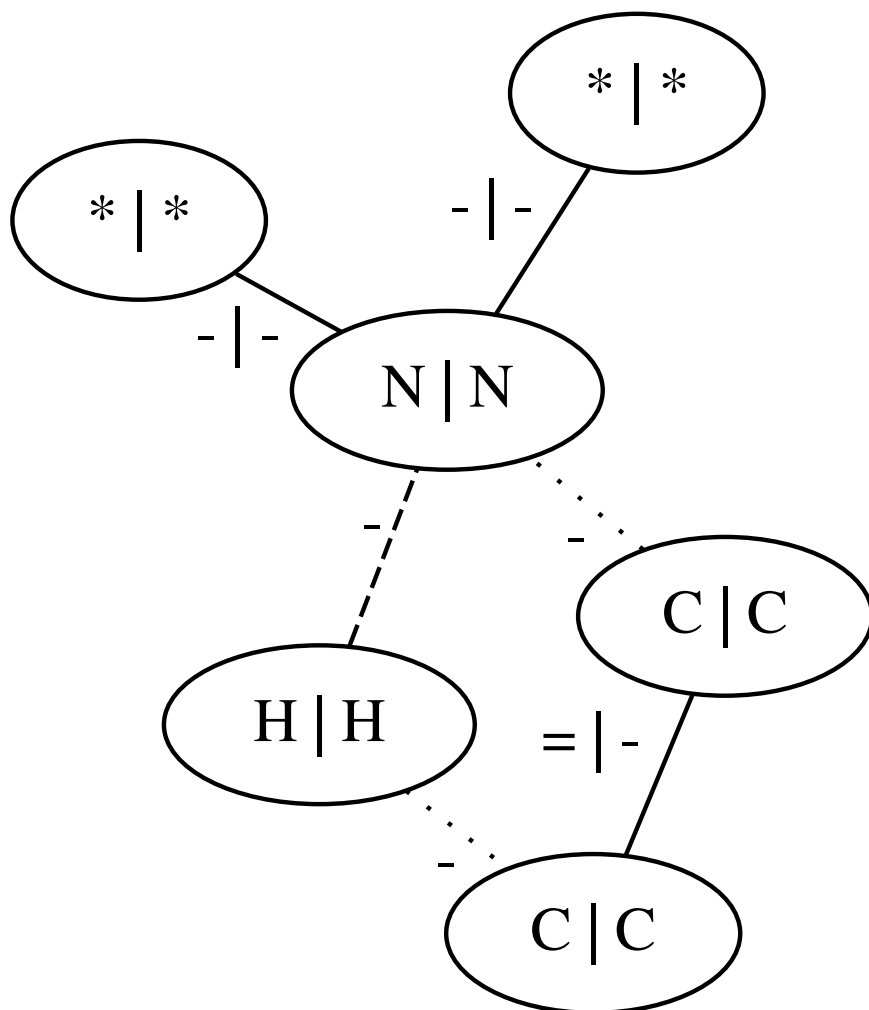
$$\begin{aligned}
& |\{e \in \text{outEdges}(4) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.101 Deamination 3 (inverse)



Files: out/401_r_104_10300110_{L, K, R}



File: out/402_r_104_combined

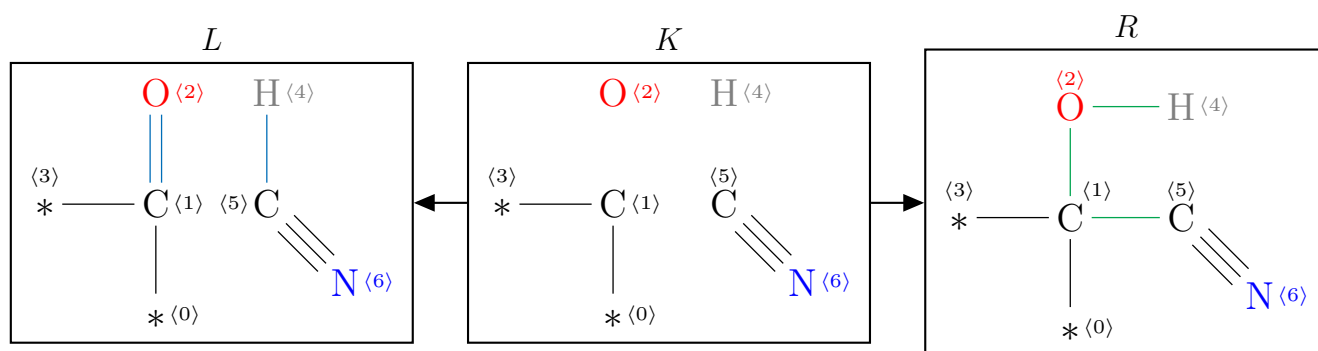
$$\begin{aligned}
 &|\{e \in \text{outEdges}(1) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
 &\quad \}| = 0
 \end{aligned}$$

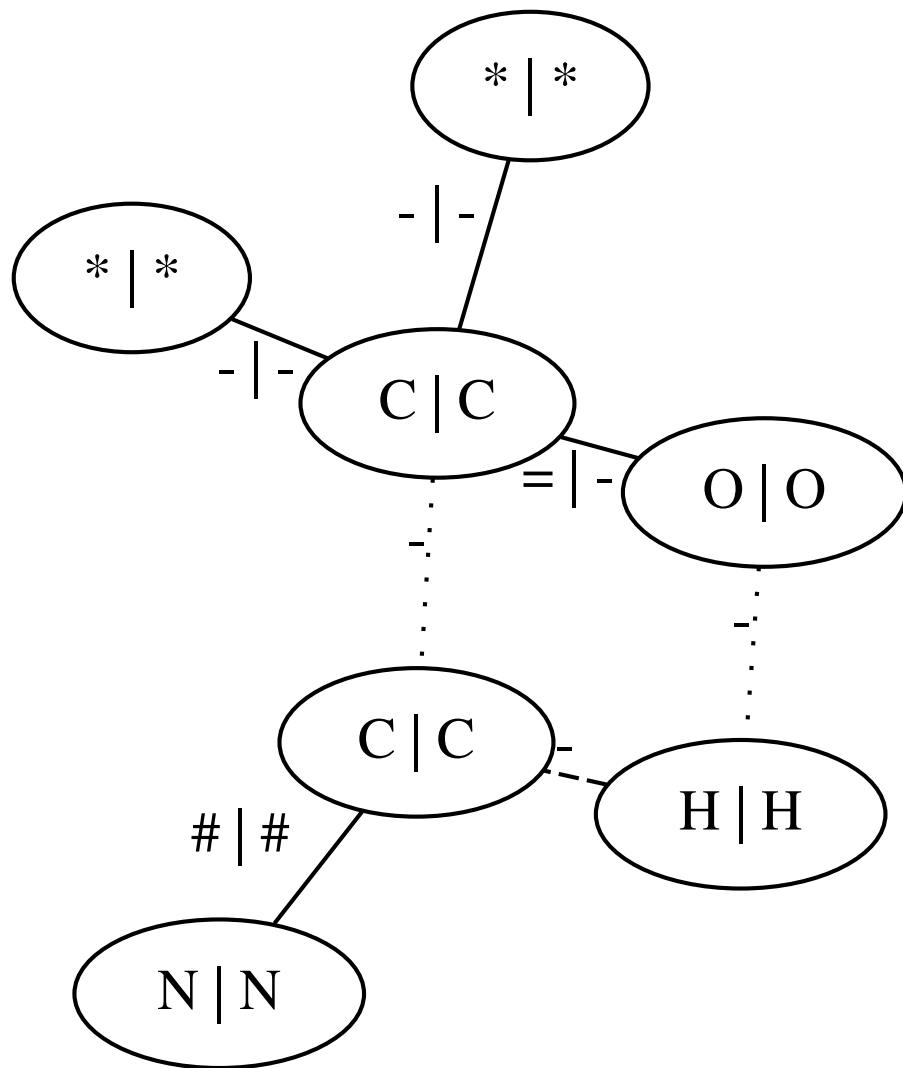
$$\begin{aligned}
&|\{e \in \text{outEdges}(2) \mid \\
&\quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'O'}}\} \\
&\quad \wedge \\
&\quad \text{label}(e) \in \{\text{'='}, \text{'-'}\} \\
&\}| = 0
\end{aligned}$$

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

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

1.0.102 Cyanohydrin Formation





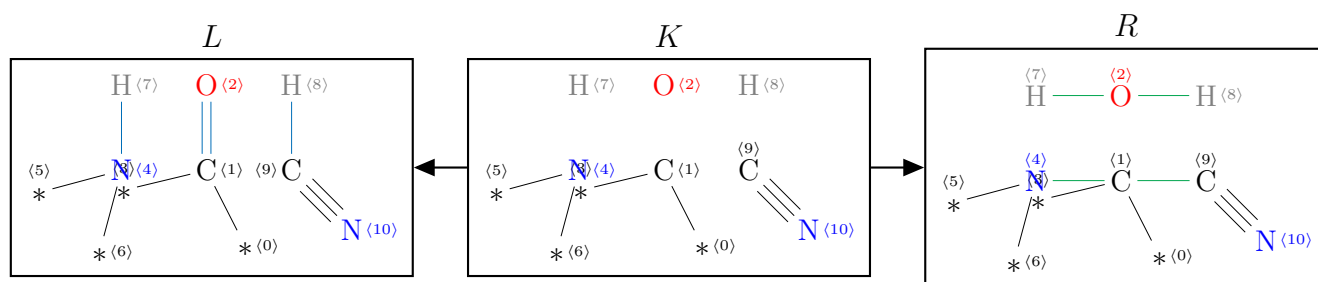
File: out/406_r_105_combined

```

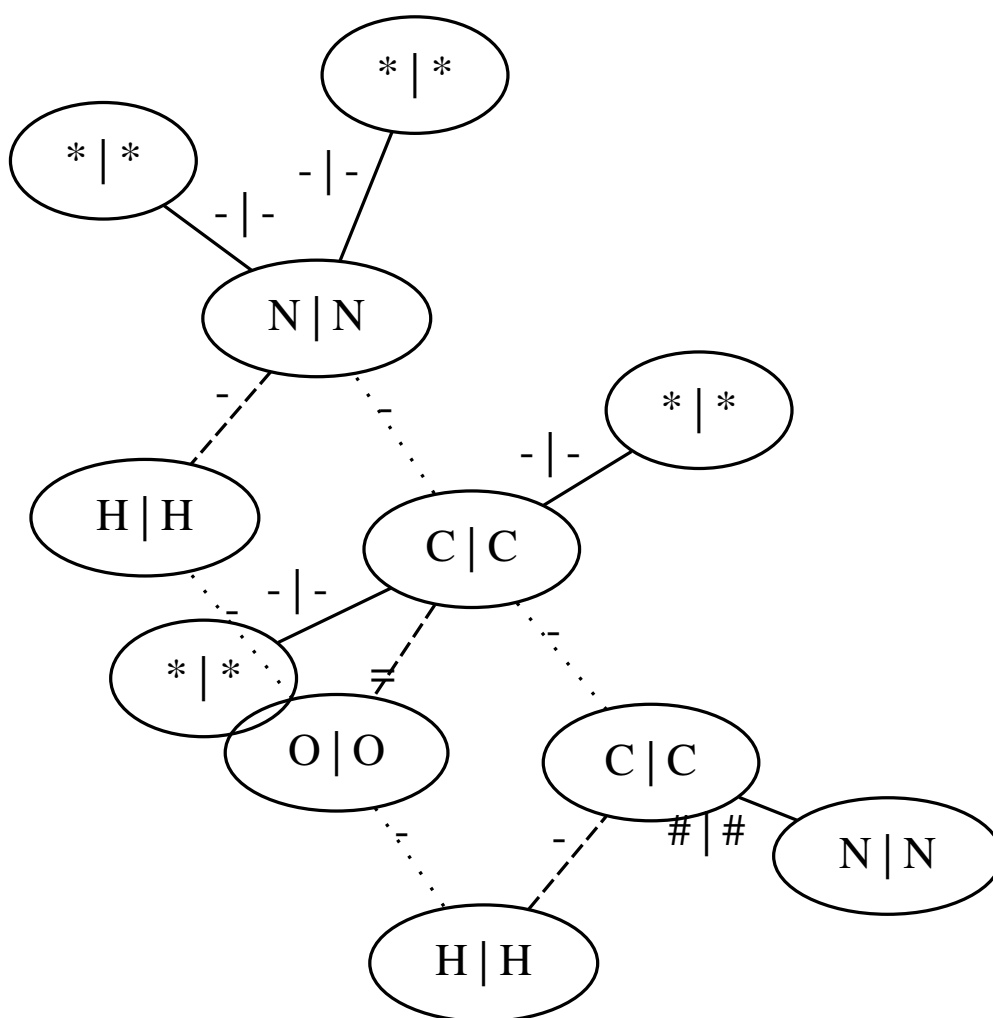
|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```

1.0.103 Strecker Synthesis



Files: out/409_r_106_10300110_{L, K, R}



File: out/410_r_106_combined

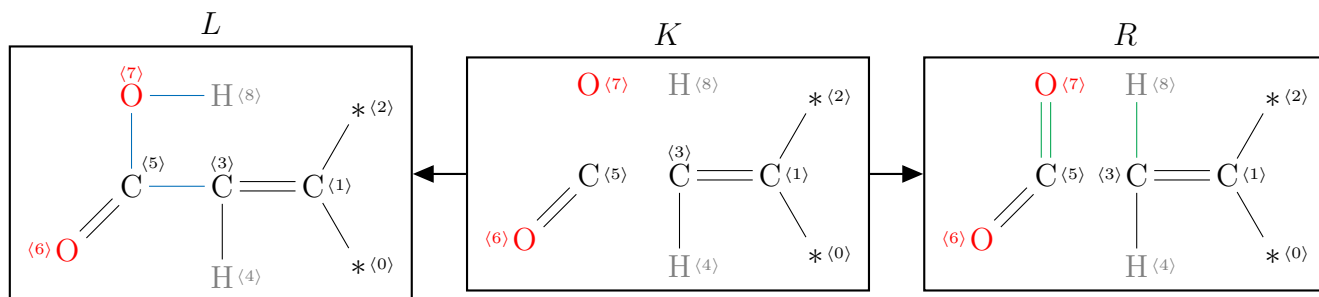
$$\begin{aligned}
 &|\{e \in \text{outEdges}(1) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\}\mid = 0
 \end{aligned}$$

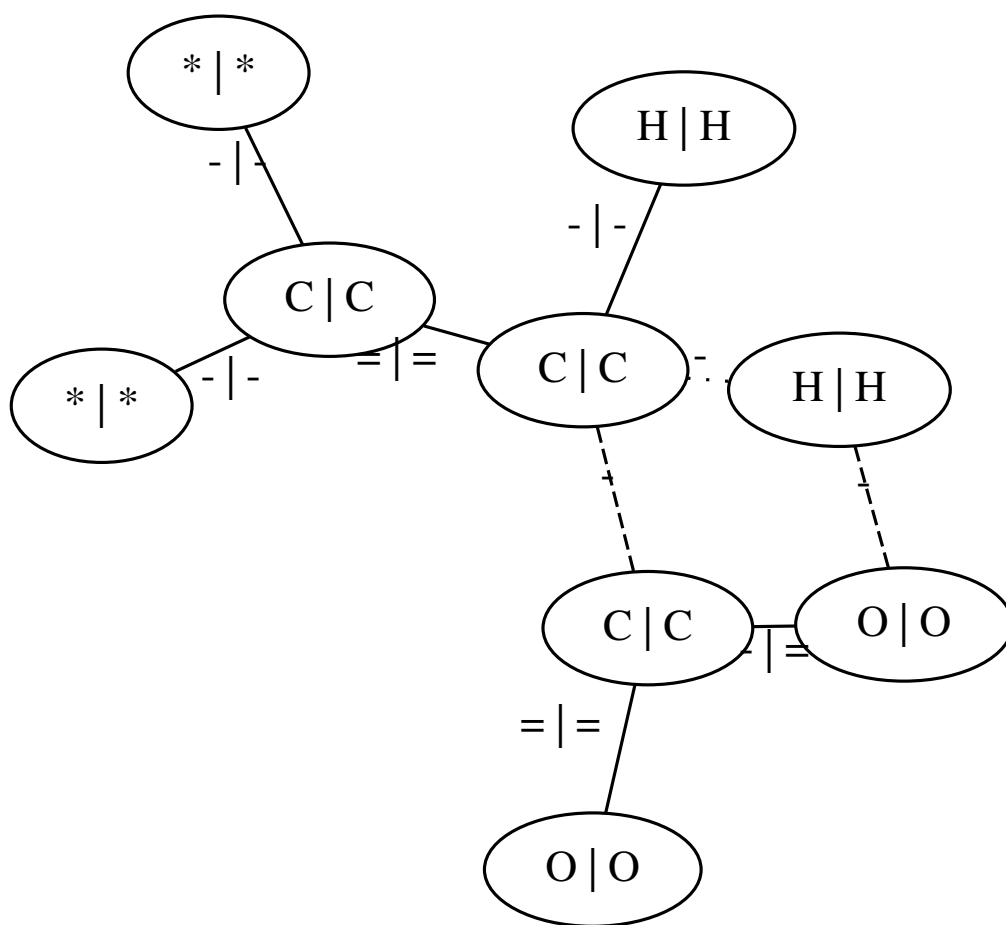
$$\begin{aligned}
 &|\{e \in \text{outEdges}(4) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\}\mid = 0
 \end{aligned}$$

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

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

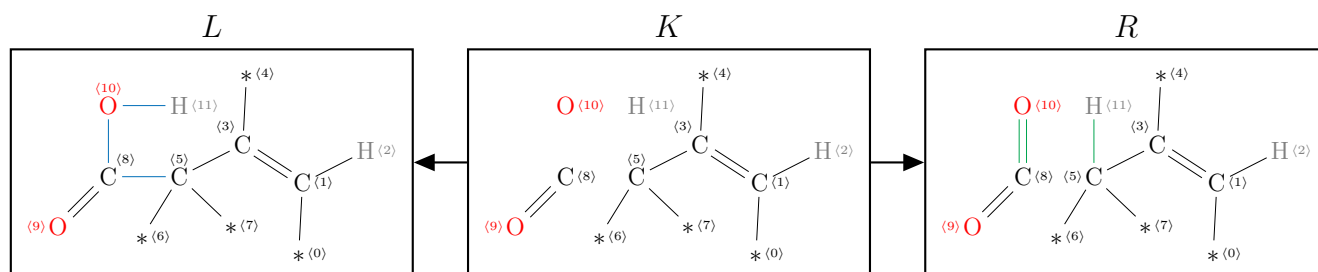
1.0.104 Alpha-Beta Unsaturated Acid Decarboxylation



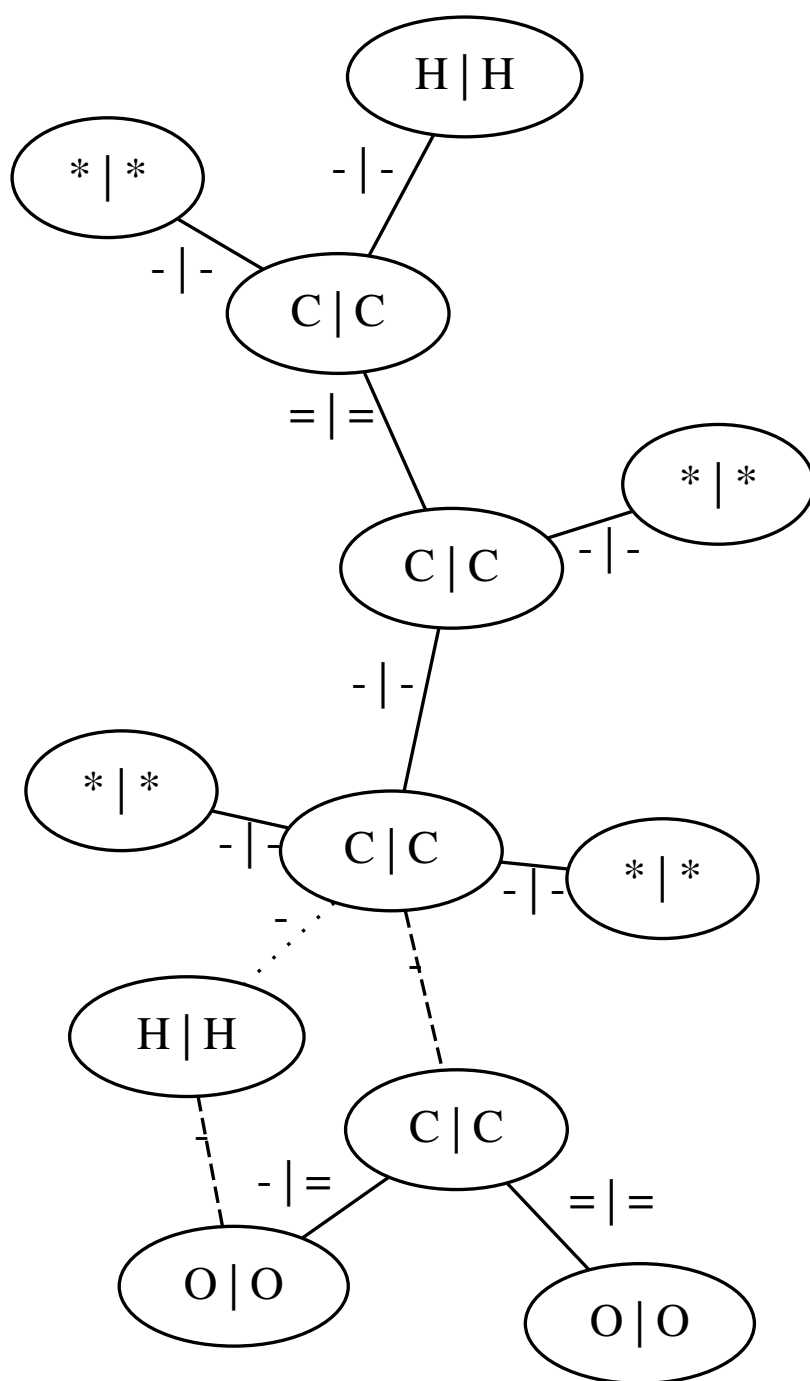


File: out/414_r_107_combined

1.0.105 Beta-gamma Unsaturated Acid Decarboxylation

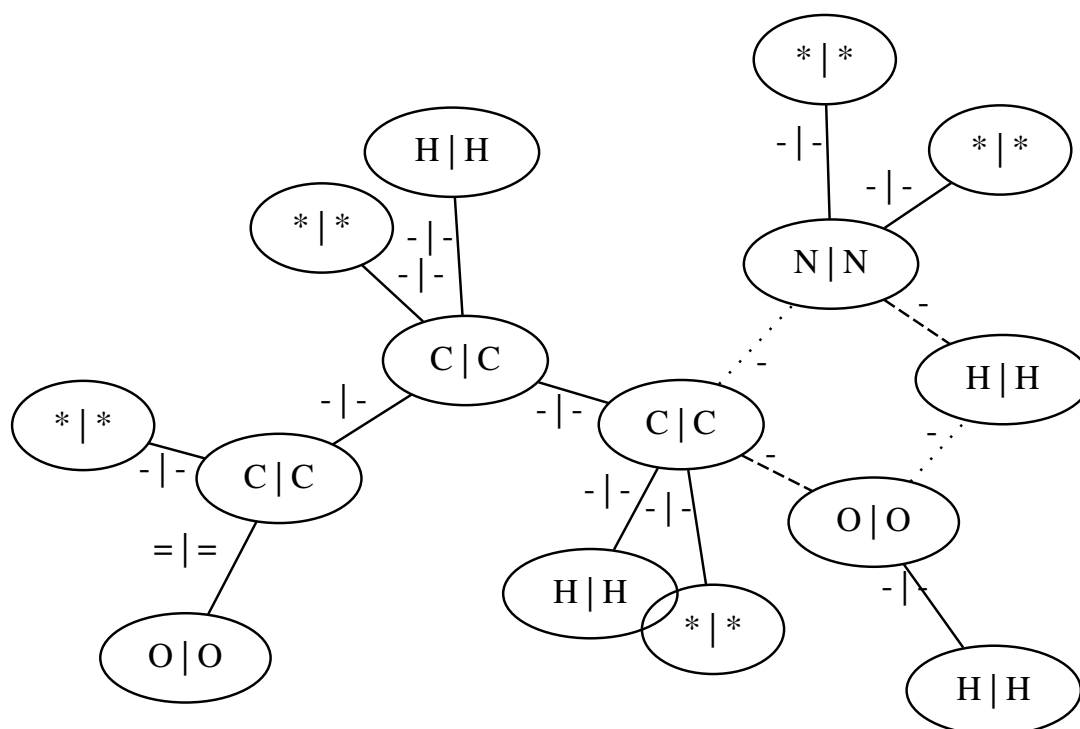
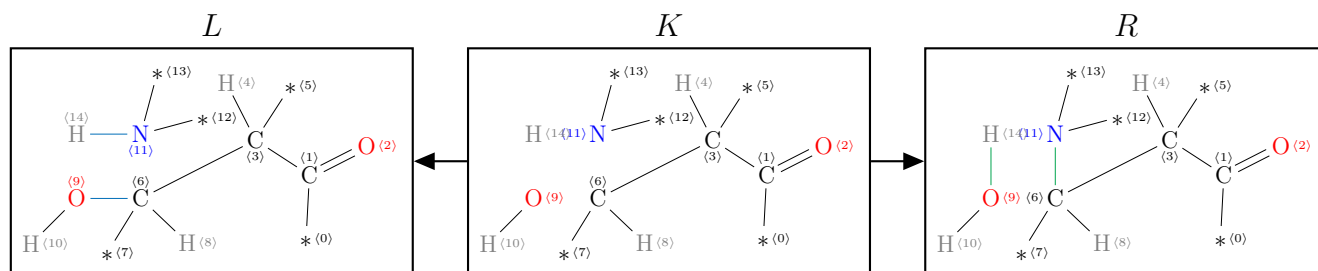


Files: out/417_r_108_10300110_{L, K, R}



File: out/418_r_108_combined

1.0.106 Mannich Addition



File: out/422_r_109_combined

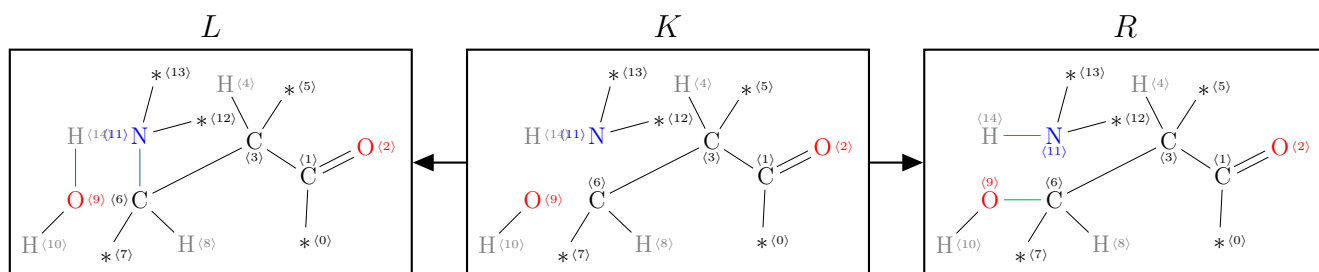
$$\begin{aligned}
 &|\{e \in \text{outEdges}(12) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\quad \}| = 1
 \end{aligned}$$

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

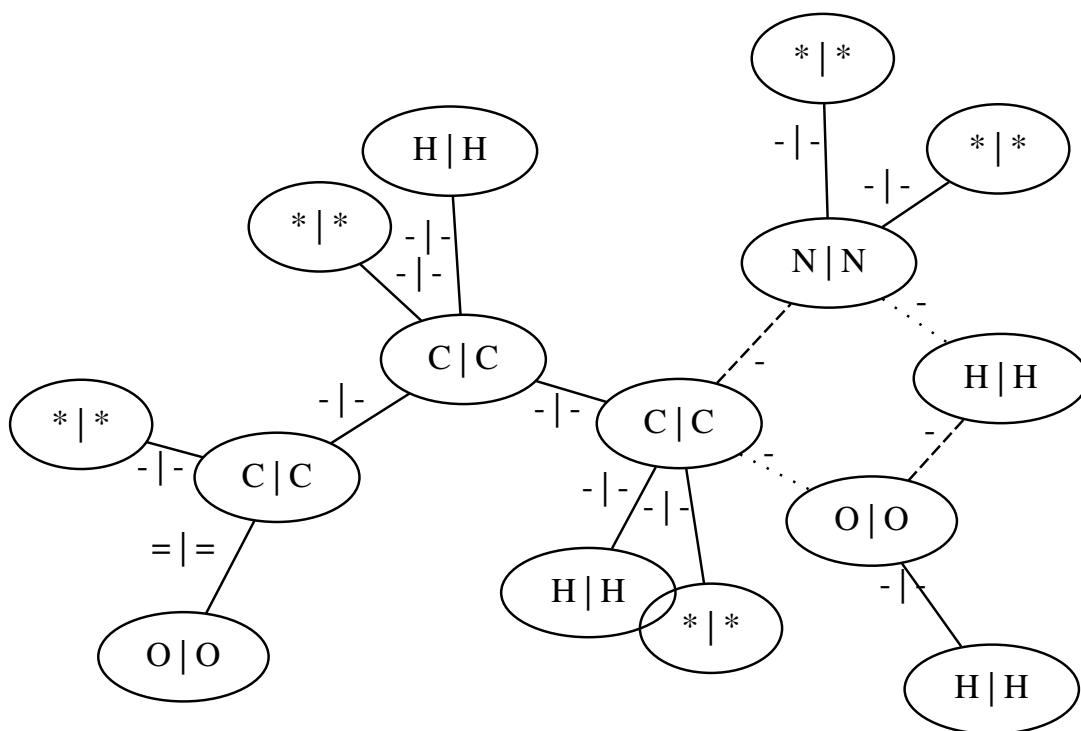
$$\begin{aligned}
& |\{e \in \text{outEdges}(13) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid = 1
\end{aligned}$$

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

1.0.107 Mannich Addition (reverse)



Files: out/425_r_110_10300110_{L, K, R}



File: out/426_r_110_combined

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

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

$$\wedge$$

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

$$\}| = 1$$

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

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

$$\wedge$$

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

$$\}| = 0$$

$$|\{e \in \text{outEdges}(13) \mid$$

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

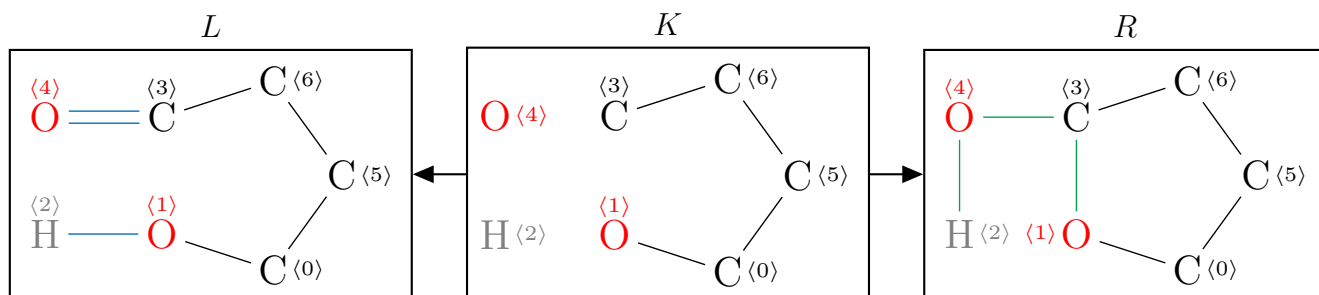
$$\wedge$$

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

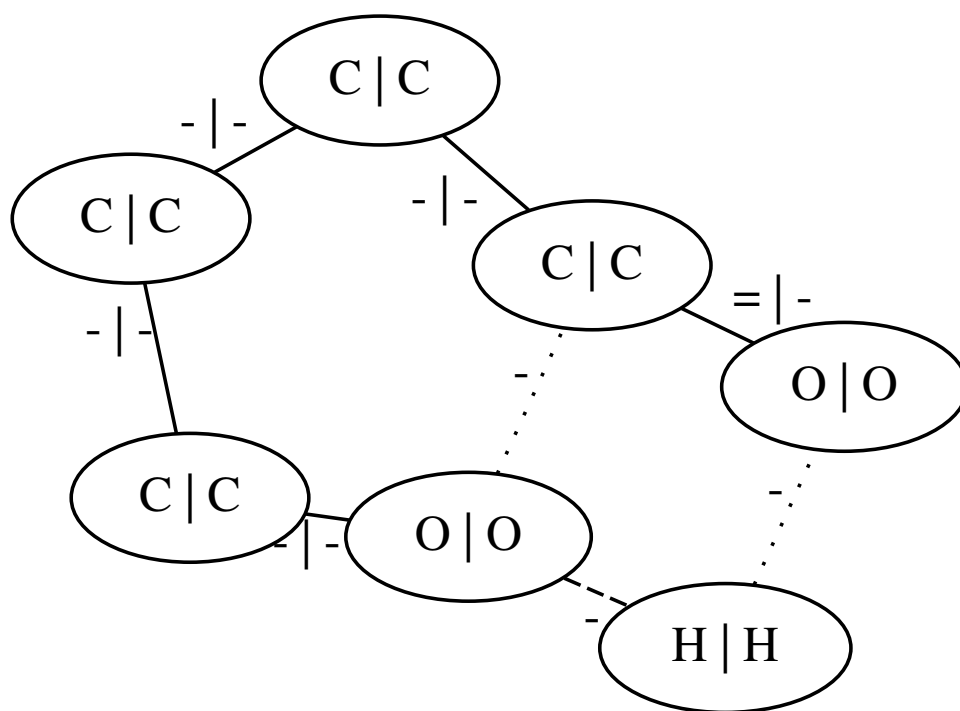
$$\}| = 1$$

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

1.0.108 Hemiacetal Formation for 5 membered rings



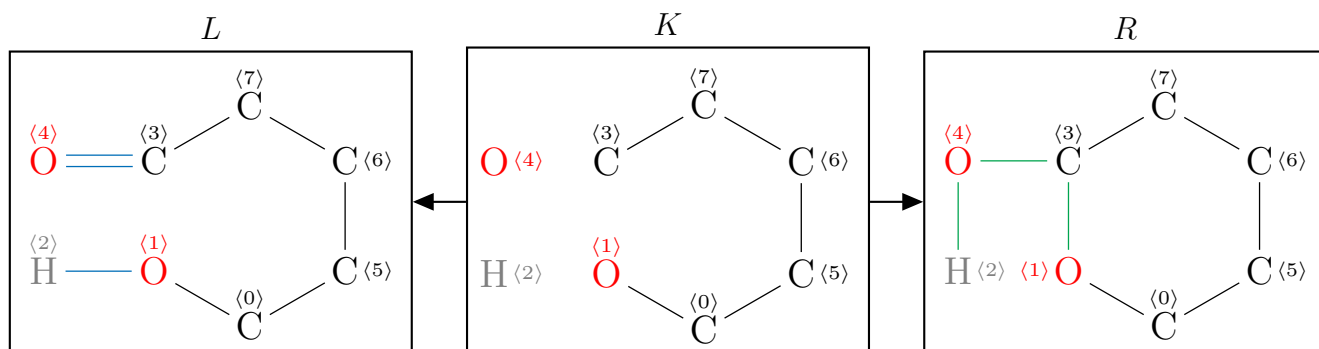
Files: out/429_r_111_10300110_{L, K, R}



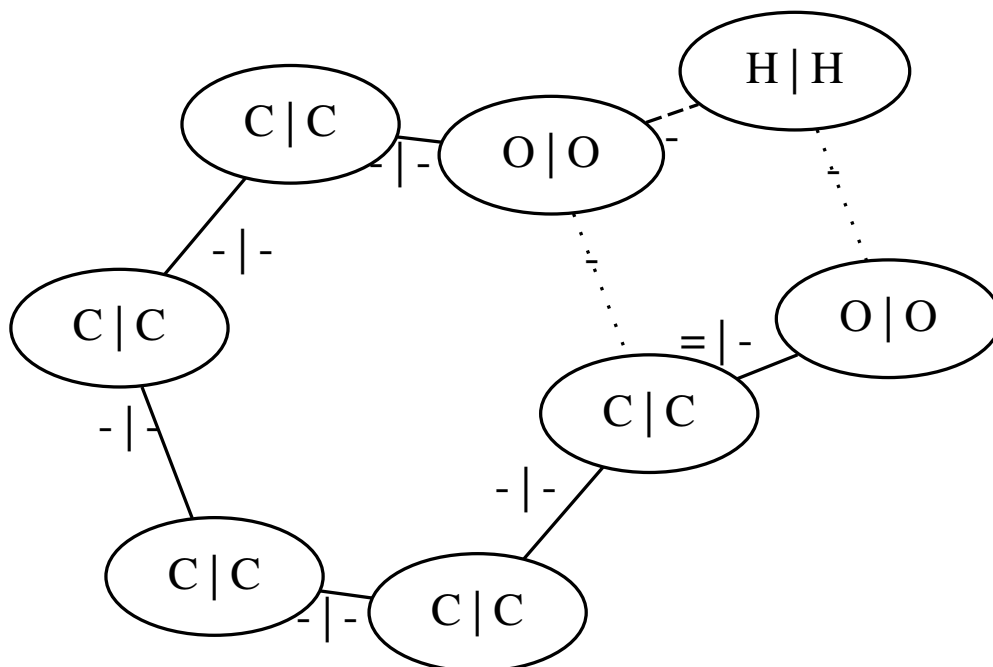
File: out/430_r_111_combined

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

1.0.109 Hemiacetal Formation for 6 membered rings



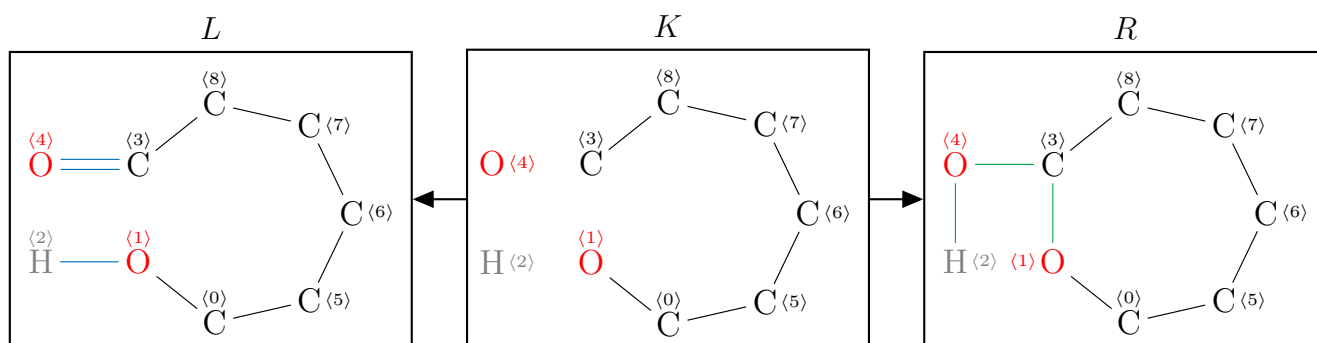
Files: out/433_r_112_10300110_{L, K, R}



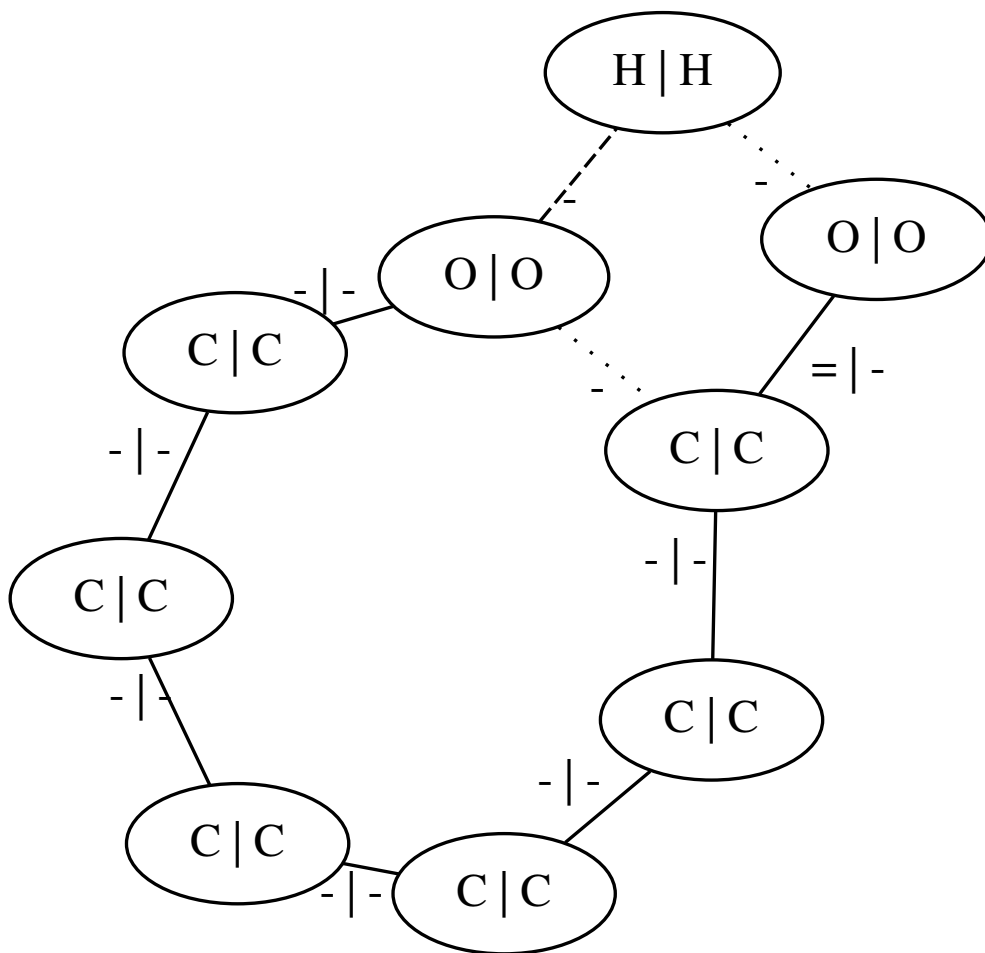
File: out/434_r_112_combined

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

1.0.110 Hemiacetal Formation for 7 membered rings



Files: out/437_r_113_10300110_{L, K, R}



File: out/438_r_113_combined

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

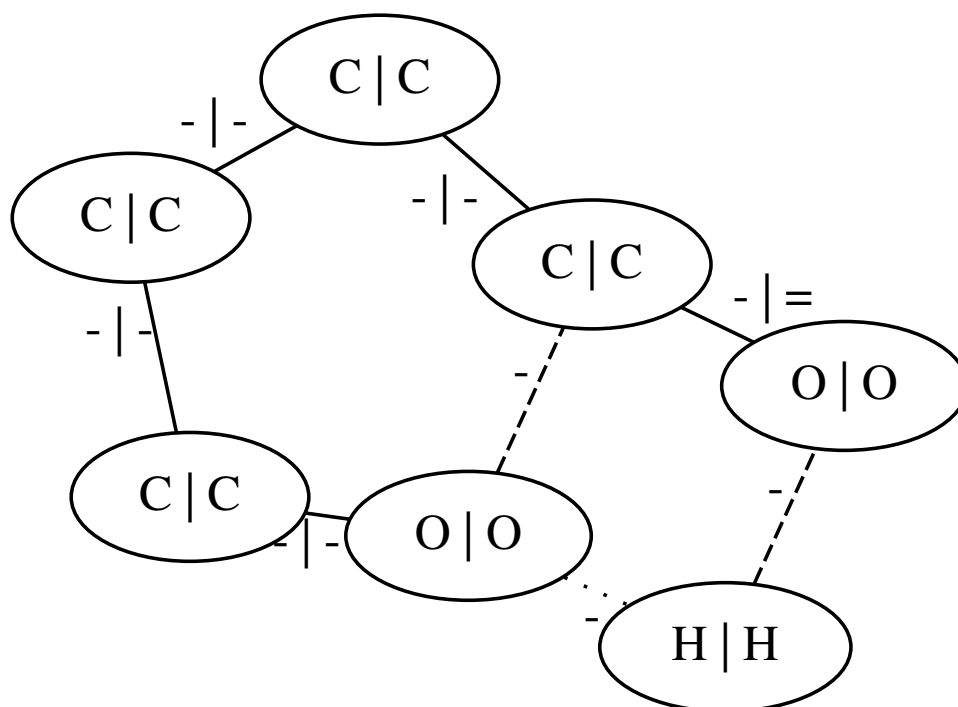
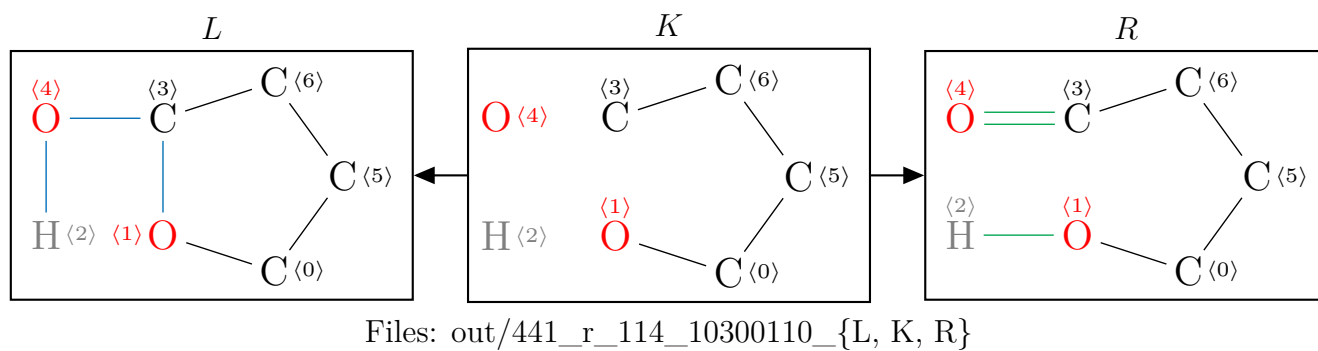
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

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

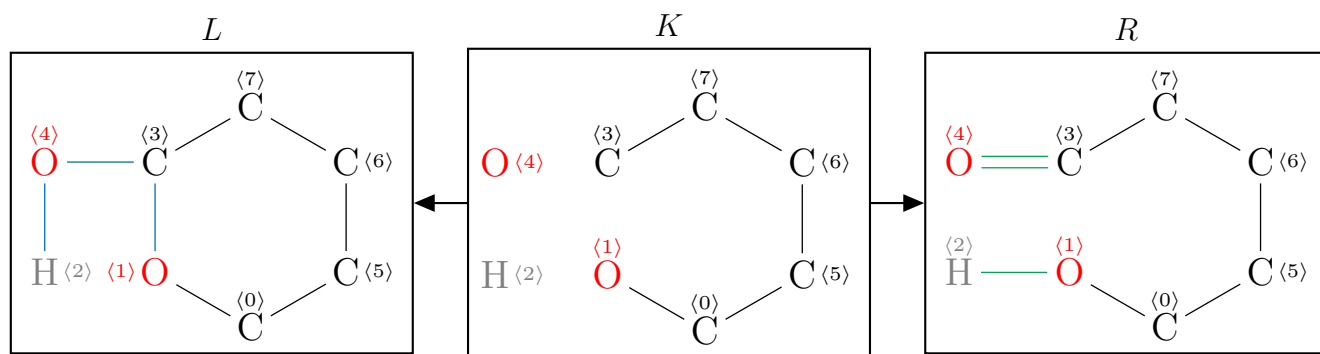
$$\}| = 0$$

1.0.111 Hemiacetal Formation for 5 membered rings, inverse

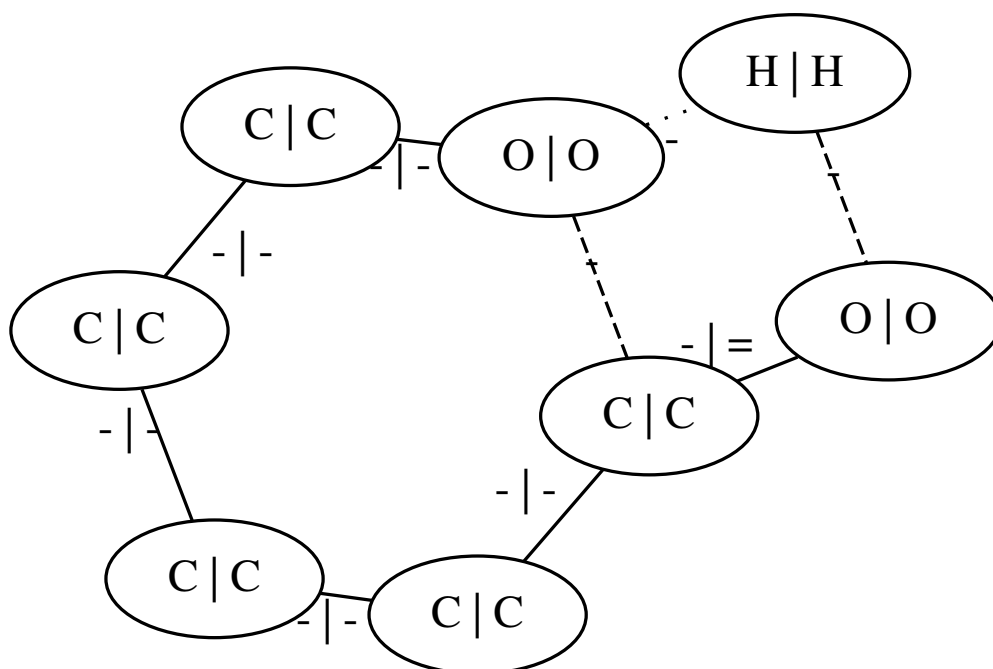


File: out/442_r_114_combined

1.0.112 Hemiacetal Formation for 6 membered rings, inverse

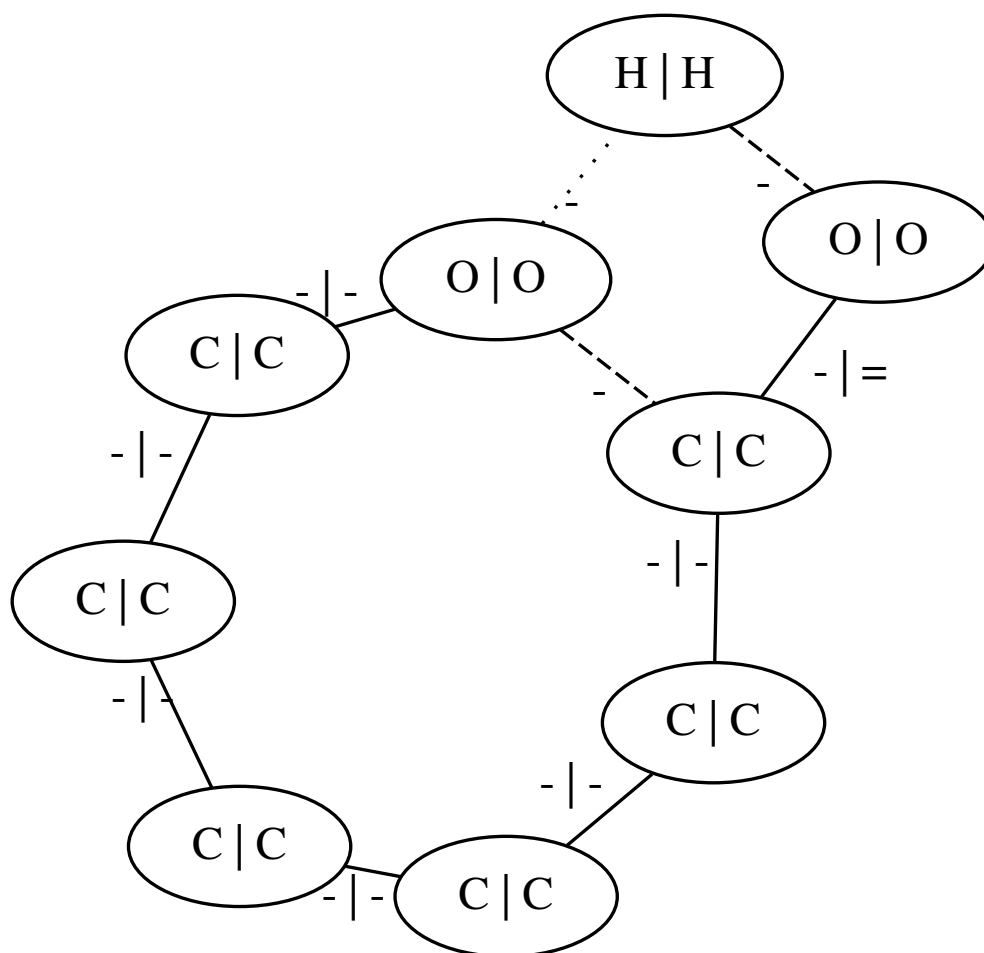
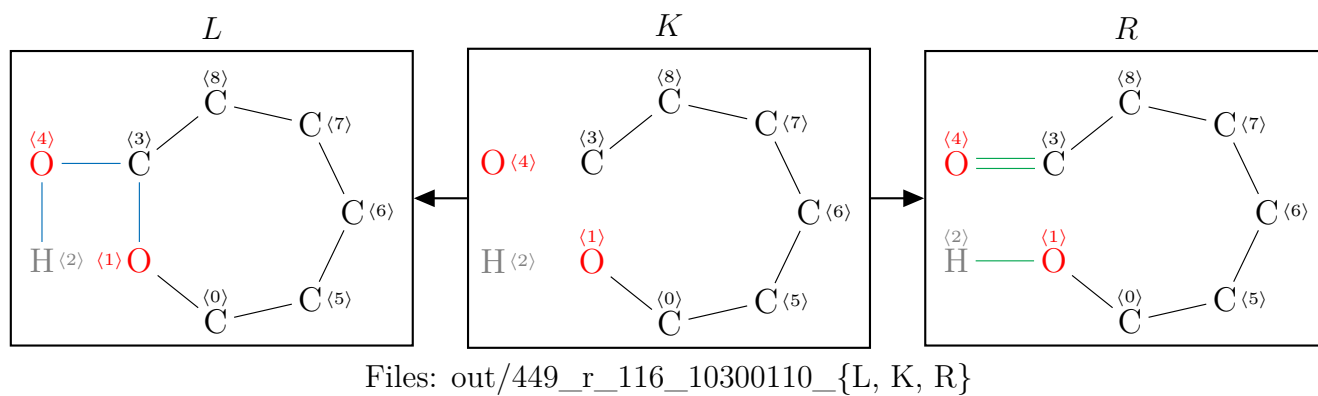


Files: out/445_r_115_10300110_{L, K, R}



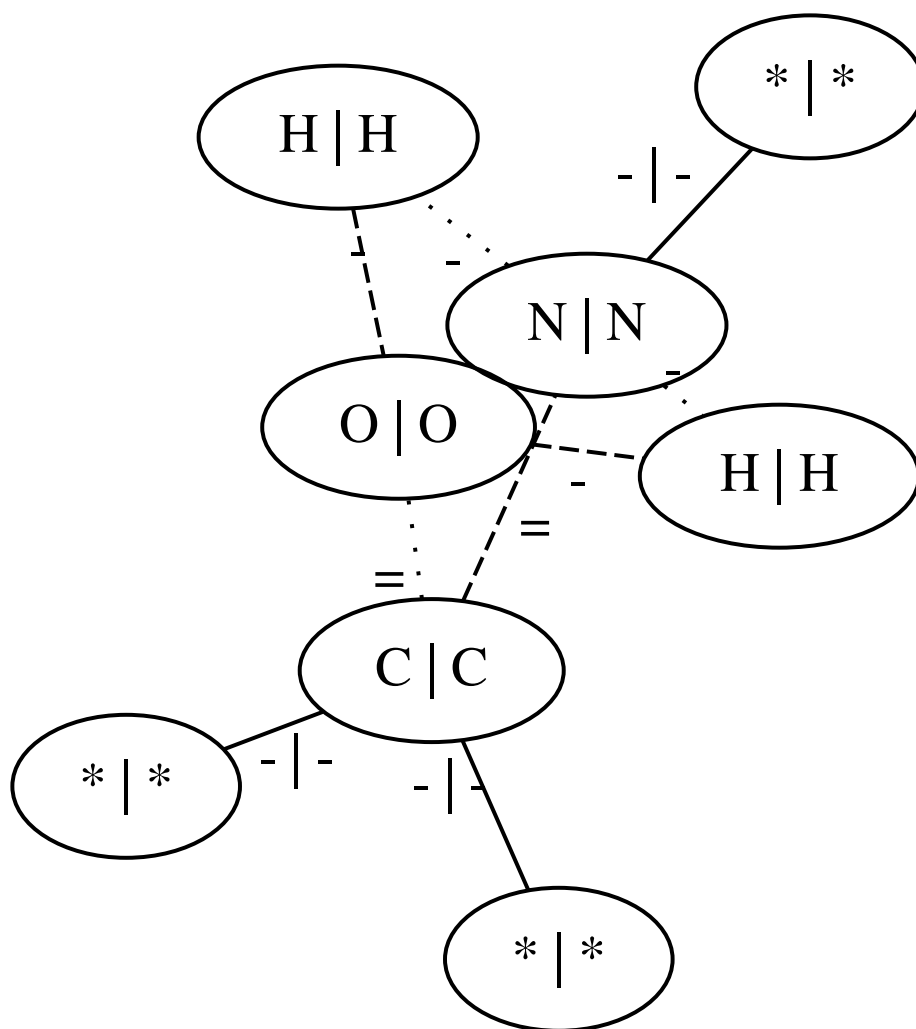
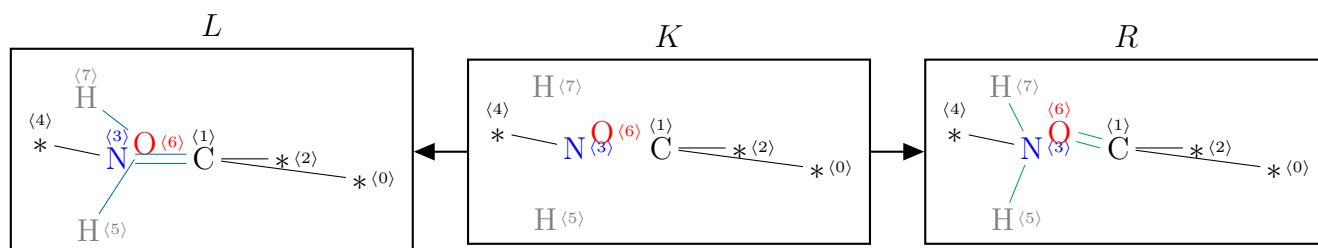
File: out/446_r_115_combined

1.0.113 Hemiacetal Formation for 7 membered rings, inverse



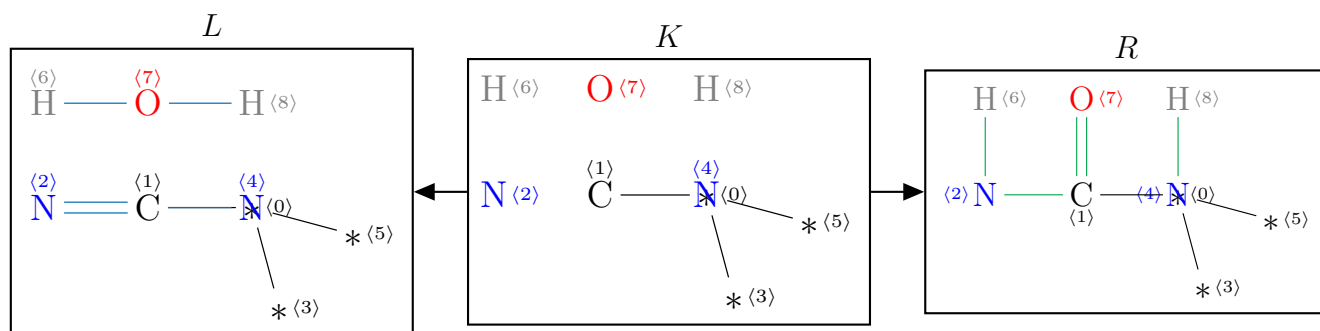
File: out/450_r_116_combined

1.0.114 Imine to Carbonyl

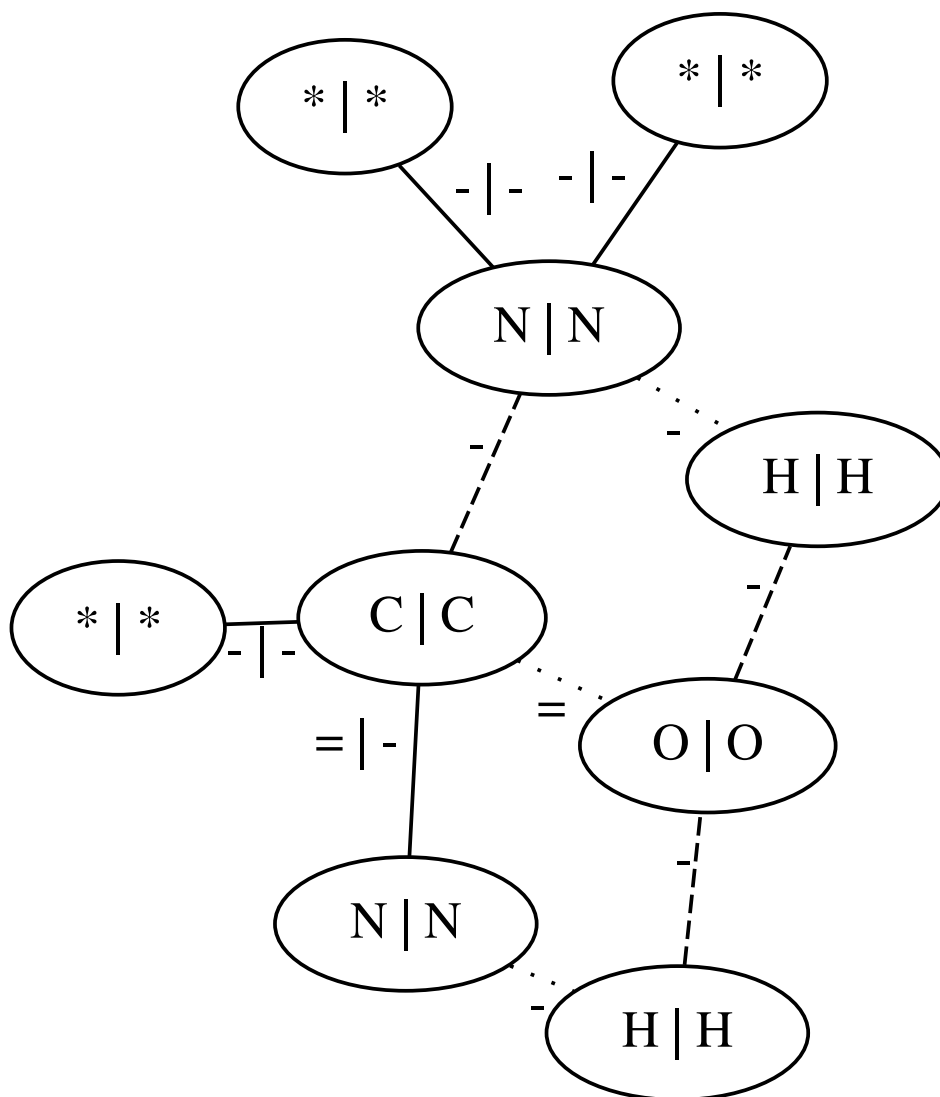


File: out/454_r_117_combined

1.0.115 Amidine to Amide Hydrolysis

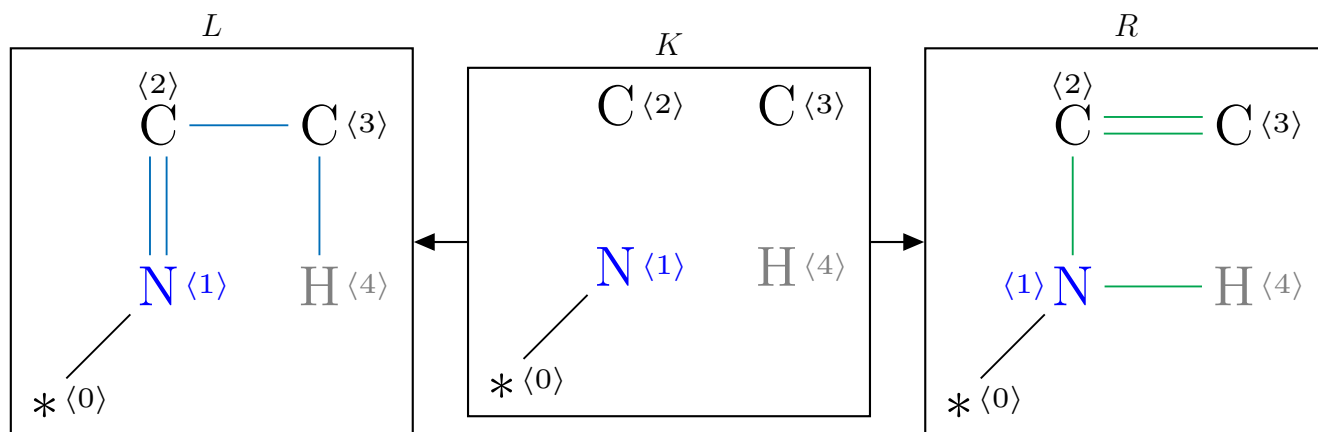


Files: out/457_r_118_10300110_{L, K, R}

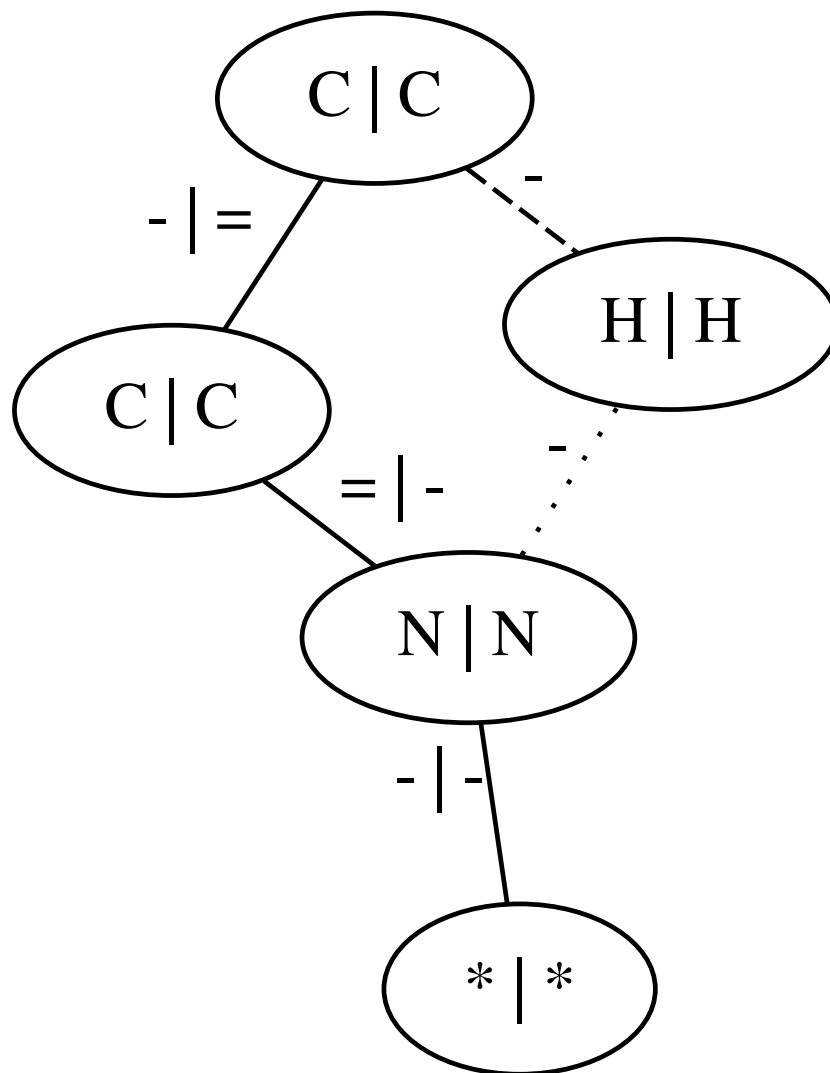


File: out/458_r_118_combined

1.0.116 Imine to Enamine



Files: out/461_r_119_10300110_{L, K, R}



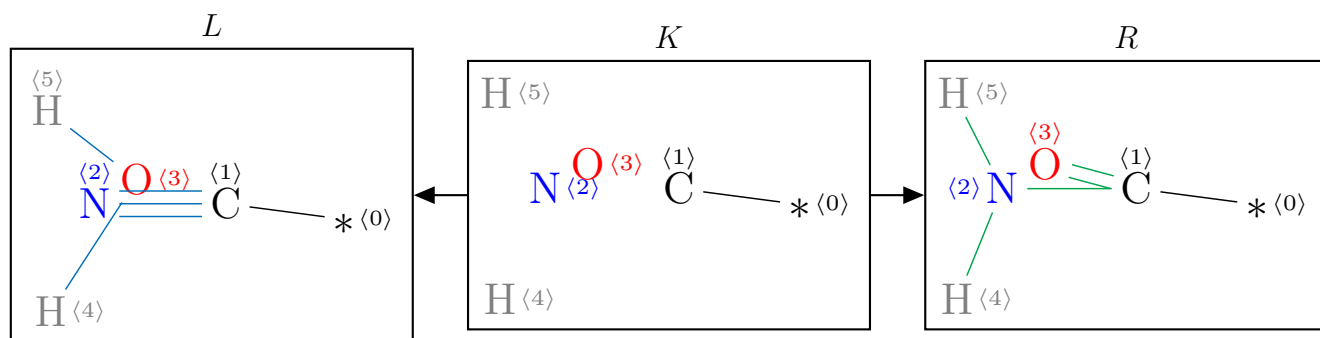
File: out/462_r_119_combined

```

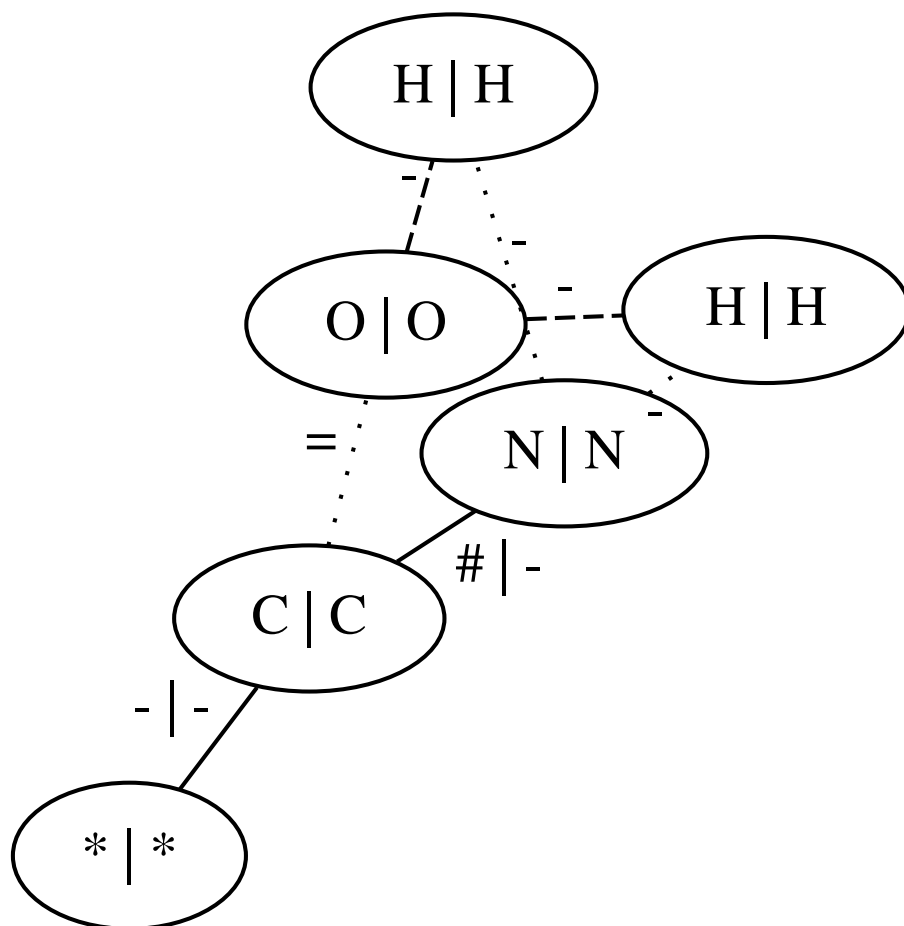
|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```

1.0.117 Nitrile Hydrolysis

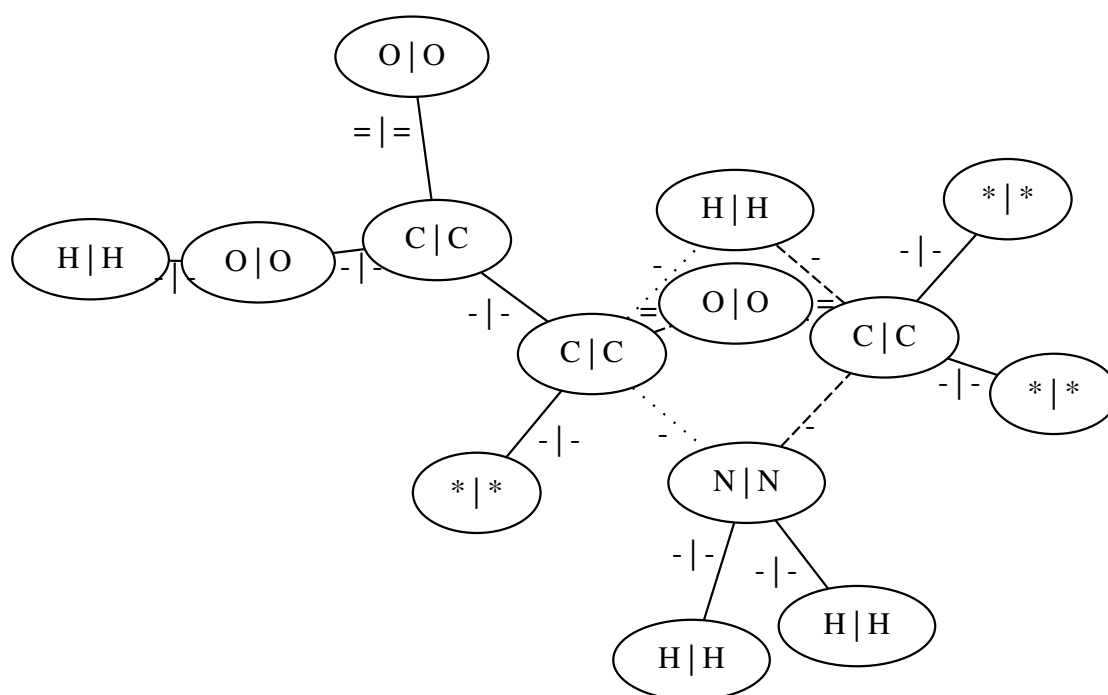
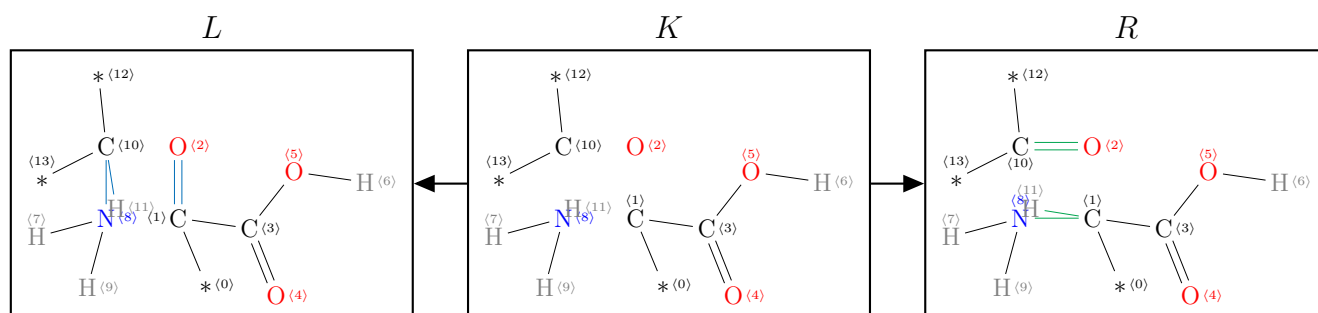


Files: out/465_r_120_10300110_{L, K, R}



File: out/466_r_120_combined

1.0.118 Transamination



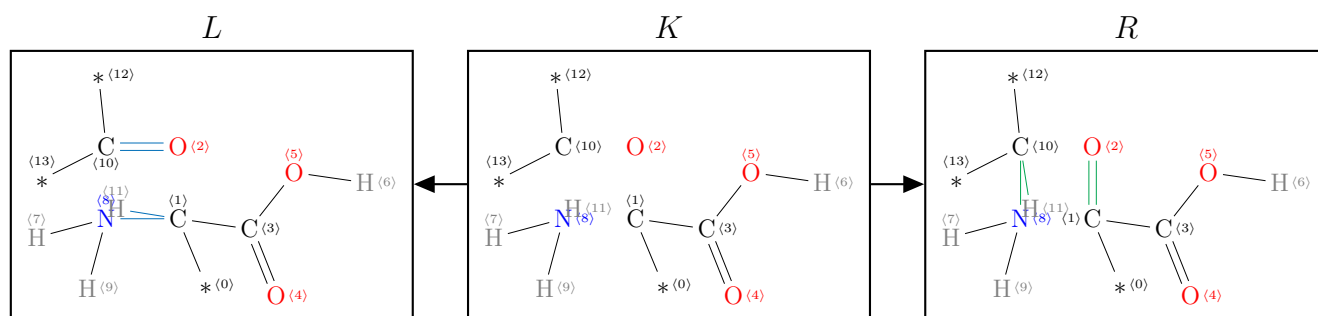
File: out/470_r_121_combined

```

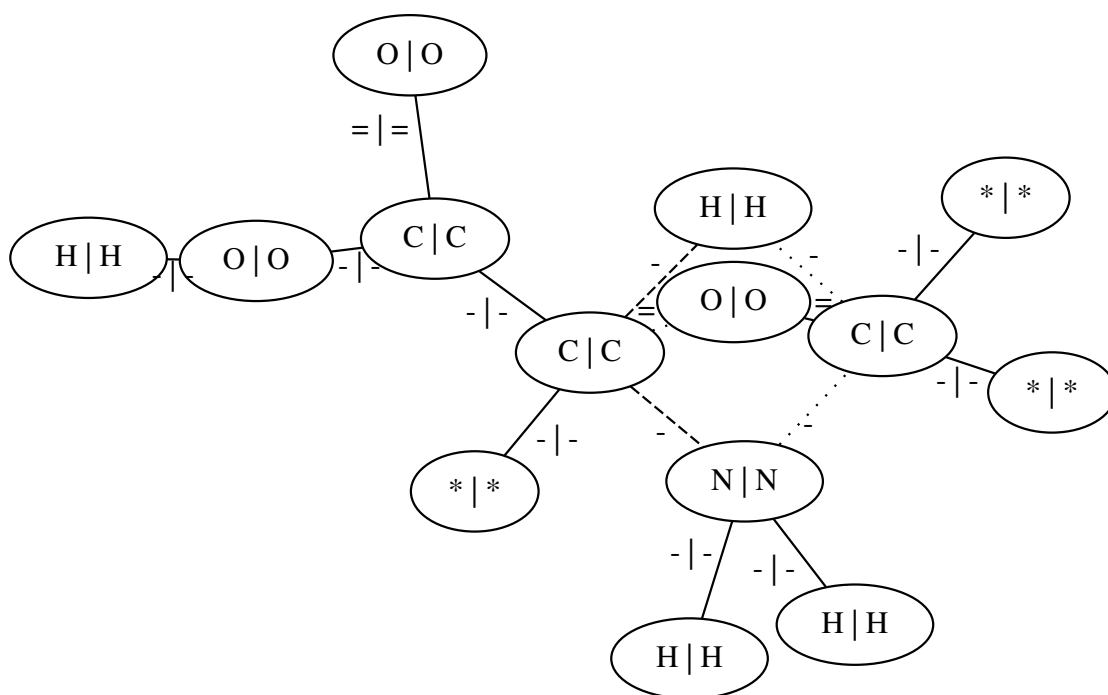
|{e ∈ outEdges(1) |
  label(target(e)) ∈ {'S', 'O', 'N'}
  ∧
  label(e) ∈ {'-'}
}| = 0

```

1.0.119 Transamination (inverse)



Files: out/473_r_122_10300110_{L, K, R}



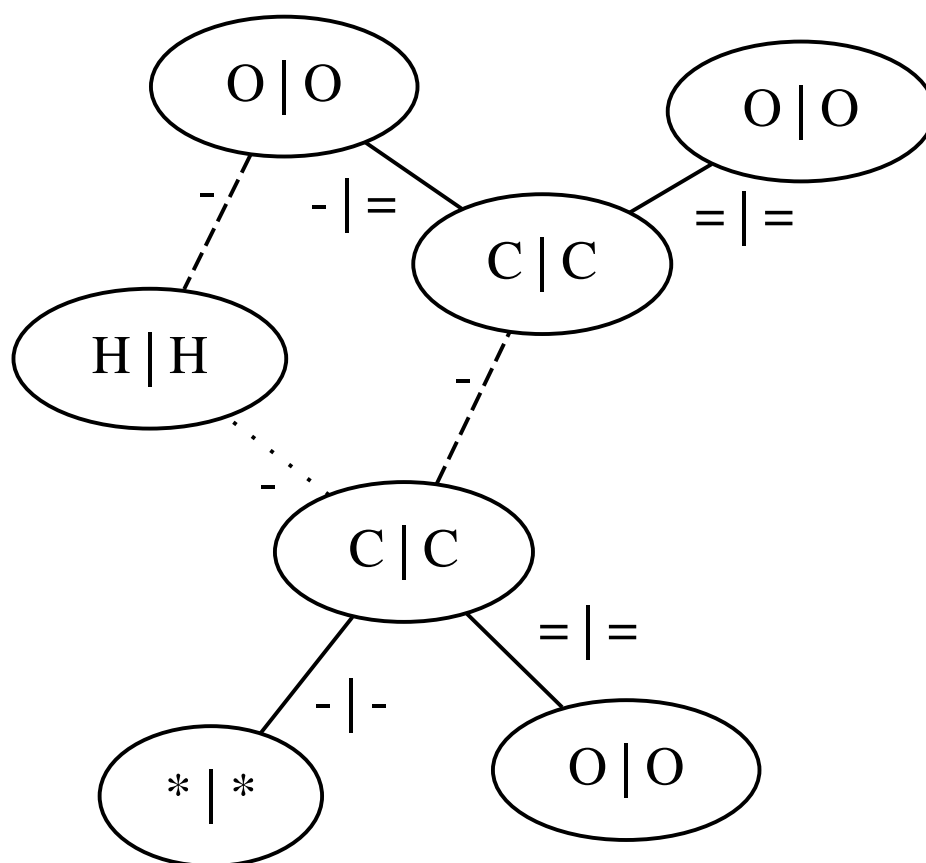
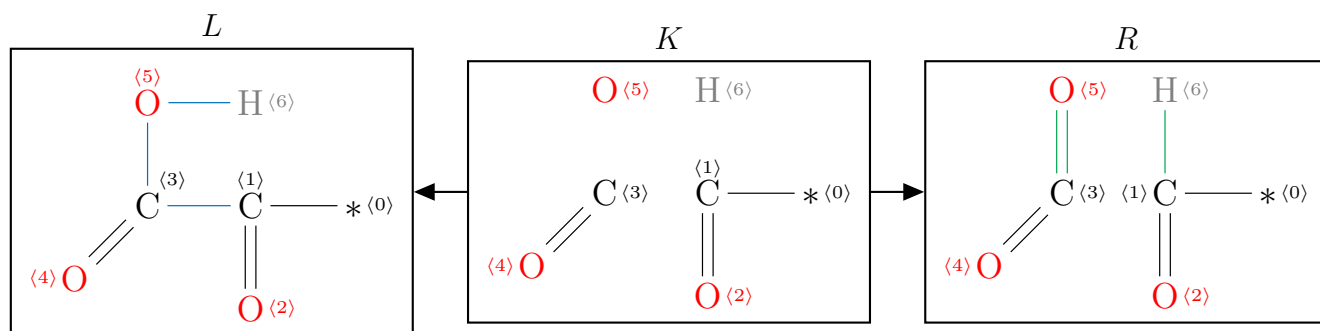
File: out/474_r_122_combined

```

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

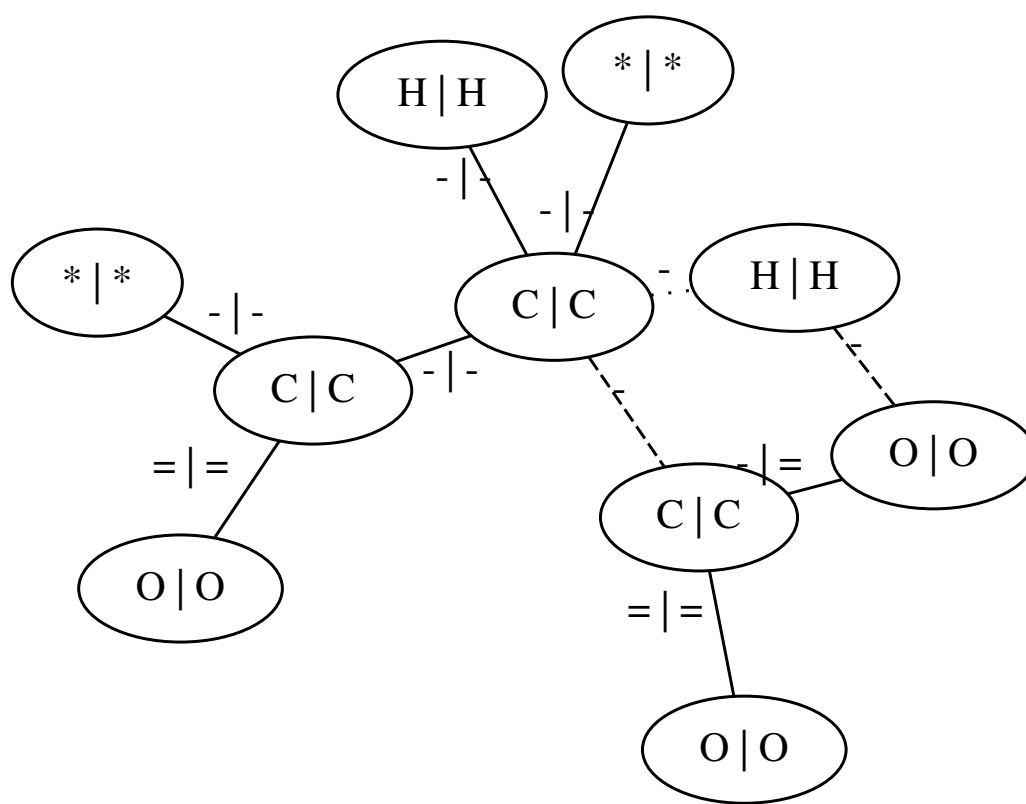
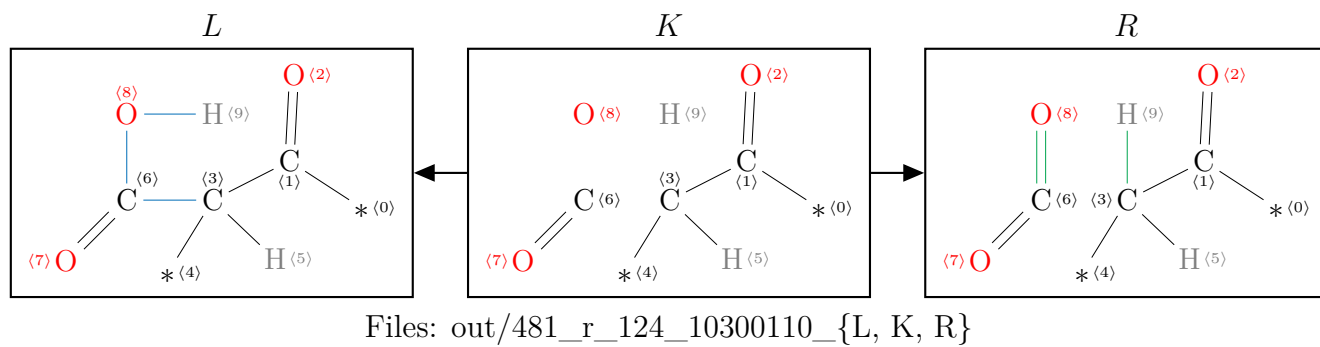
```

1.0.120 Alpha-Keto Acid Decarboxylation



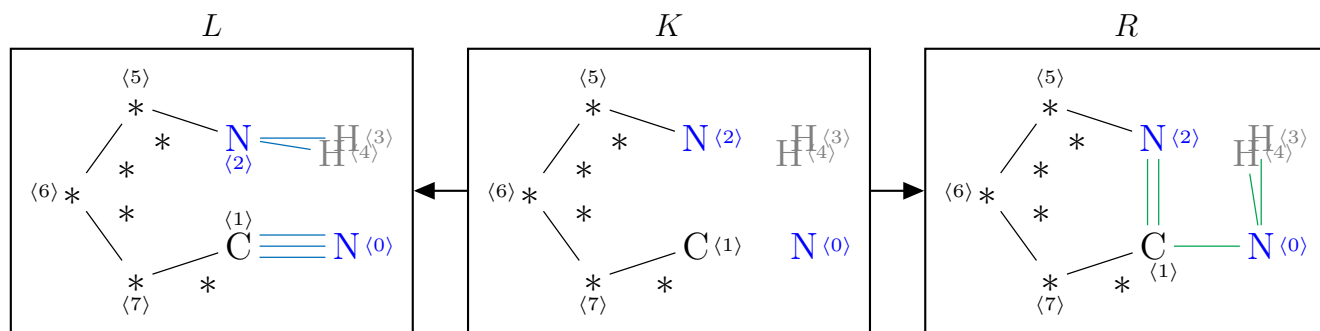
File: out/478_r_123_combined

1.0.121 Beta Decarboxylation

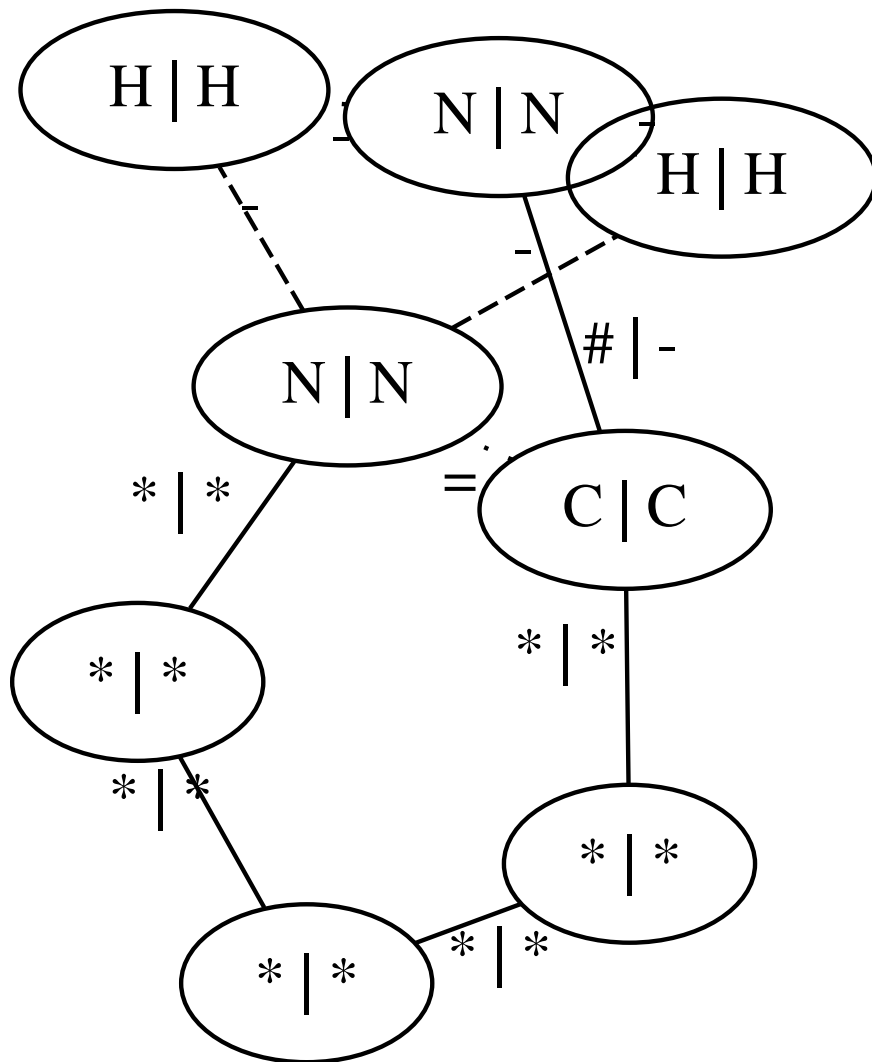


File: out/482_r_124_combined

1.0.122 Nitrile Ring Closure 5



Files: out/485_r_125_10300110_{L, K, R}



File: out/486_r_125_combined

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

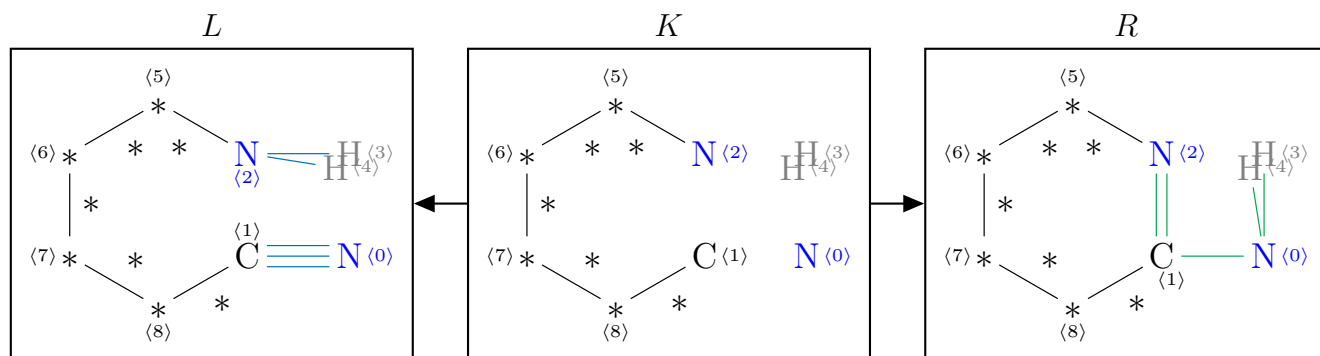
$$\text{label}(\text{target}(e)) \in \{'0'\}$$

$$\wedge$$

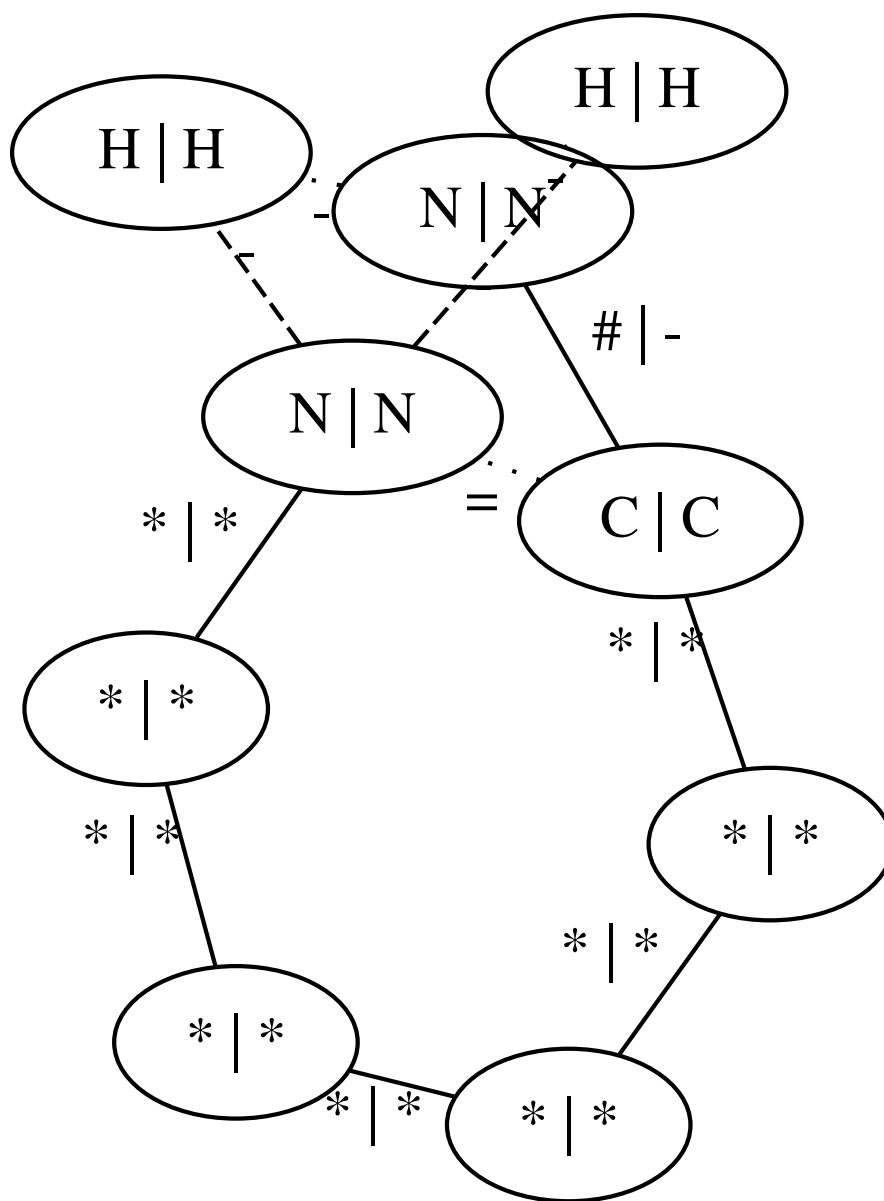
$$\text{label}(e) \in \{'=\'}\}$$

$$| = 0$$

1.0.123 Nitrile Ring Closure 6



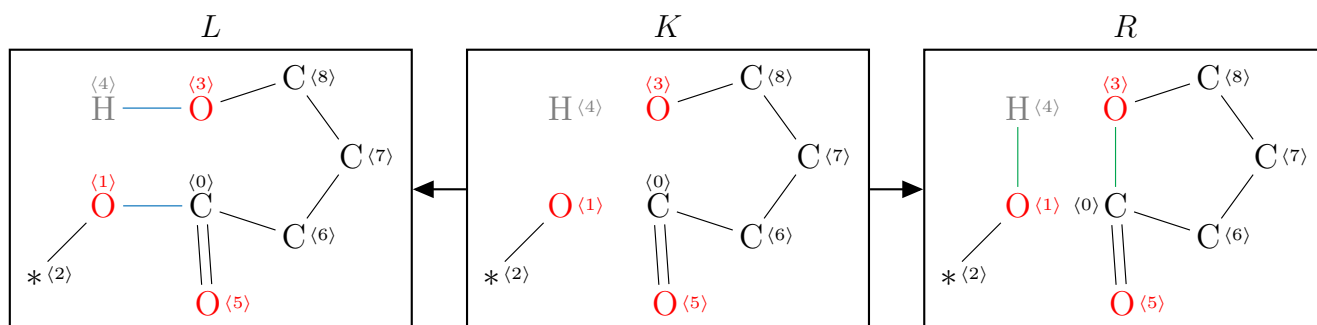
Files: out/489_r_126_10300110_{L, K, R}



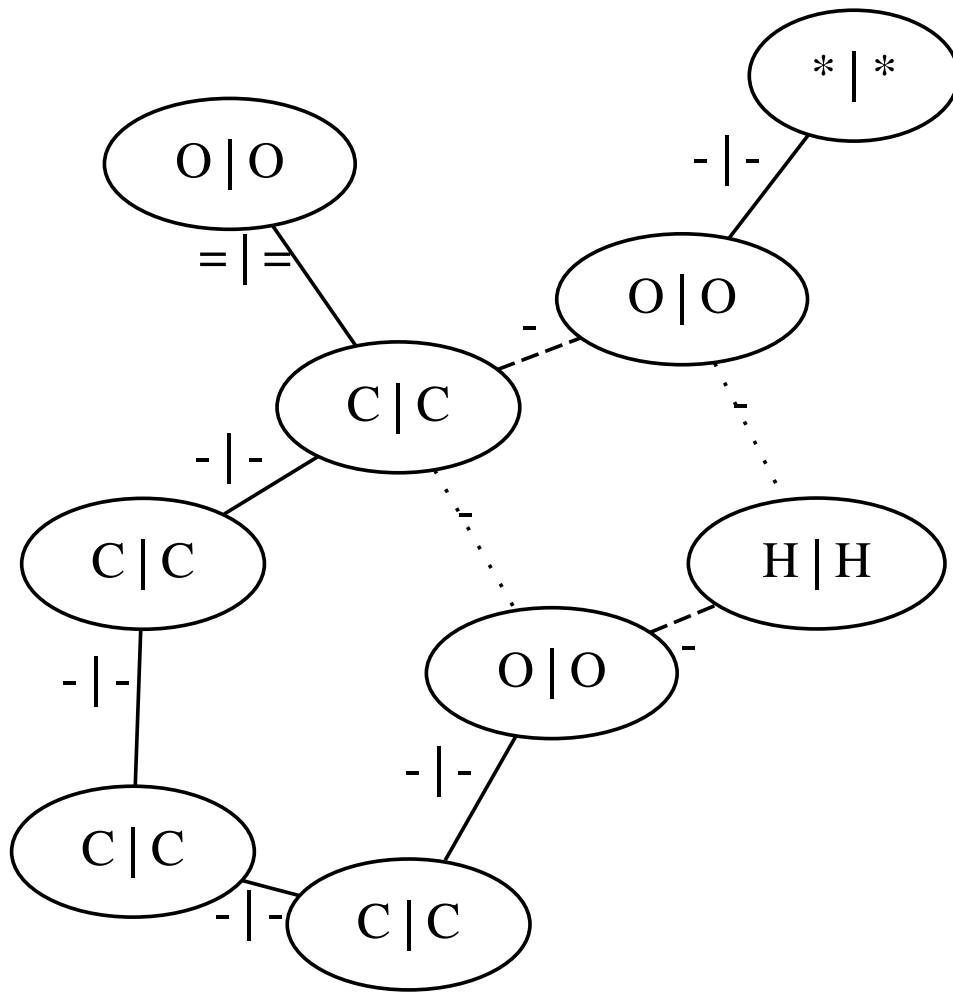
File: out/490_r_126_combined

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

1.0.124 Ring Closure 5 membered O, O



Files: out/493_r_127_10300110_{L, K, R}



File: out/494_r_127_combined

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

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

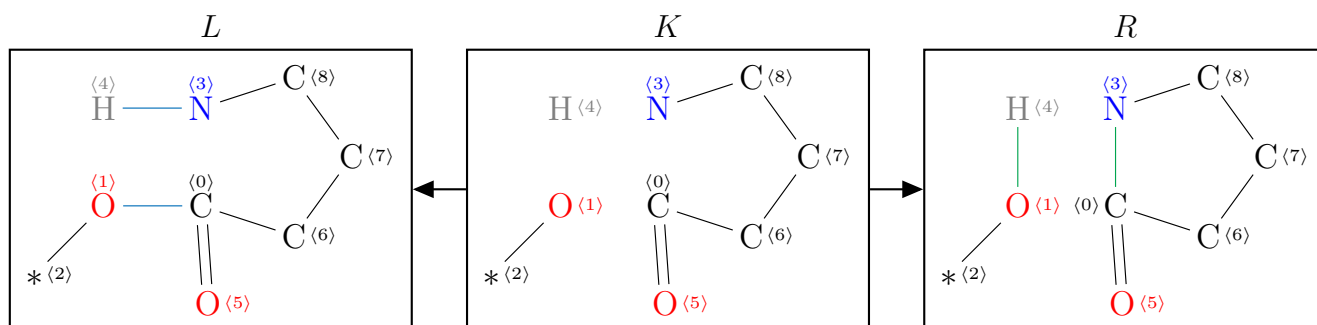
$$\wedge$$

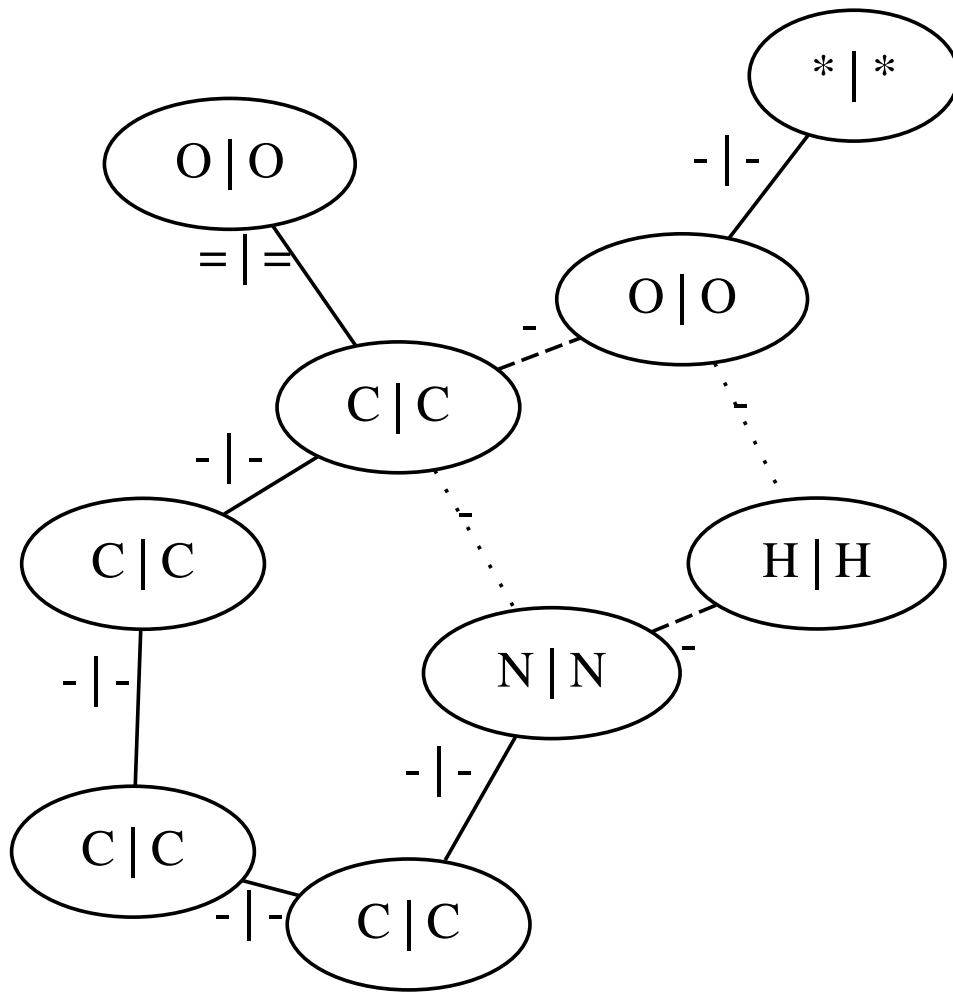
$$\text{label}(e) \in \{ '-' \}$$

$$\}| = 1$$

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

1.0.125 Ring Closure 5 membered O, N





File: out/498_r_128_combined

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

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

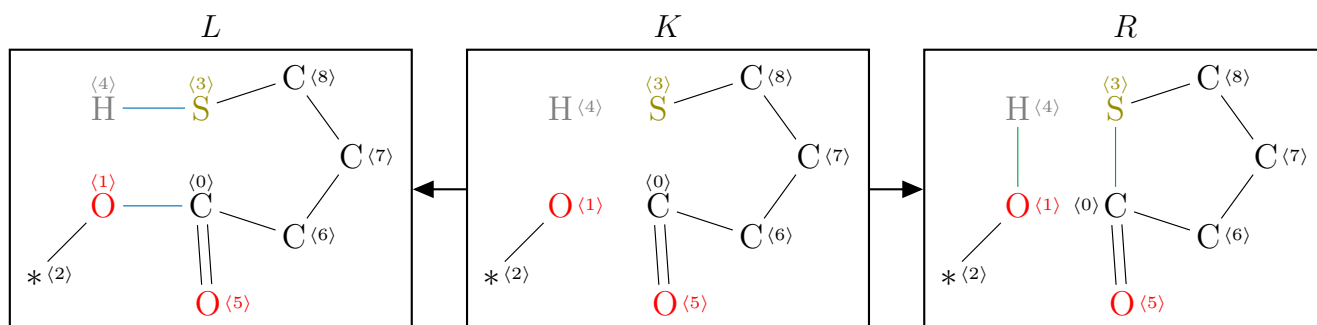
$$\wedge$$

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

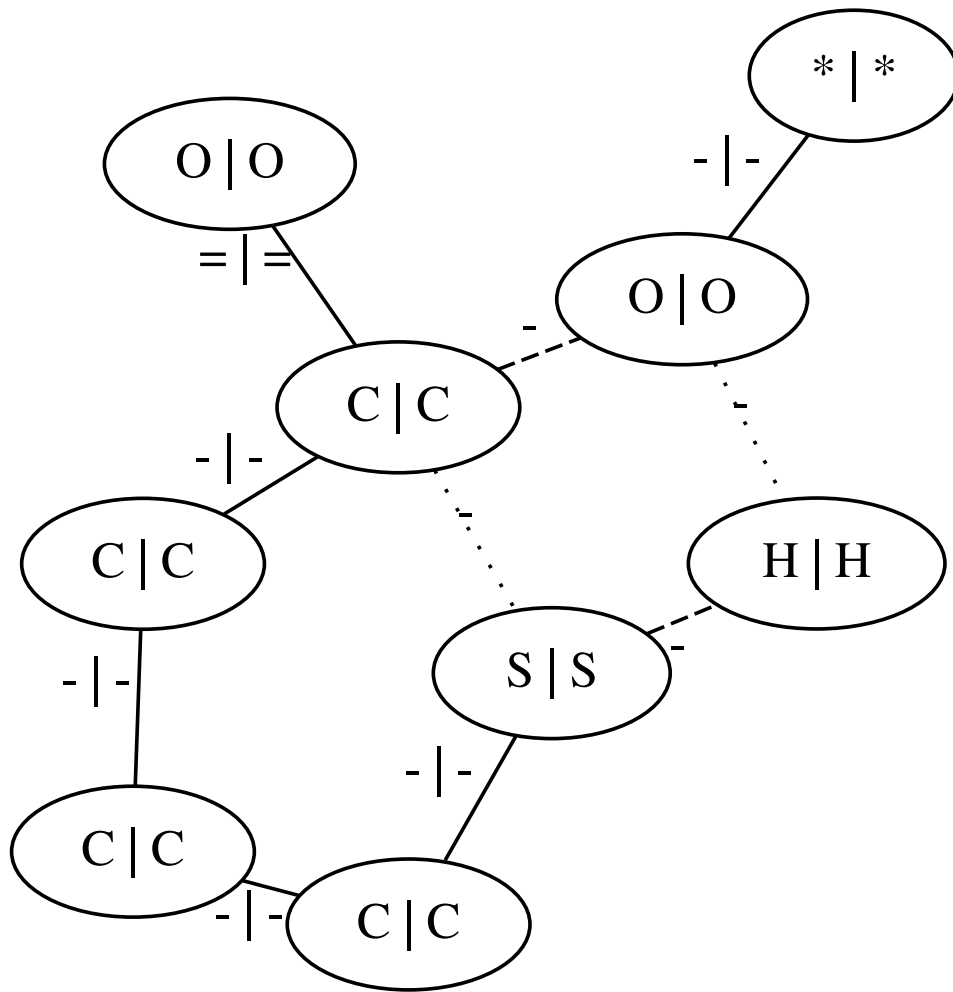
$$\}| = 1$$

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

1.0.126 Ring Closure 5 membered O, S



Files: out/501_r_129_10300110_{L, K, R}



File: out/502_r_129_combined

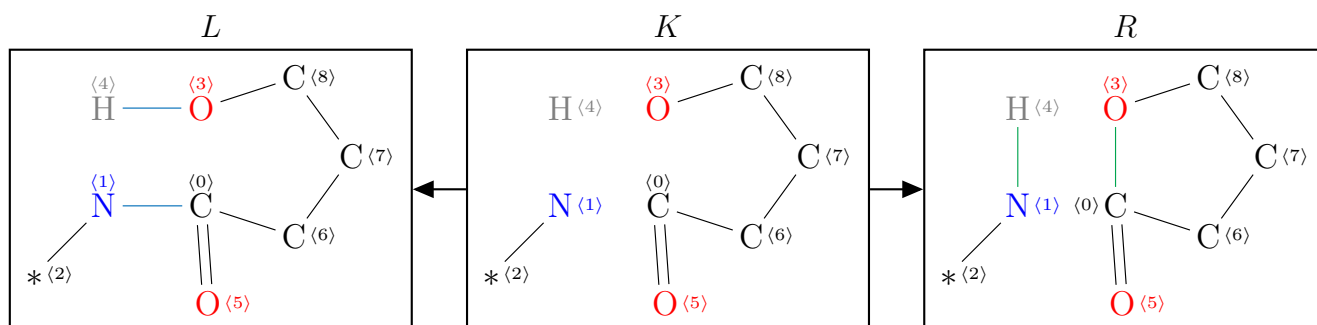
```

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

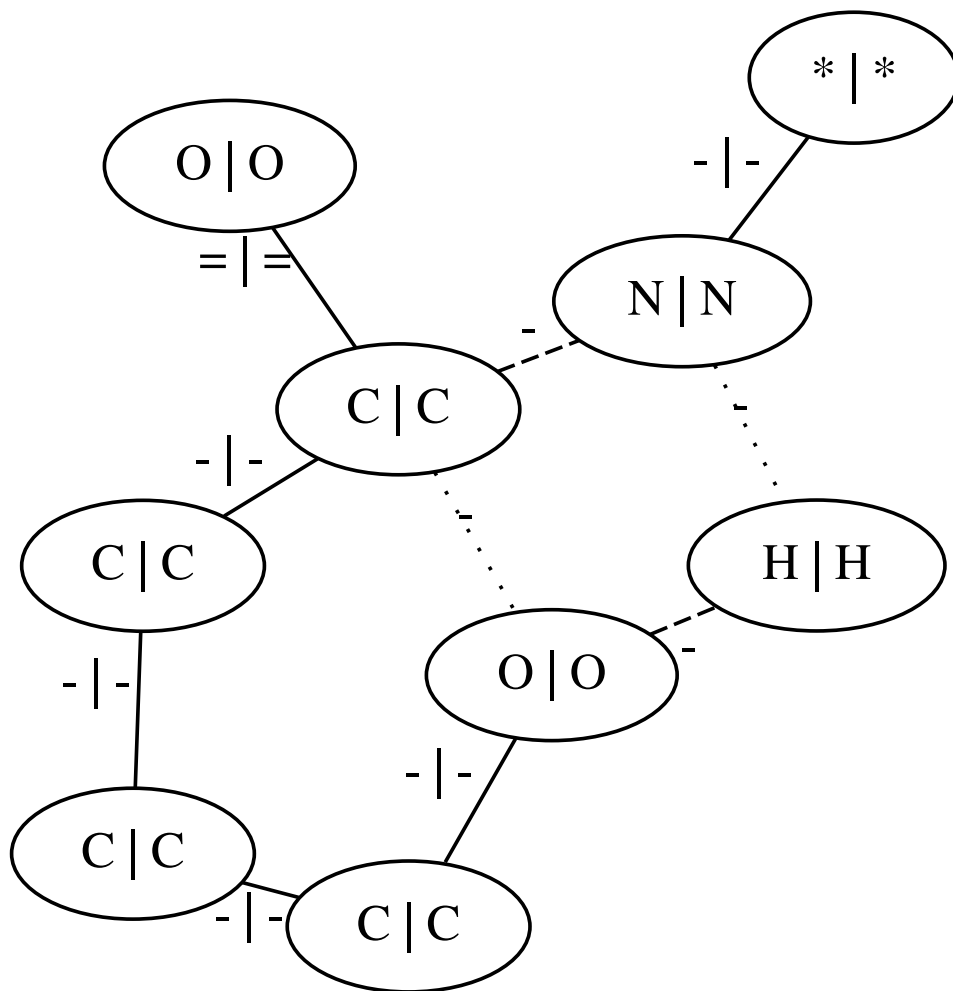
```

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

1.0.127 Ring Closure 5 membered N, O



Files: out/505_r_130_10300110_{L, K, R}



File: out/506_r_130_combined

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

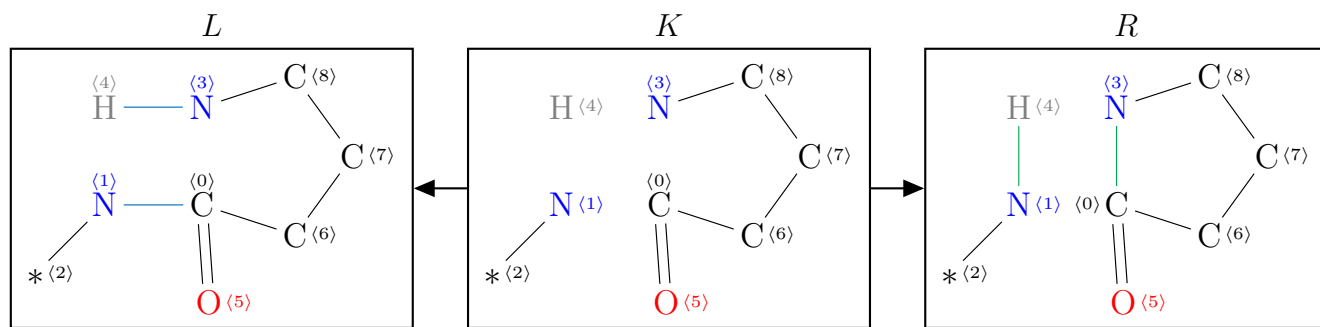
$$\text{label}(\text{target}(e)) \in \{\text{'N'}\}$$

$$\wedge$$

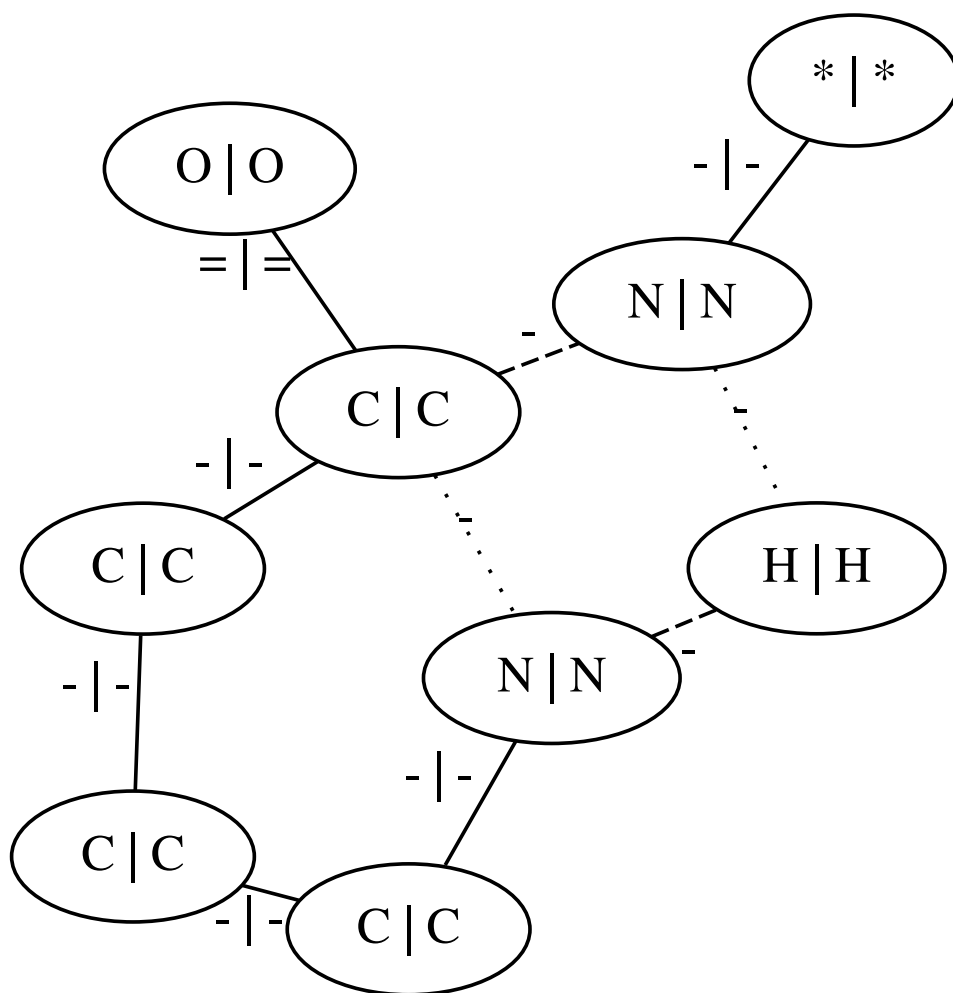
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 1$$

1.0.128 Ring Closure 5 membered N, N



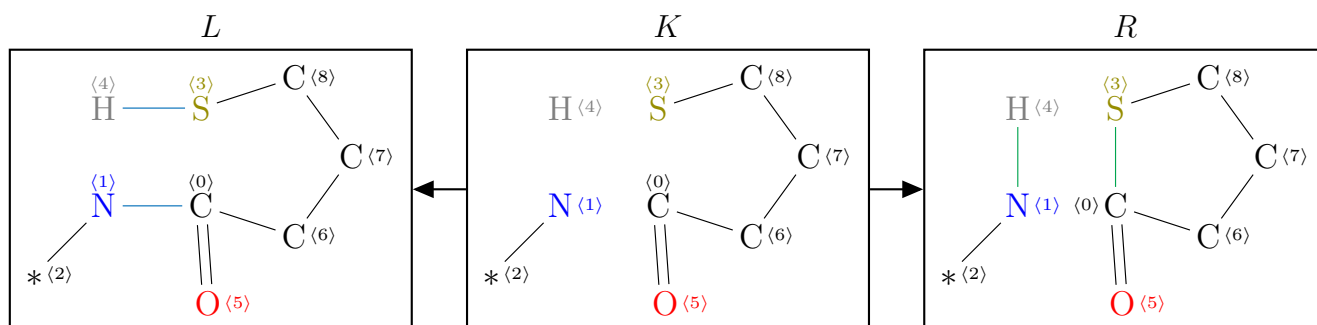
Files: out/509_r_131_10300110_{L, K, R}

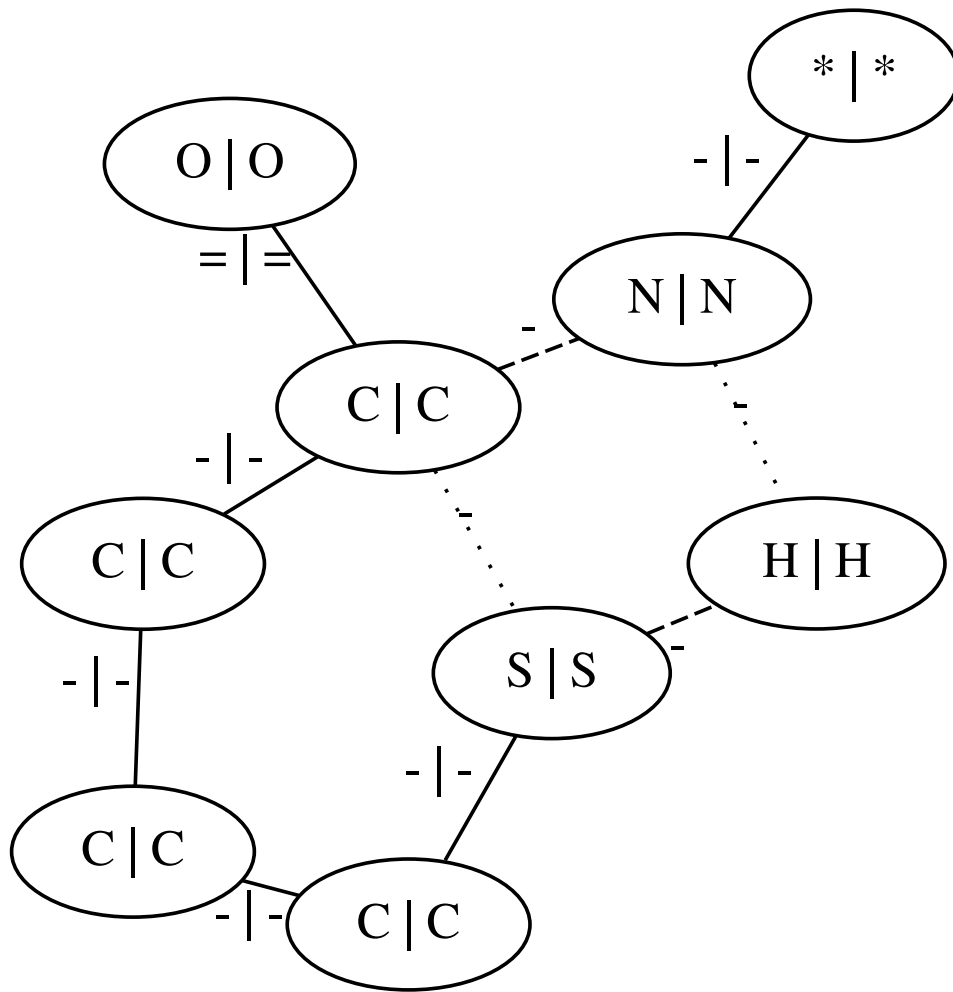


File: out/510_r_131_combined

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

1.0.129 Ring Closure 5 membered N, S





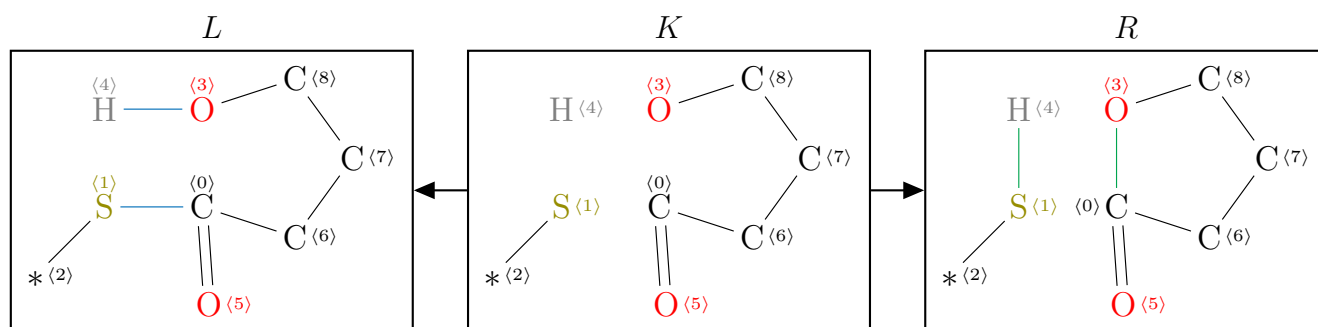
File: out/514_r_132_combined

```

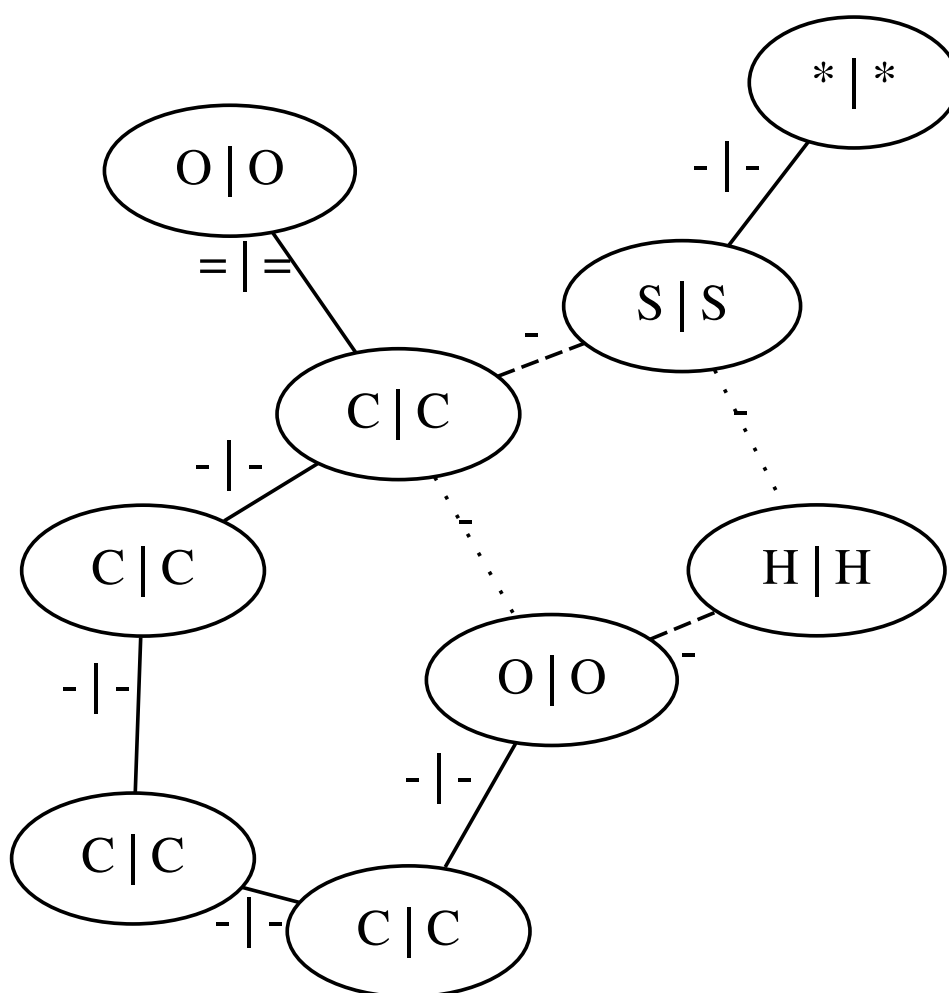
|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'N'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```


1.0.130 Ring Closure 5 membered S, O



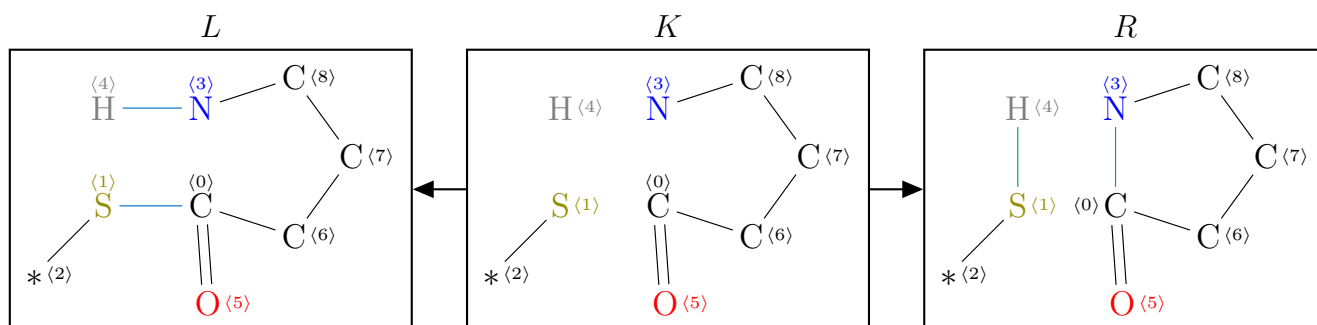
Files: out/517_r_133_10300110_{L, K, R}

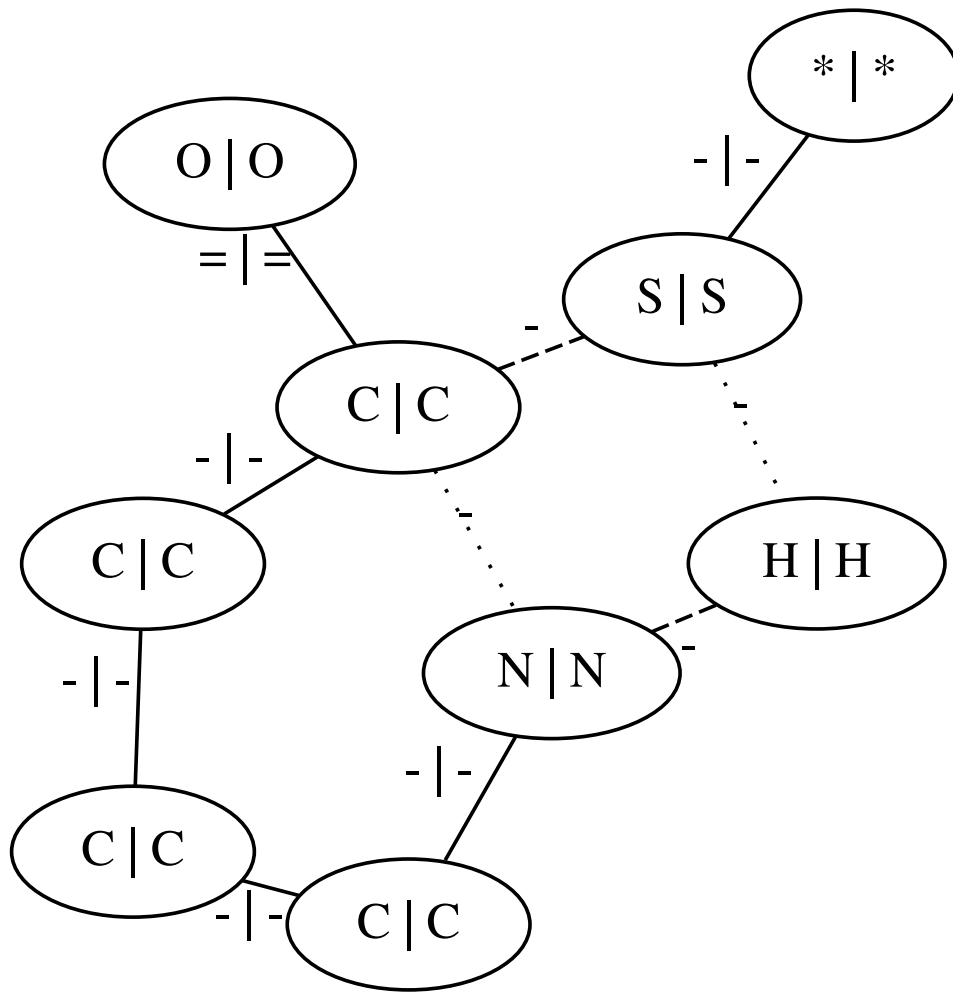


File: out/518_r_133_combined

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

1.0.131 Ring Closure 5 membered S, N





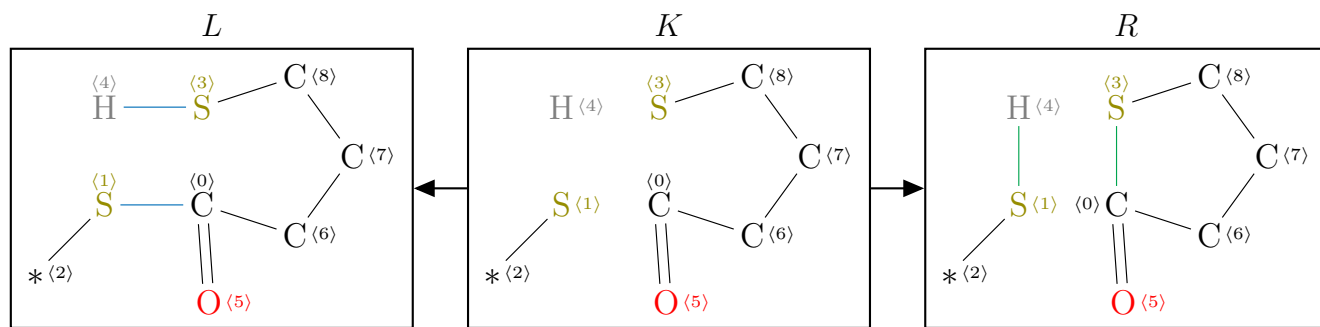
File: out/522_r_134_combined

```

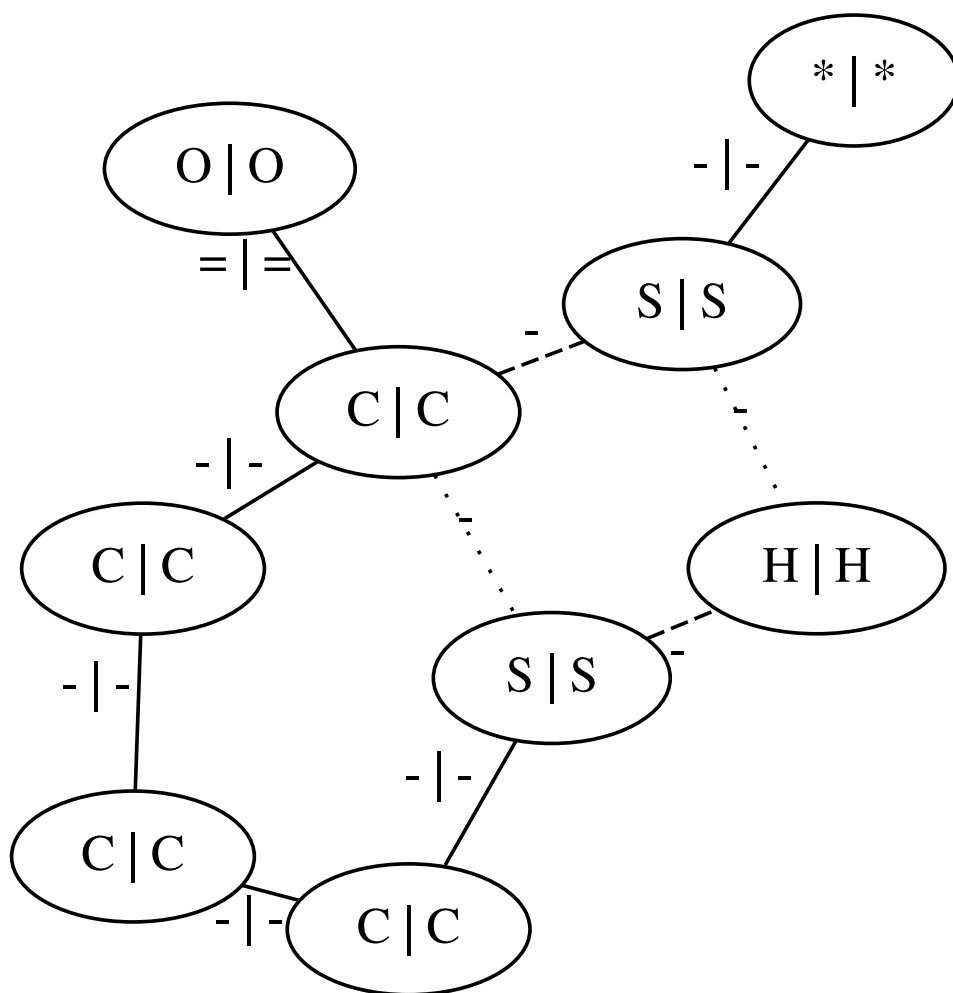
|{e ∈ outEdges(2) |
  label(target(e)) ∈ {'S'}
  ∧
  label(e) ∈ {'-'}
}| = 1

```

1.0.132 Ring Closure 5 membered S, S



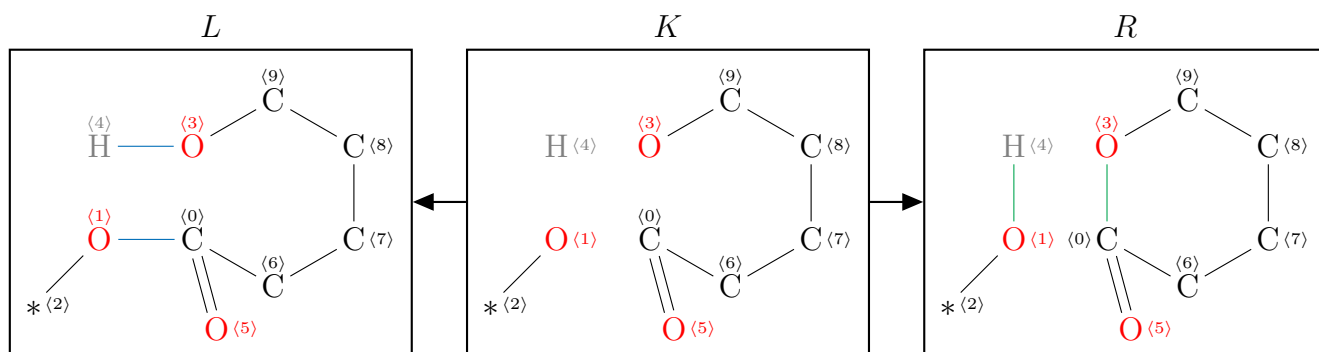
Files: out/525_r_135_10300110_{L, K, R}



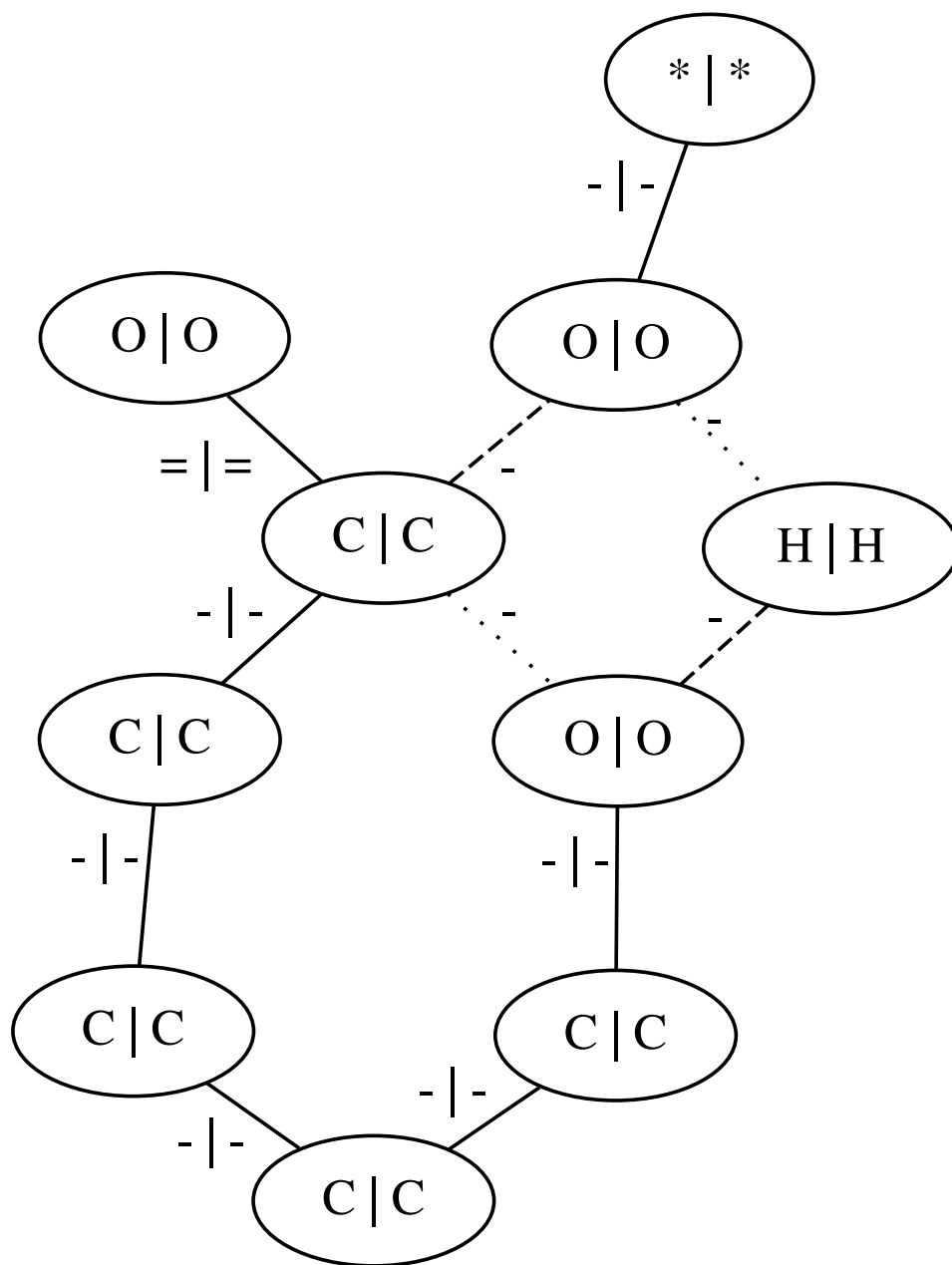
File: out/526_r_135_combined

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

1.0.133 Ring Closure 6 membered O, O



Files: out/529_r_136_10300110_{L, K, R}

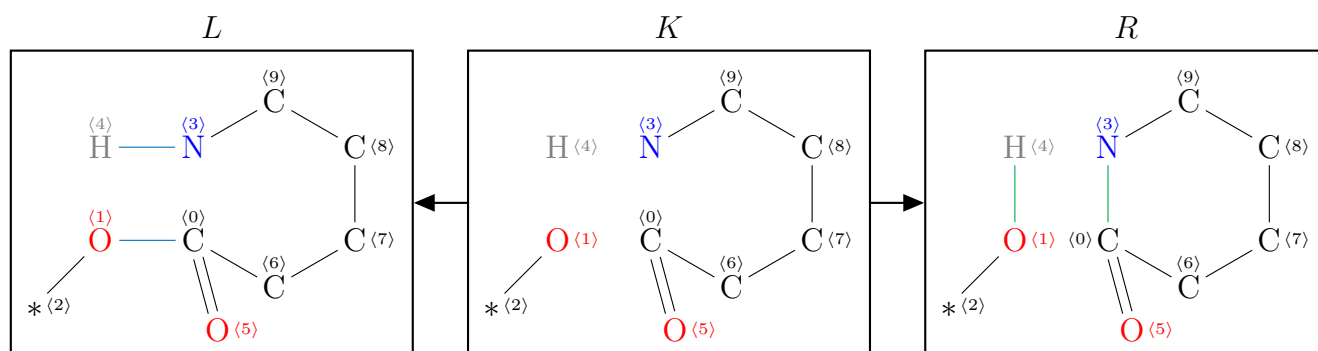


File: out/530_r_136_combined

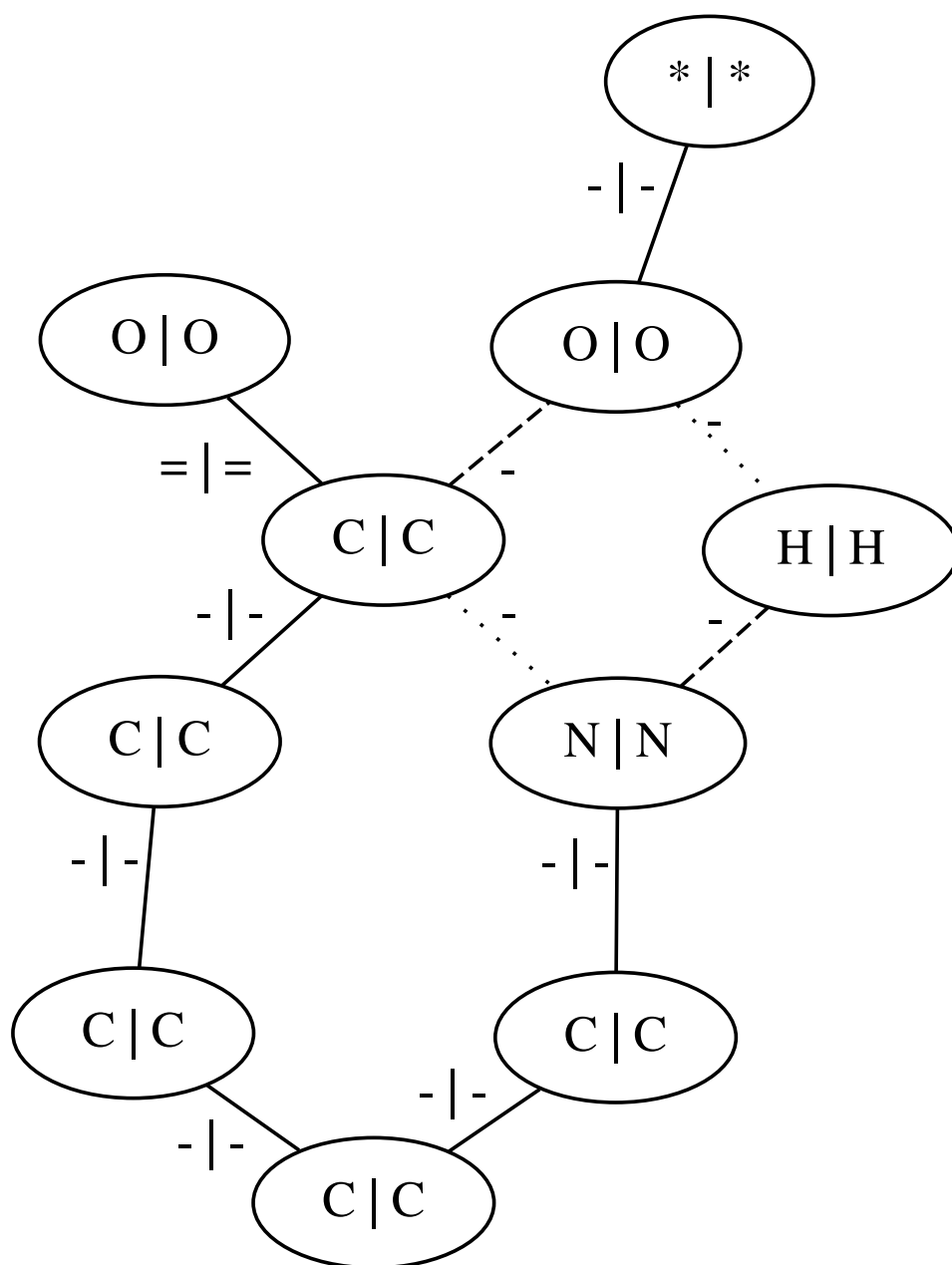
$$\begin{aligned}
 &|\{e \in \text{outEdges}(2) \mid \\
 &\quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
 &\quad \wedge \\
 &\quad \text{label}(e) \in \{\text{'-'}\} \\
 &\}\mid = 1
 \end{aligned}$$

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

1.0.134 Ring Closure 6 membered O, N



Files: out/533_r_137_10300110_{L, K, R}

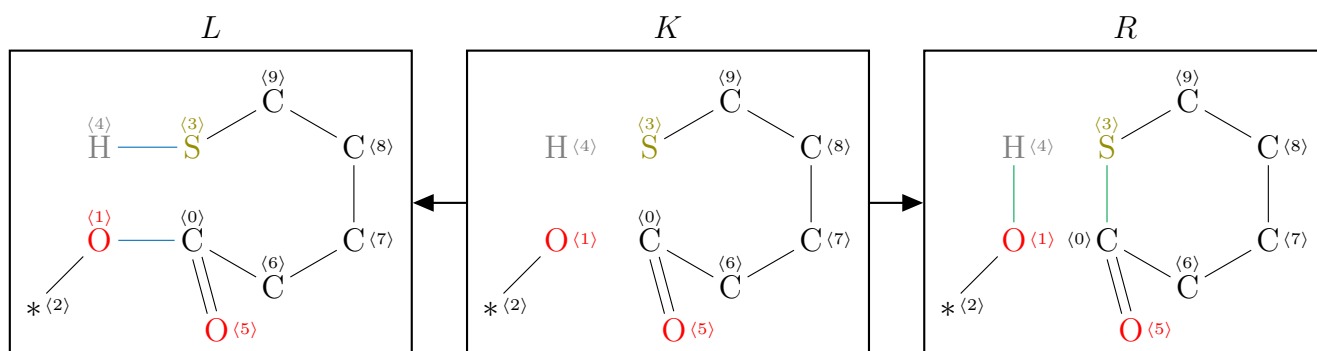


File: out/534_r_137_combined

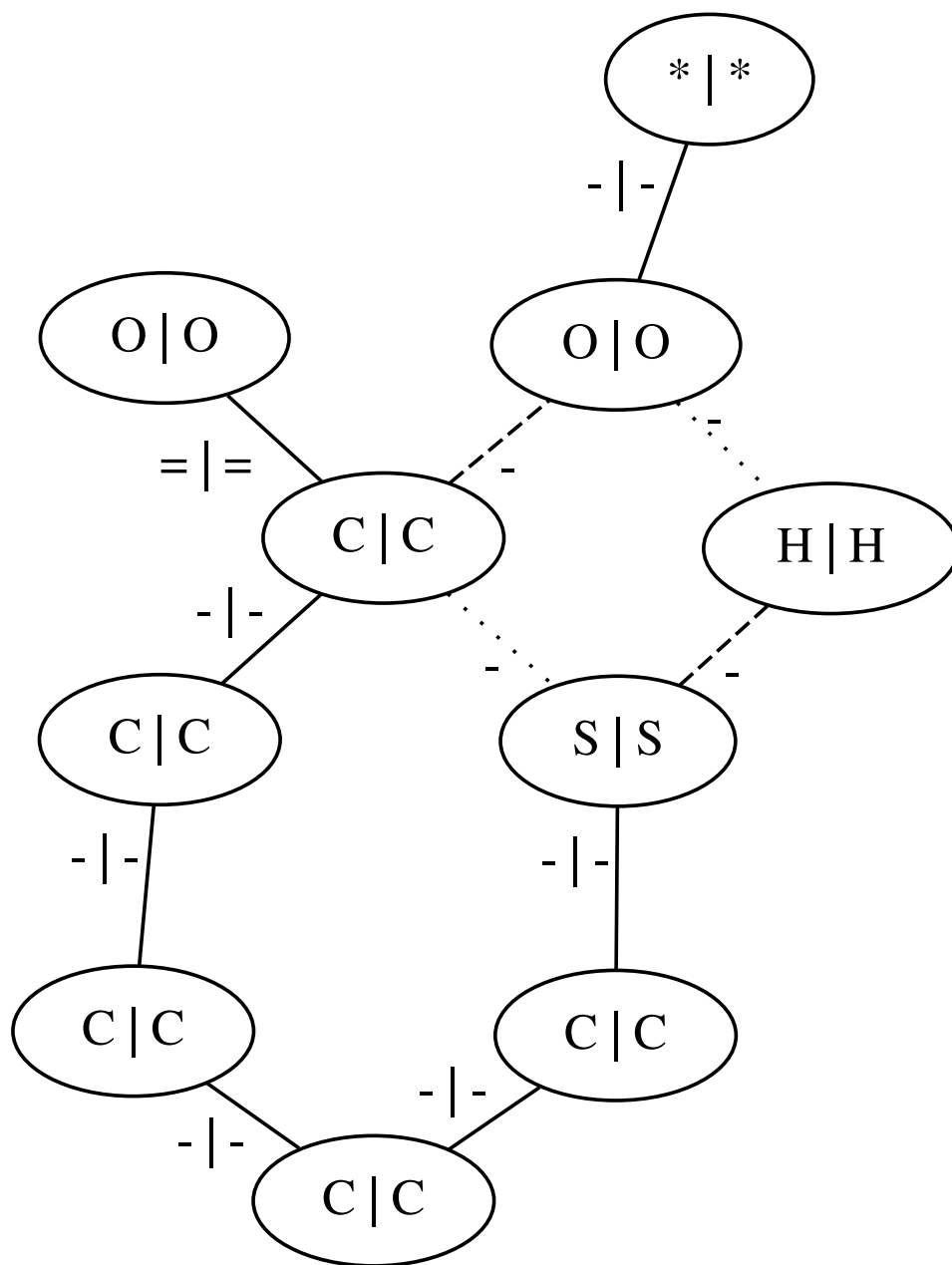
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid = 1
\end{aligned}$$

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

1.0.135 Ring Closure 6 membered O, S



Files: out/537_r_138_10300110_{L, K, R}

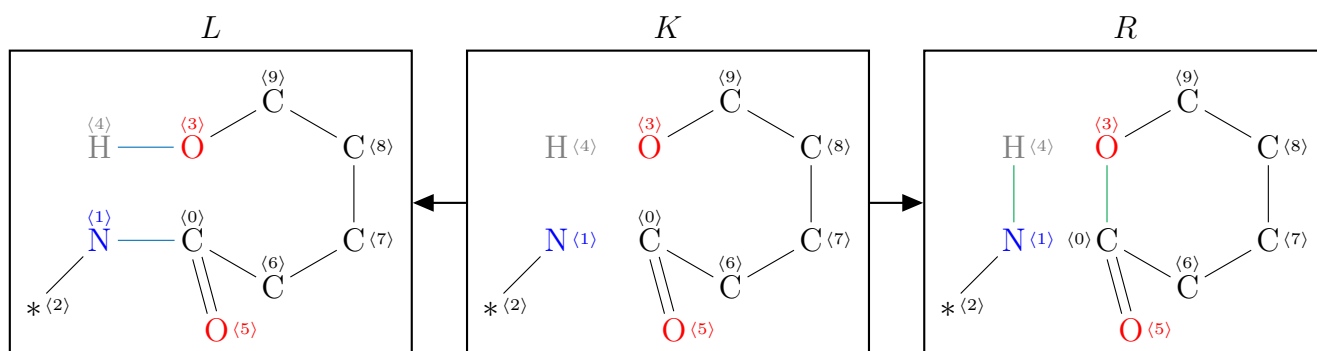


File: out/538_r_138_combined

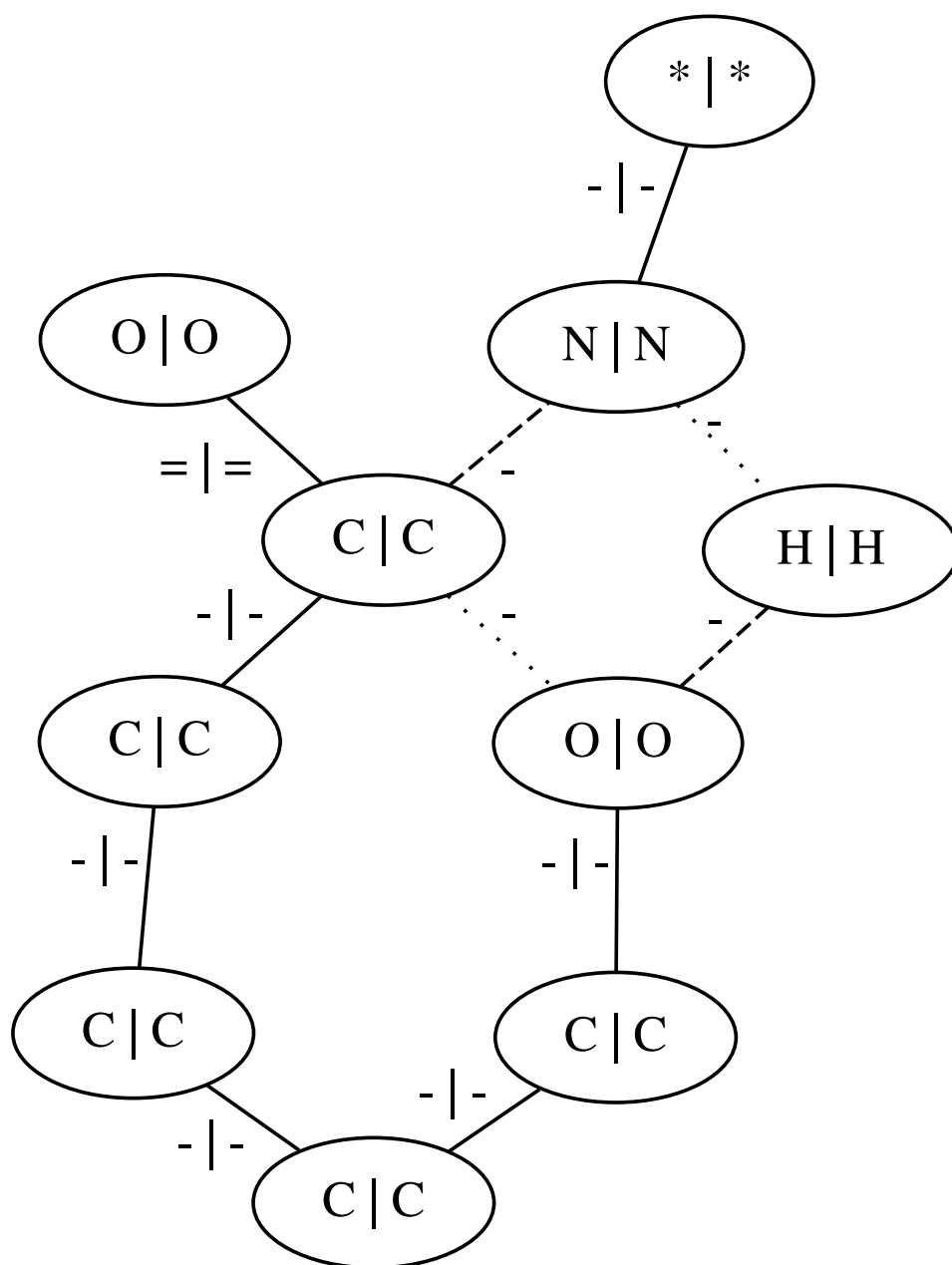
$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid = 1
\end{aligned}$$

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

1.0.136 Ring Closure 6 membered N, O



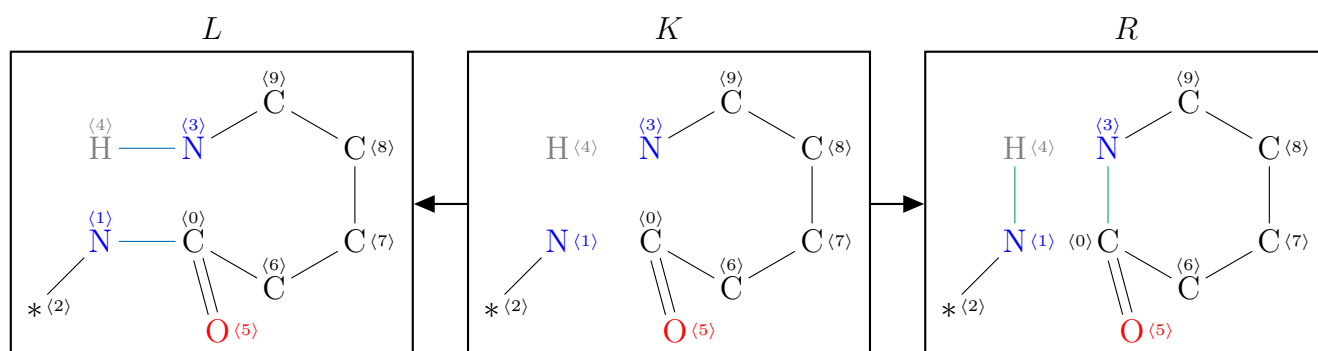
Files: out/541_r_139_10300110_{L, K, R}

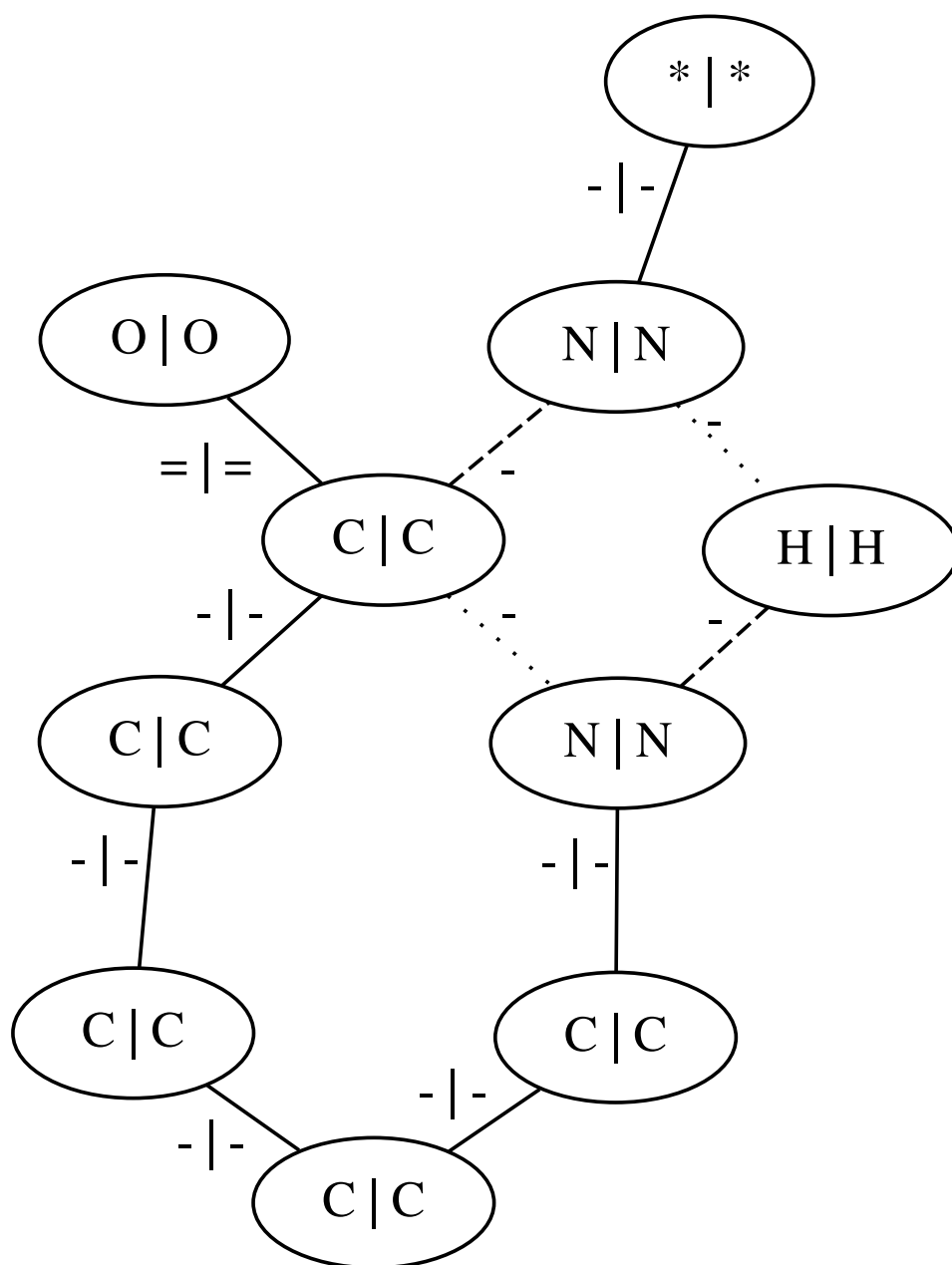


File: out/542_r_139_combined

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

1.0.137 Ring Closure 6 membered N, N

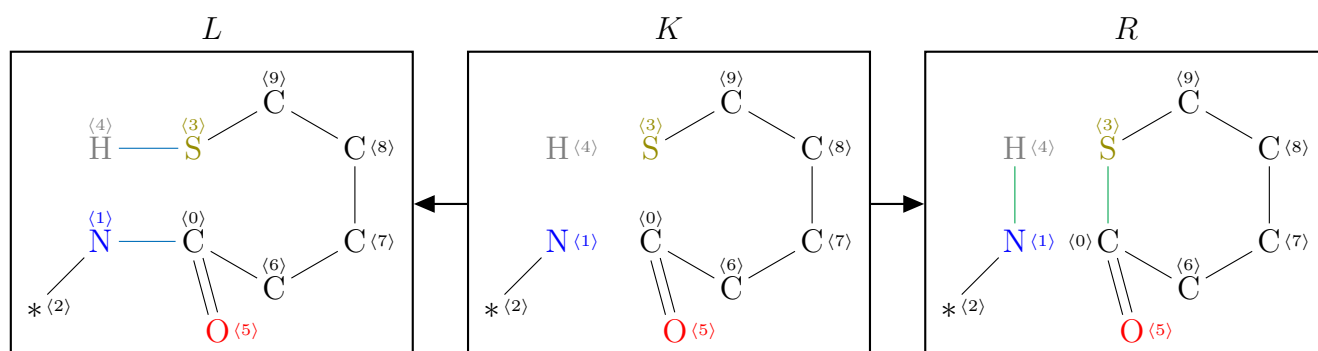


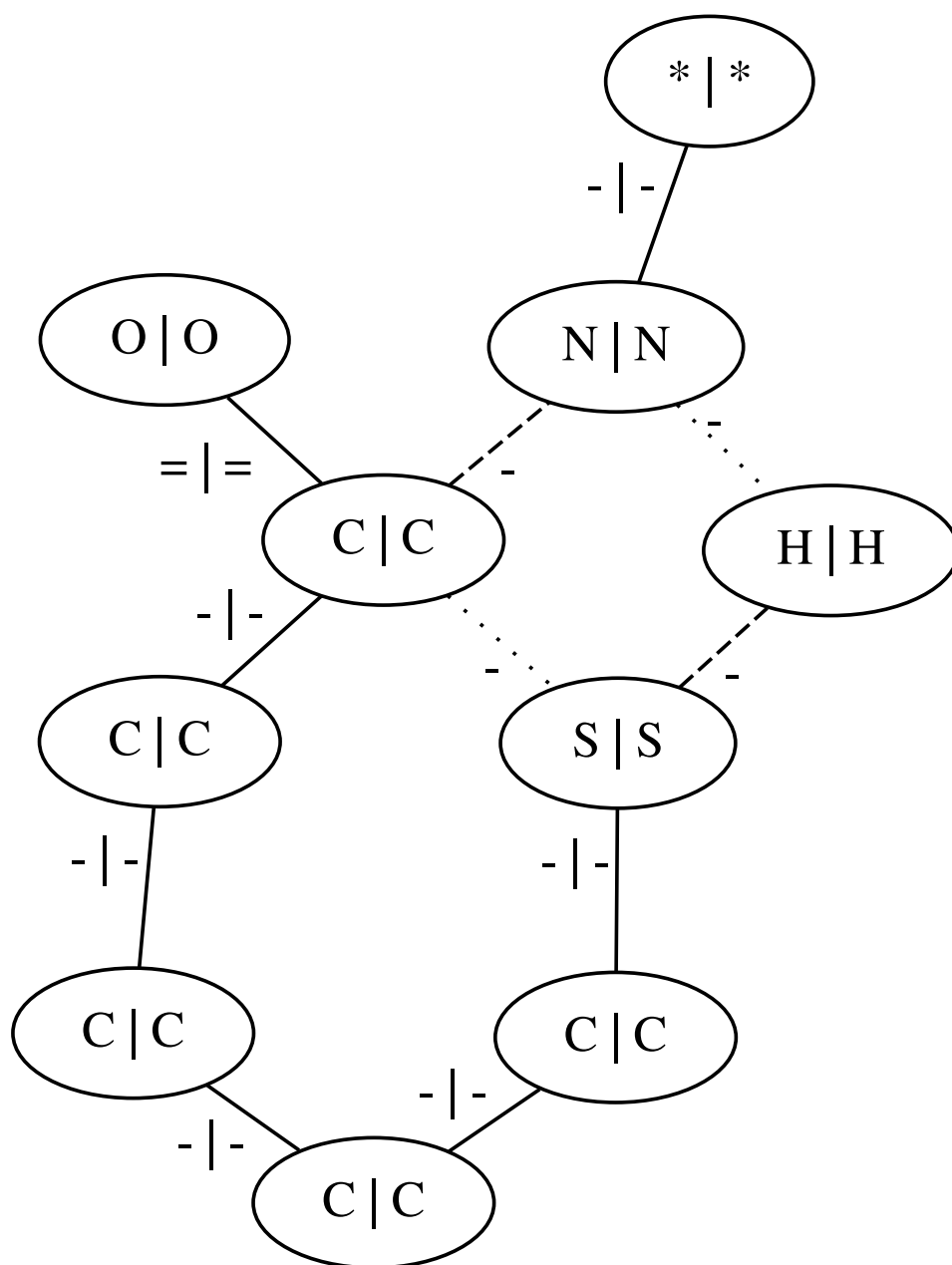


File: out/546_r_140_combined

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

1.0.138 Ring Closure 6 membered N, S

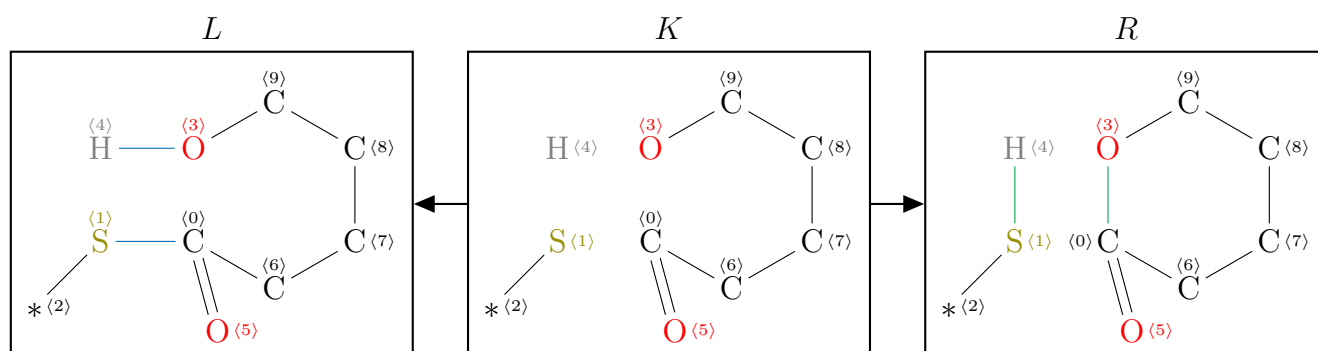




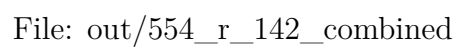
File: out/550_r_141_combined

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

1.0.139 Ring Closure 6 membered S, O

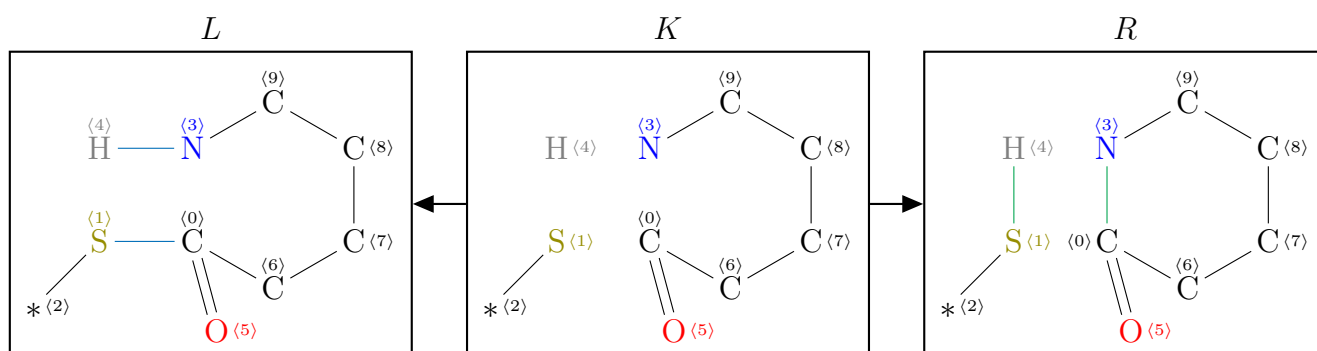


Files: out/553_r_142_10300110_{L, K, R}

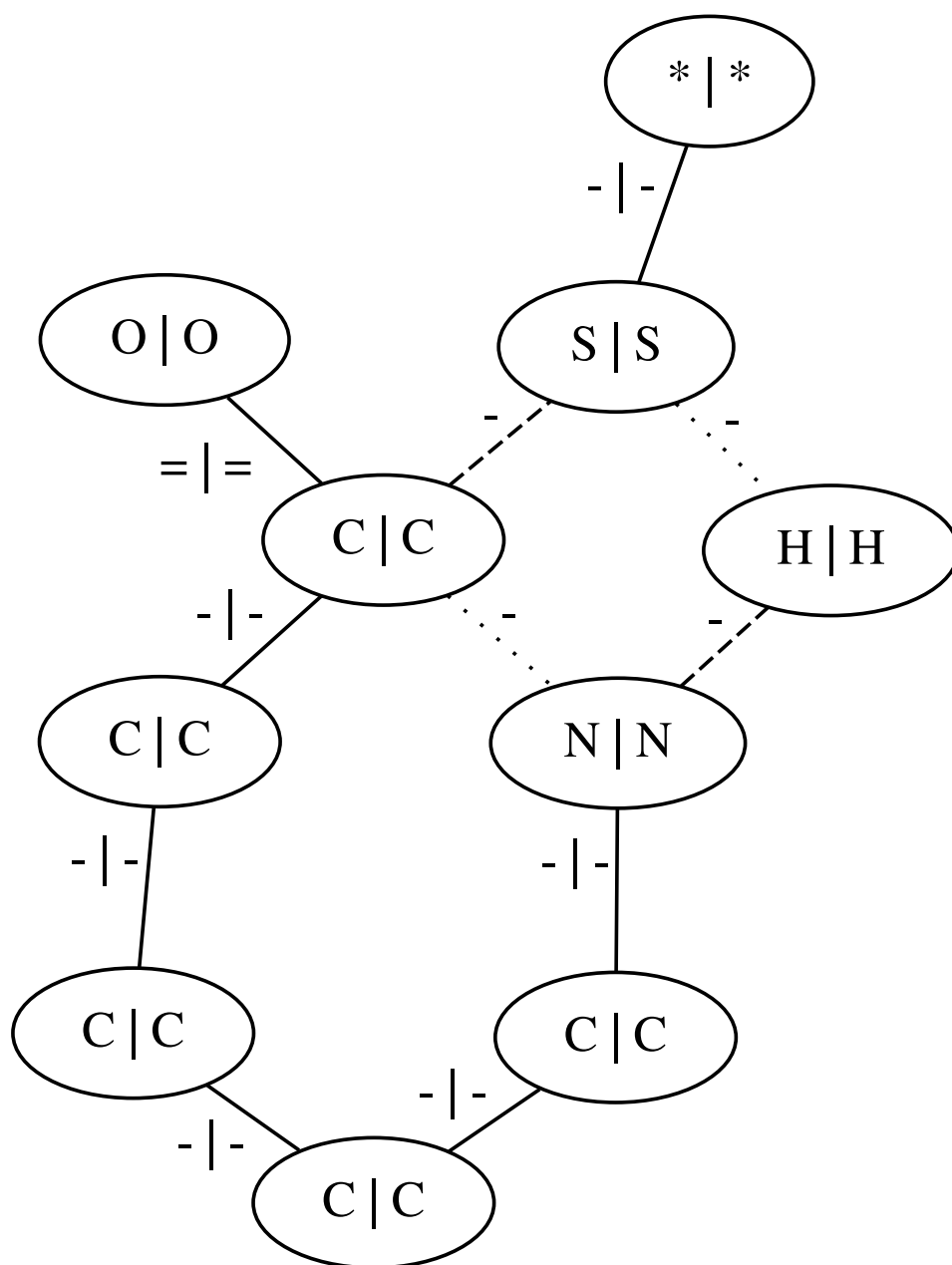


$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 1
\end{aligned}$$

1.0.140 Ring Closure 6 membered S, N



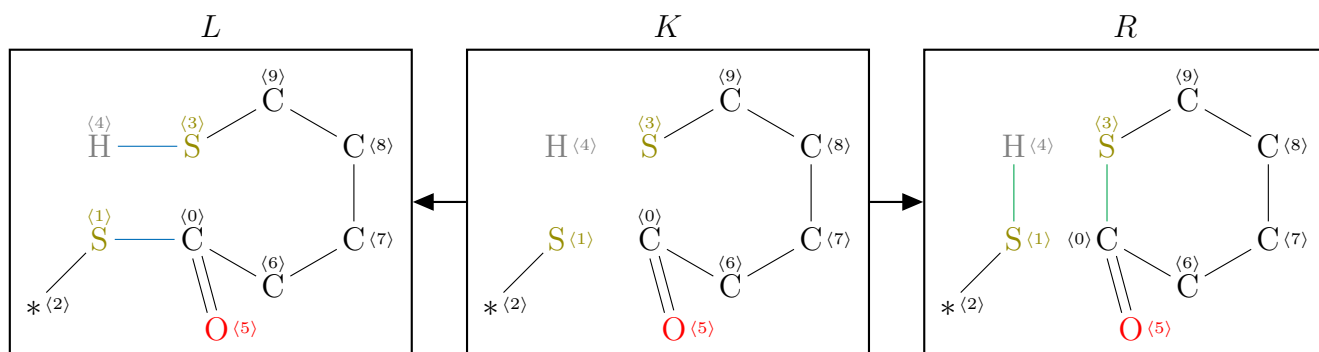
Files: out/557_r_143_10300110_{L, K, R}

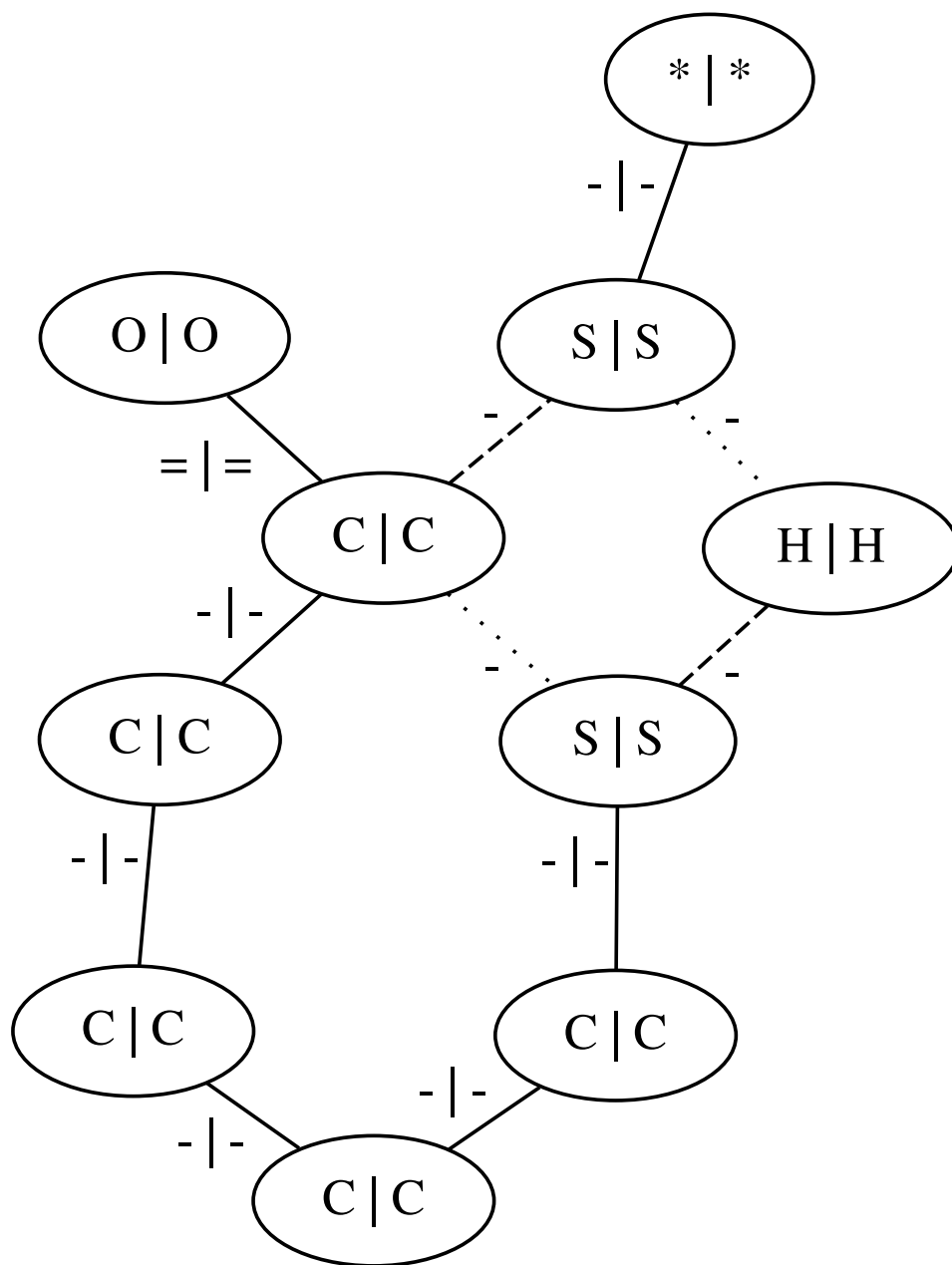


File: out/558_r_143_combined

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

1.0.141 Ring Closure 6 membered S, S

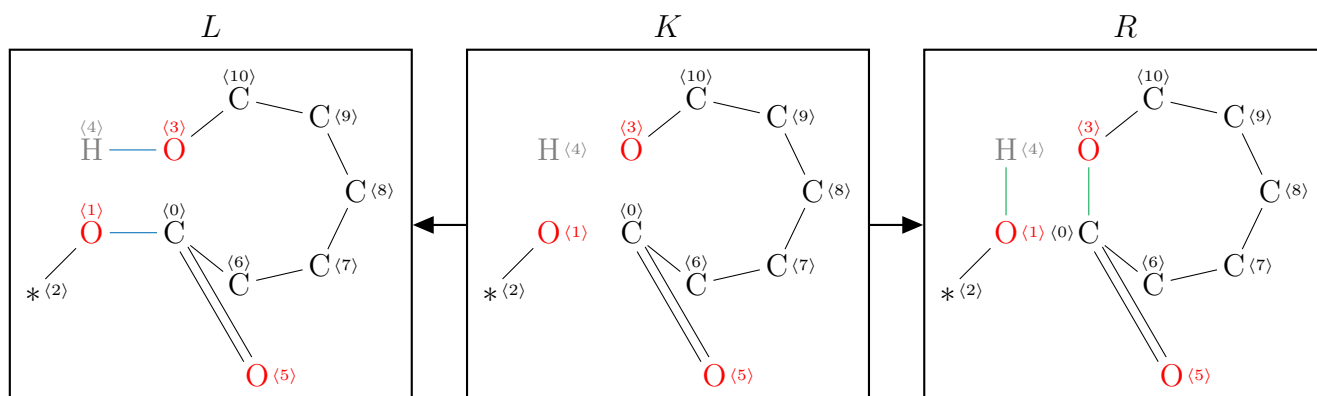




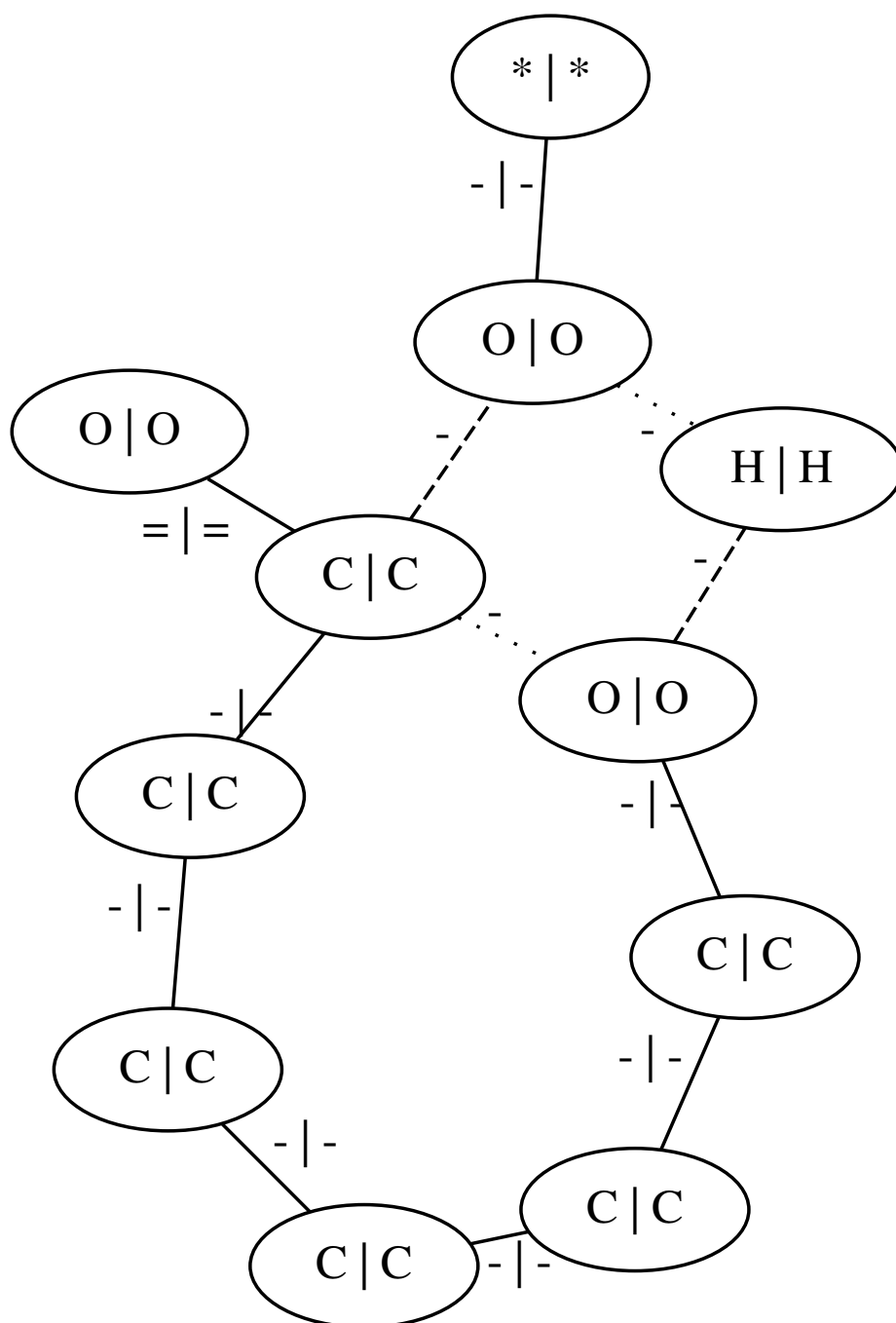
File: out/562_r_144_combined

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

1.0.142 Ring Closure 7 membered O, O



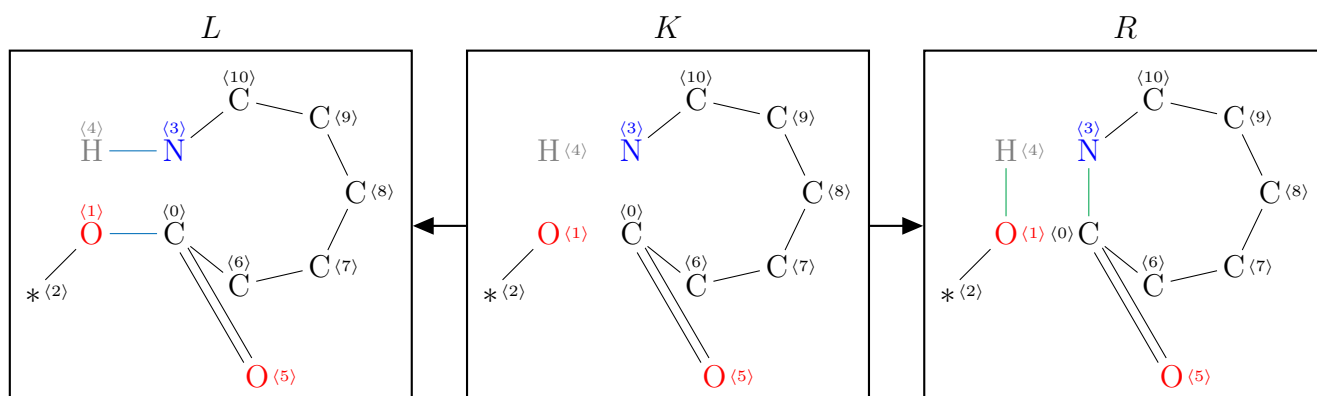
Files: out/565_r_145_10300110_{L, K, R}



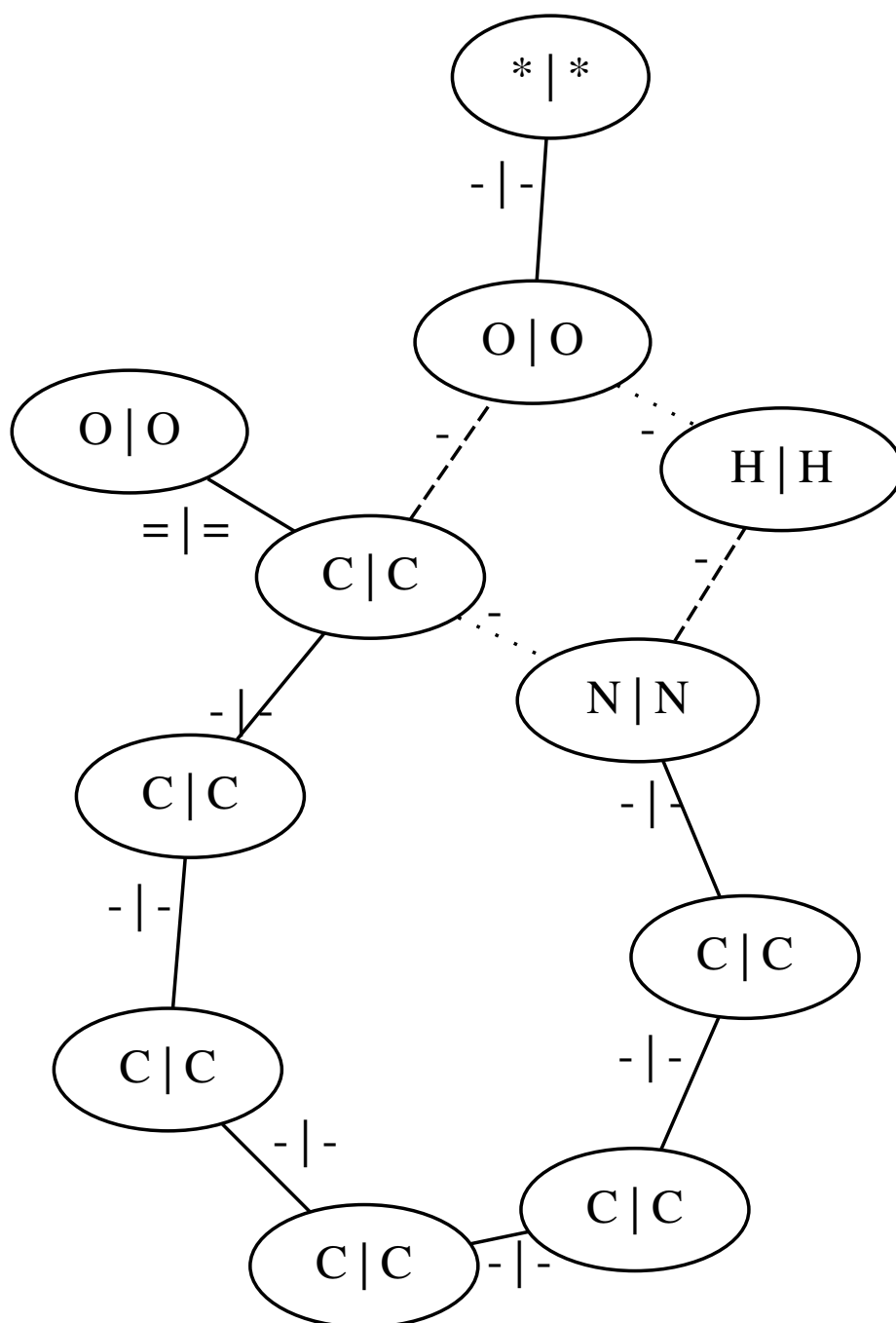
File: out/566_r_145_combined

$$\begin{aligned} & |\{e \in \text{outEdges}(2) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'-'}\} \\ & \quad \}| = 1 \end{aligned}$$
$$\begin{aligned} & |\{e \in \text{outEdges}(2) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'C'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'='}\} \\ & \quad \}| = 0 \end{aligned}$$

1.0.143 Ring Closure 7 membered O, N



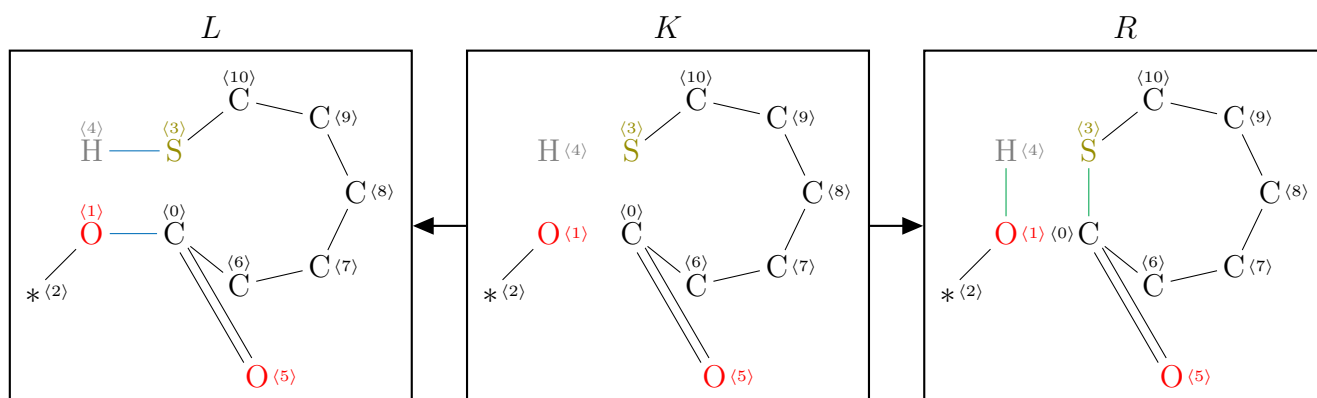
Files: out/569_r_146_10300110_{L, K, R}



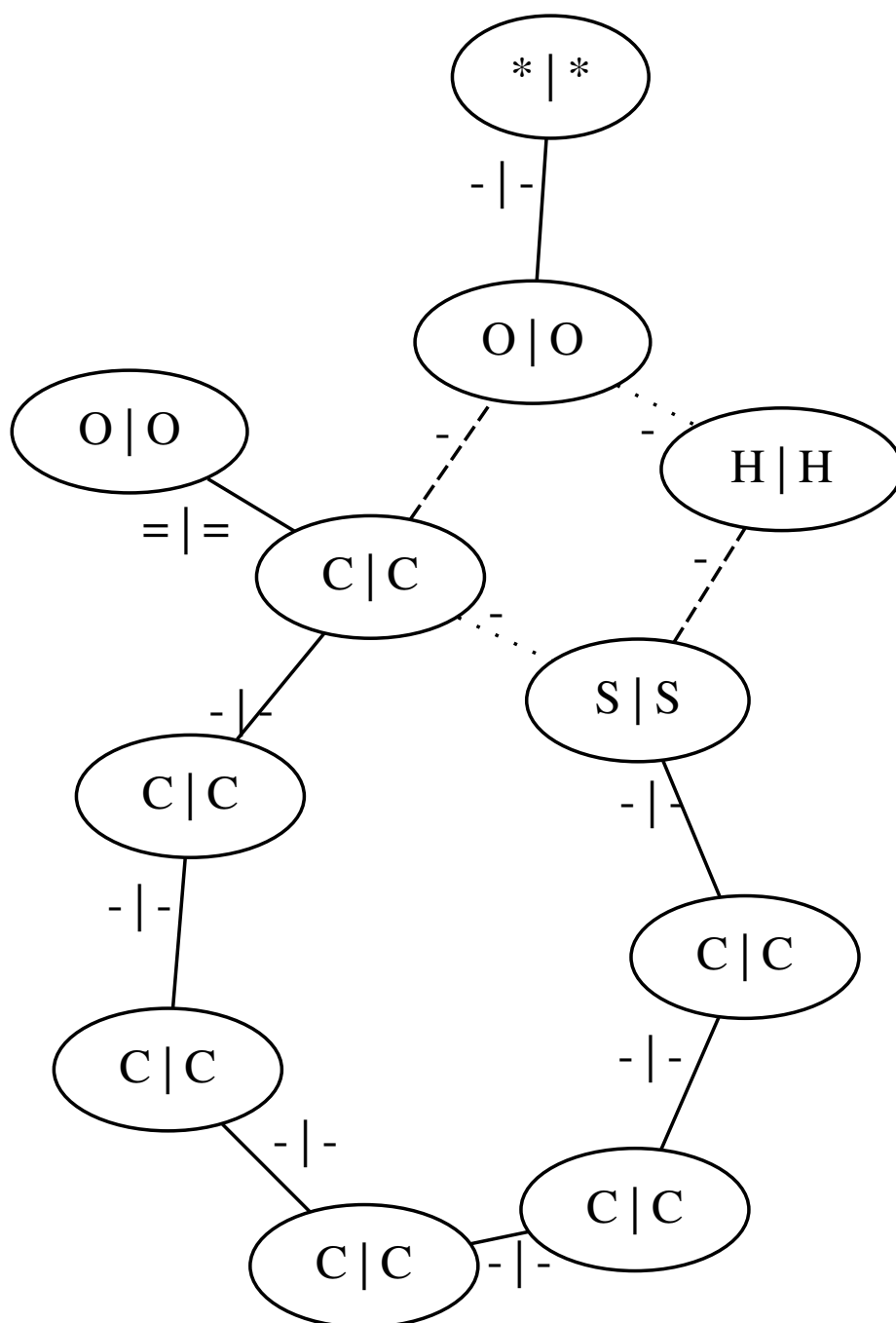
File: out/570_r_146_combined

$$\begin{aligned} & |\{e \in \text{outEdges}(2) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'-'}\} \\ & \quad \}| = 1 \end{aligned}$$
$$\begin{aligned} & |\{e \in \text{outEdges}(2) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'C'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'='}\} \\ & \quad \}| = 0 \end{aligned}$$

1.0.144 Ring Closure 7 membered O, S



Files: out/573_r_147_10300110_{L, K, R}

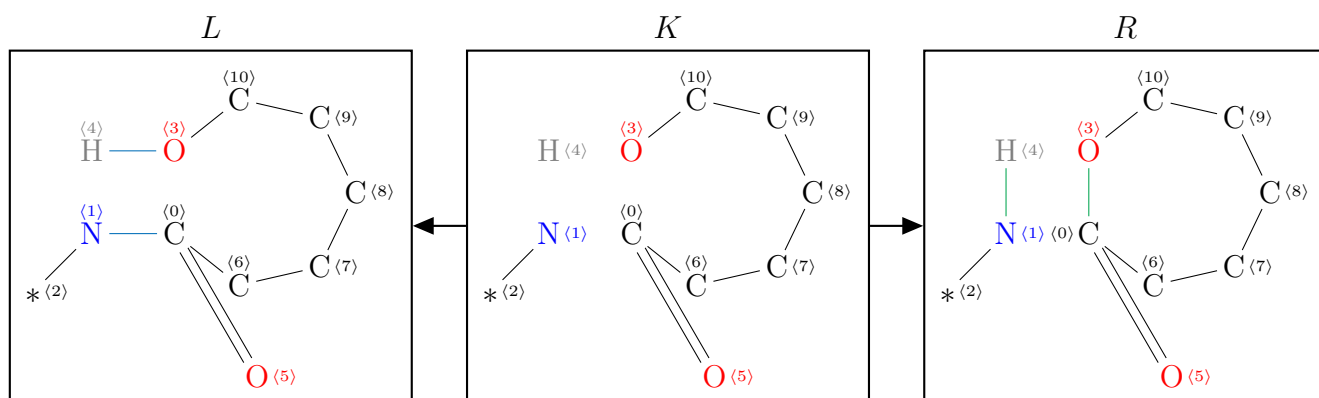


File: out/574_r_147_combined

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

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

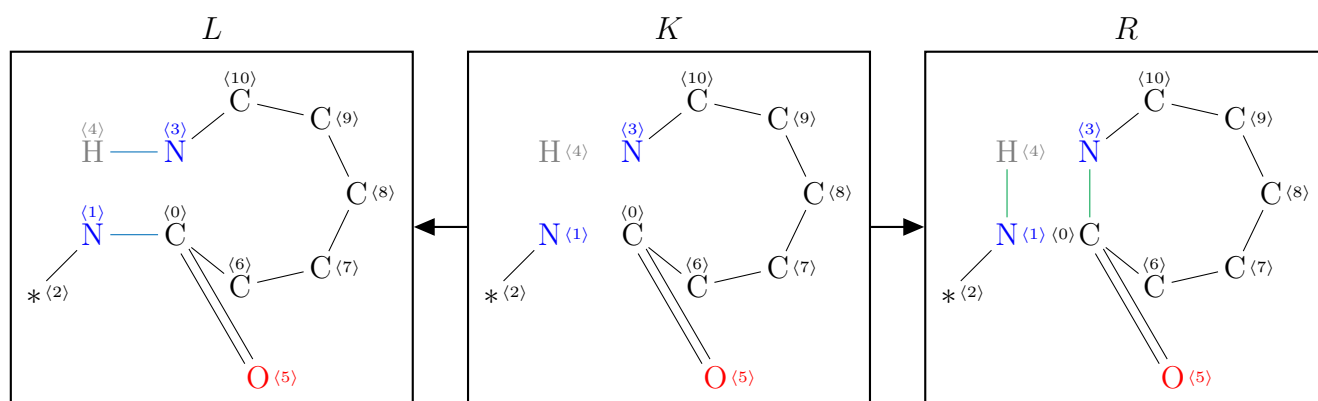
1.0.145 Ring Closure 7 membered N, O

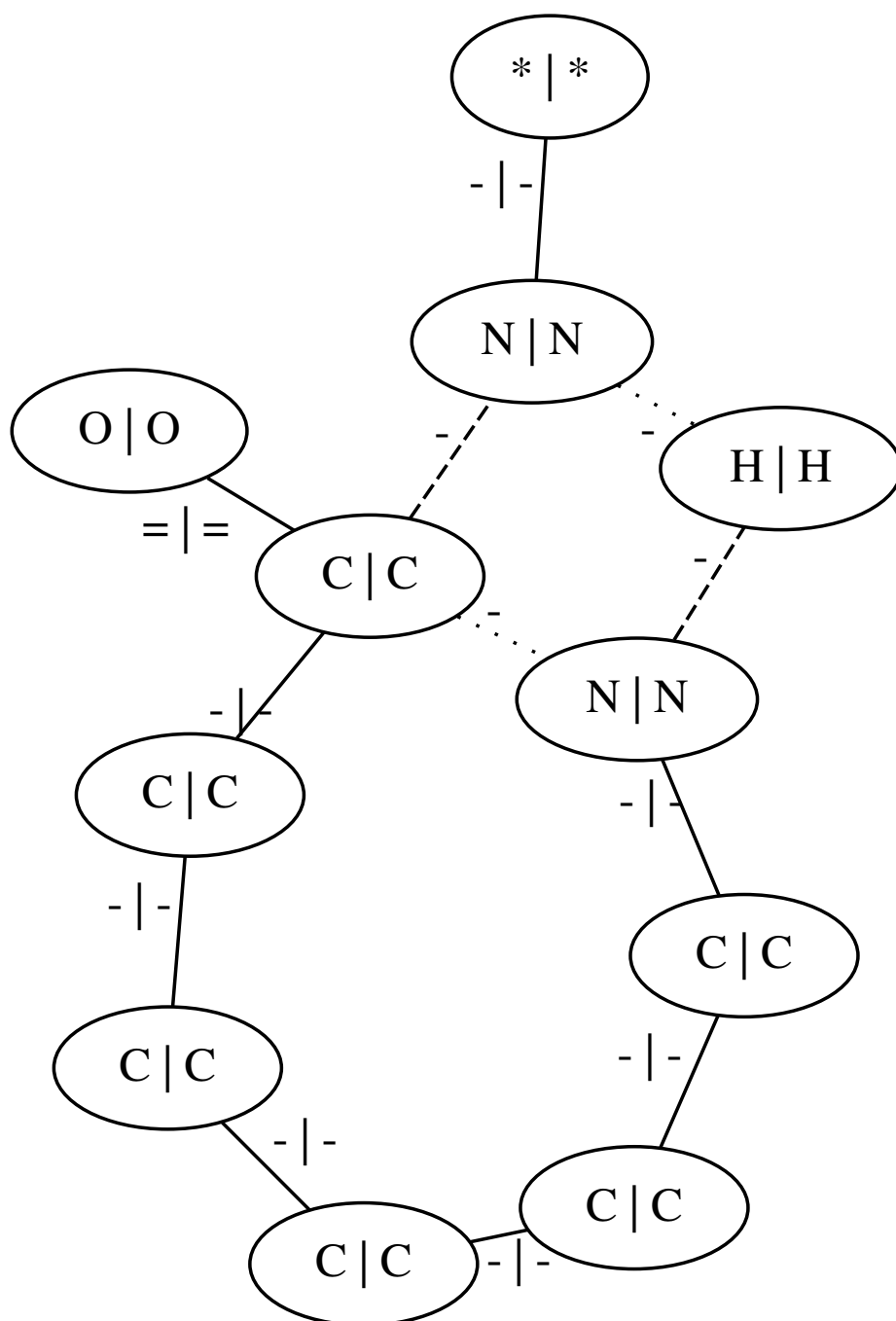


Files: out/577_r_148_10300110_{L, K, R}

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

1.0.146 Ring Closure 7 membered N, N

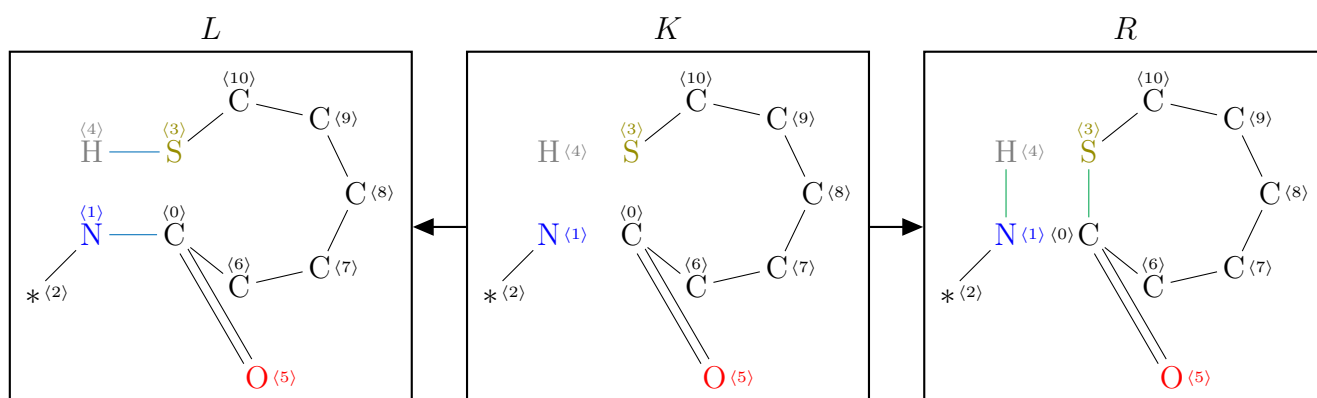




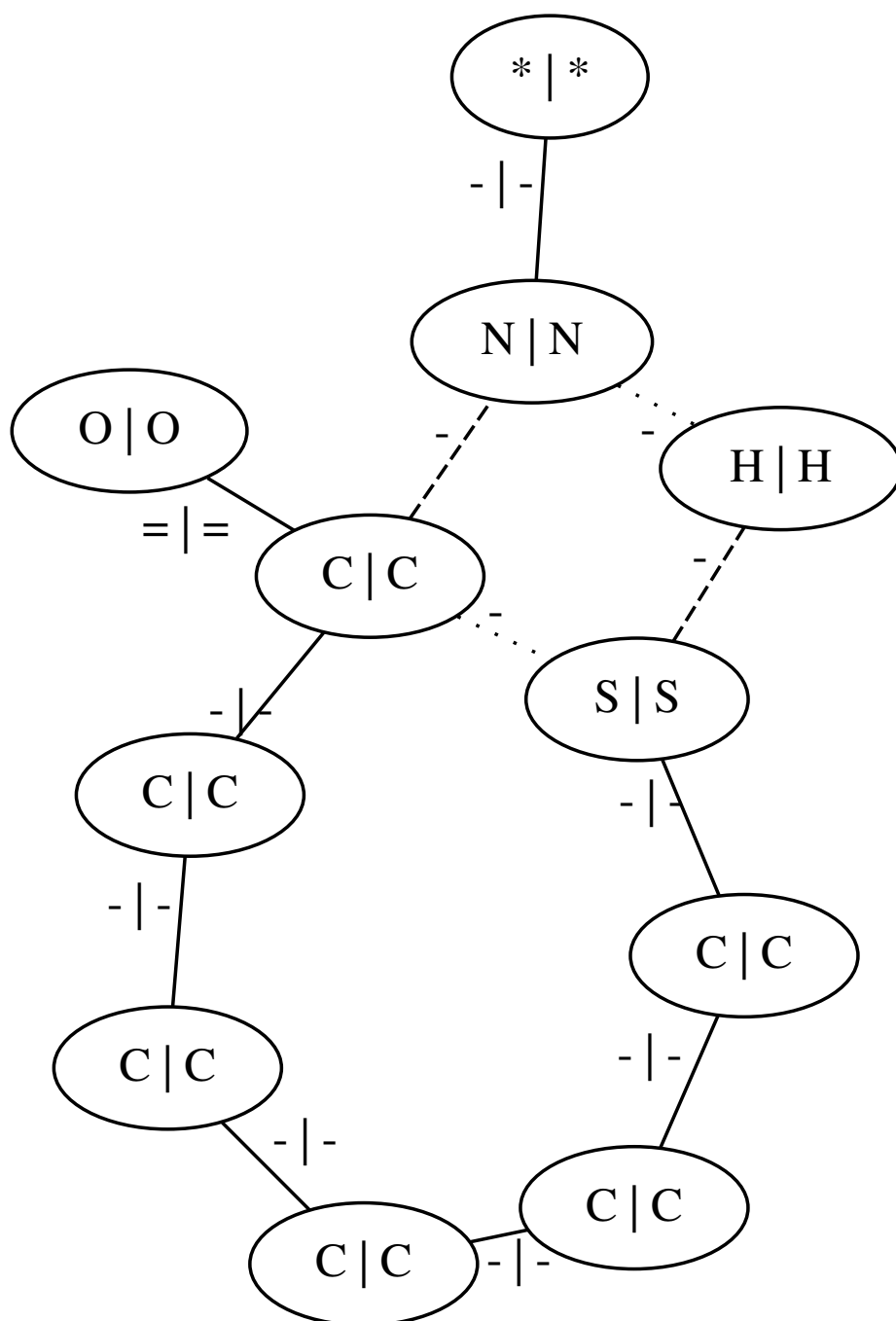
File: out/582_r_149_combined

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

1.0.147 Ring Closure 7 membered N, S



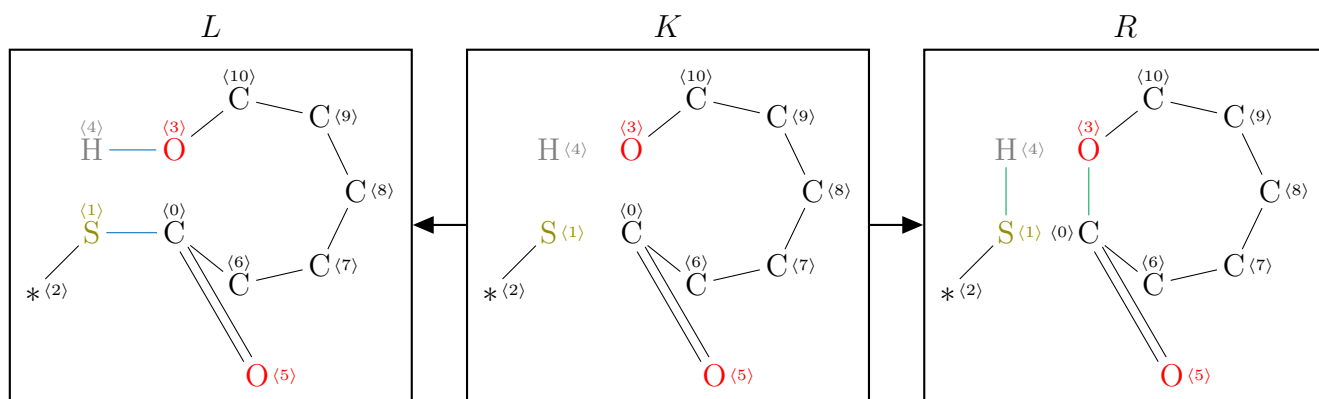
Files: out/585_r_150_10300110_{L, K, R}

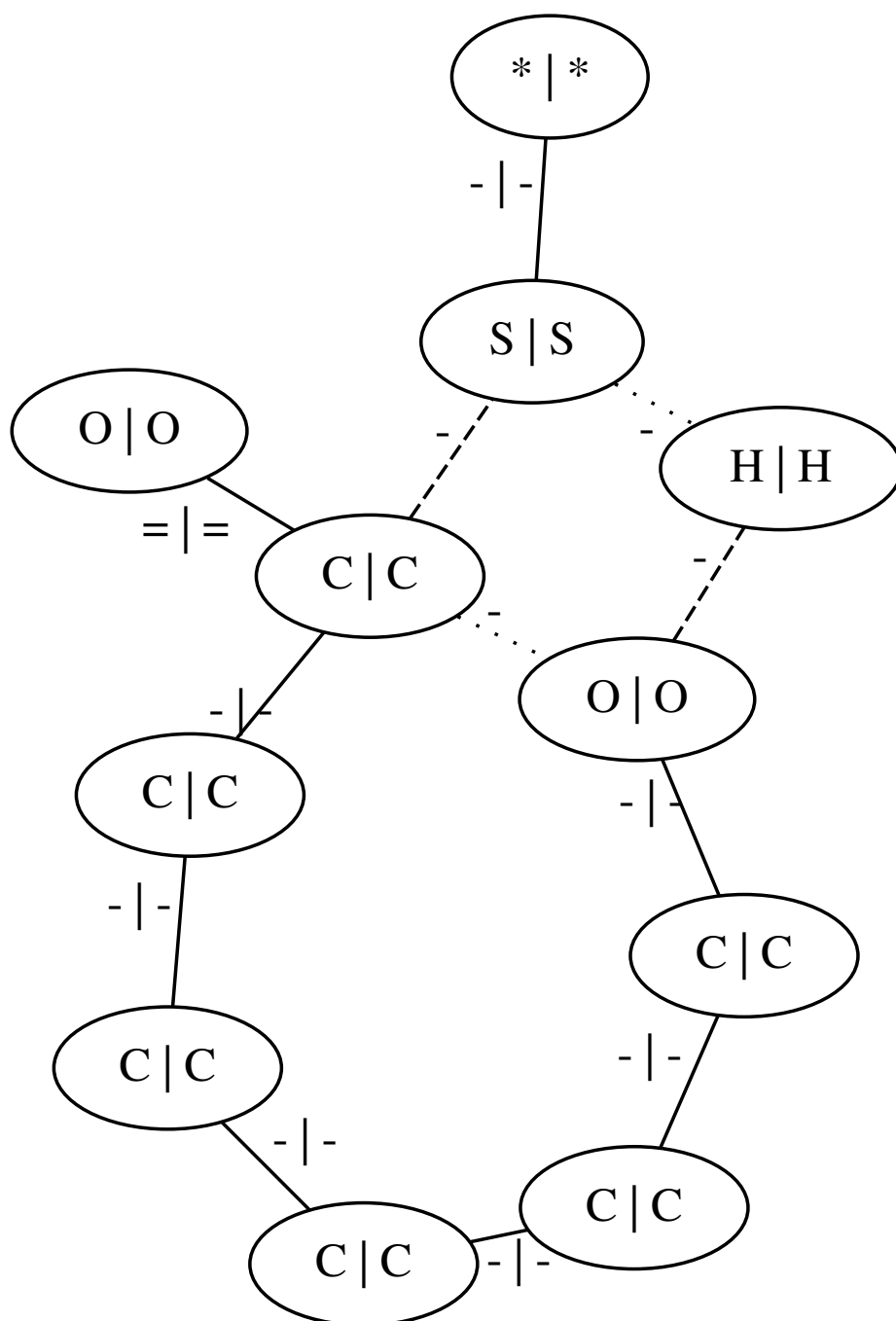


File: out/586_r_150_combined

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

1.0.148 Ring Closure 7 membered S, O

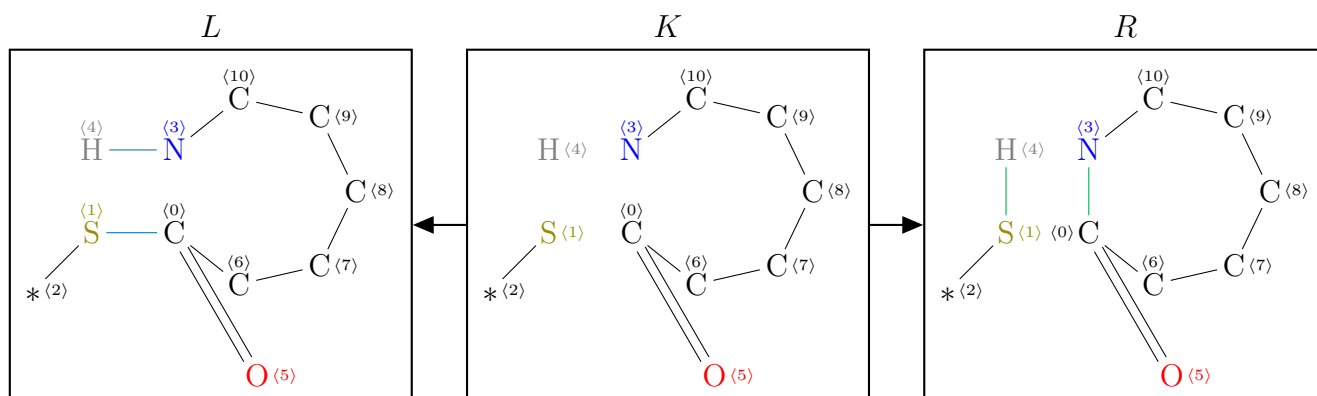




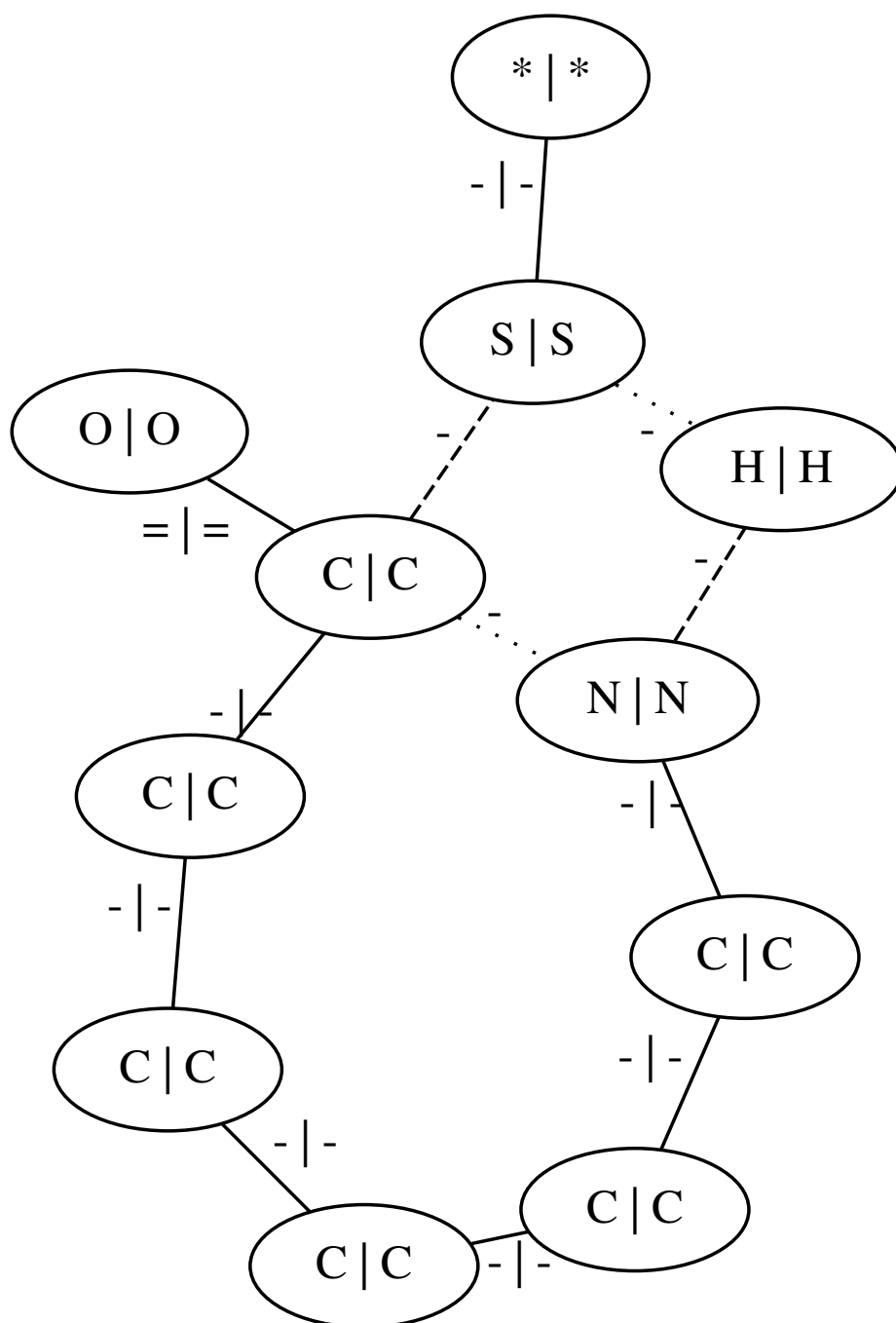
File: out/590_r_151_combined

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

1.0.149 Ring Closure 7 membered S, N



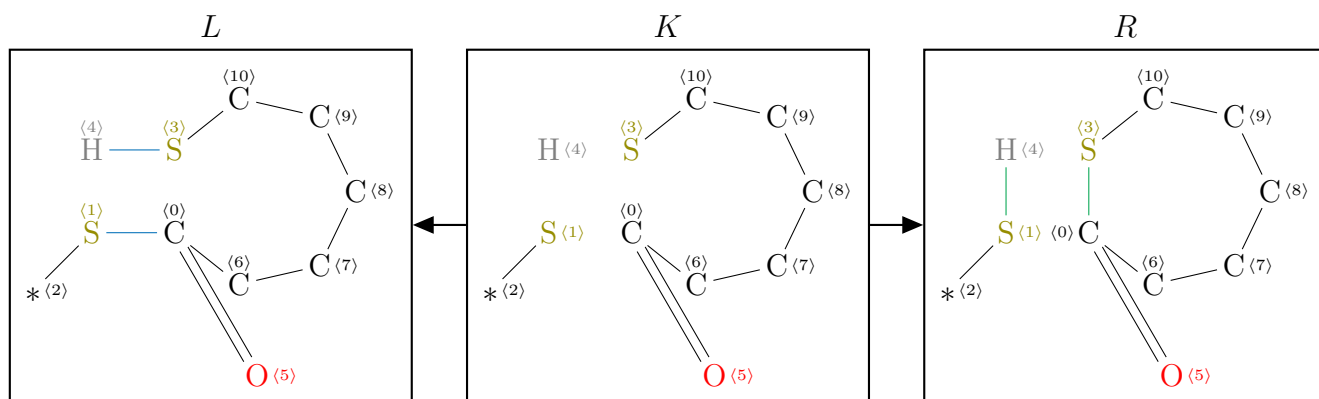
Files: out/593_r_152_10300110_{L, K, R}



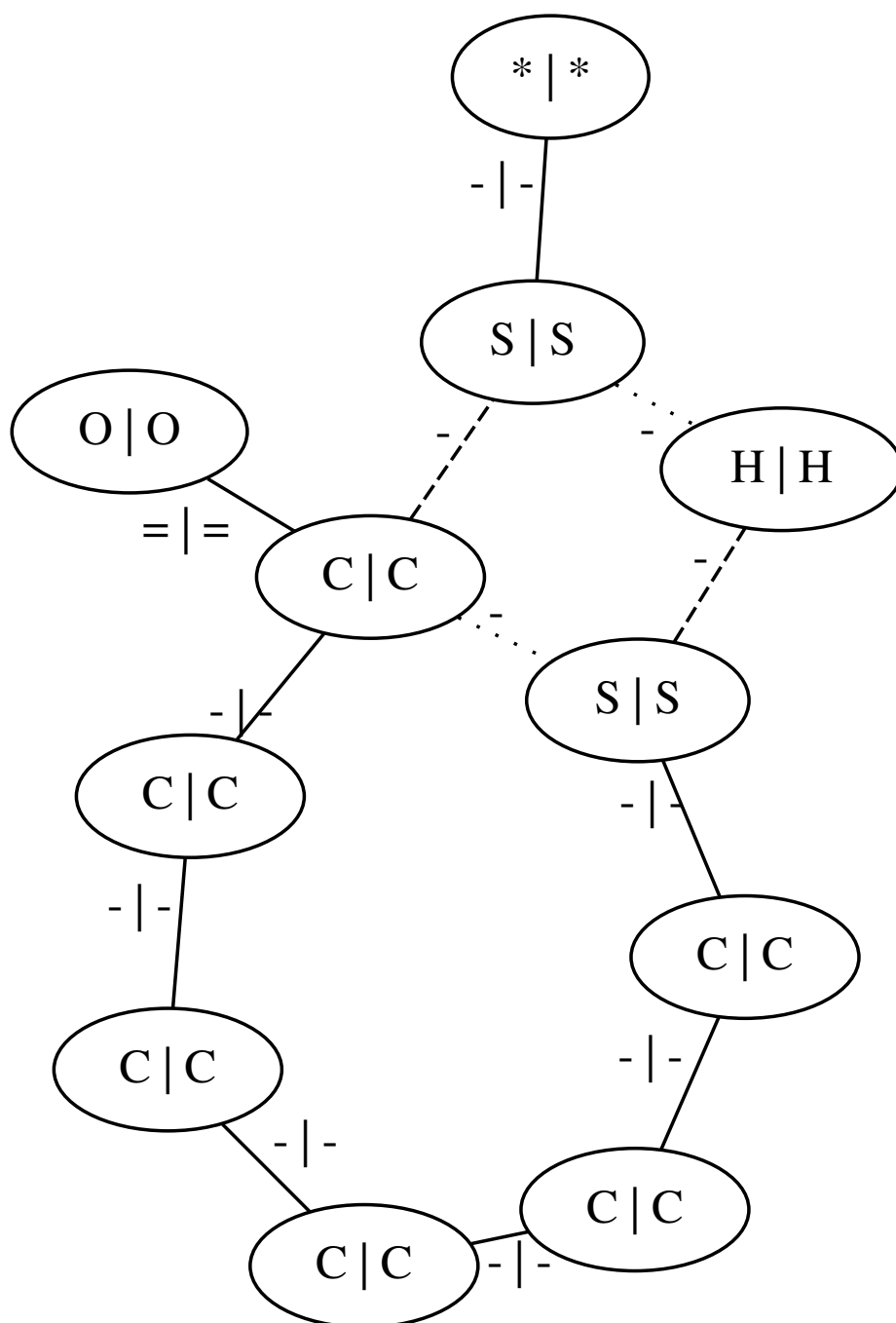
File: out/594_r_152_combined

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

1.0.150 Ring Closure 7 membered S, S



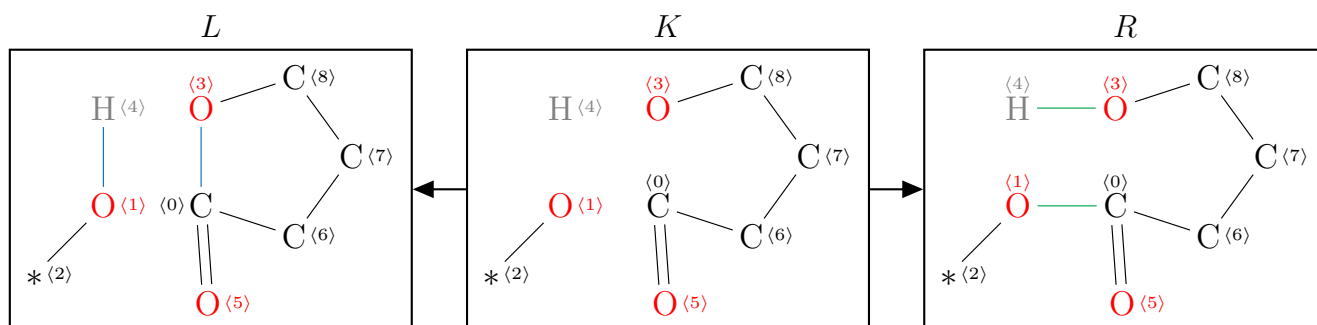
Files: out/597_r_153_10300110_{L, K, R}

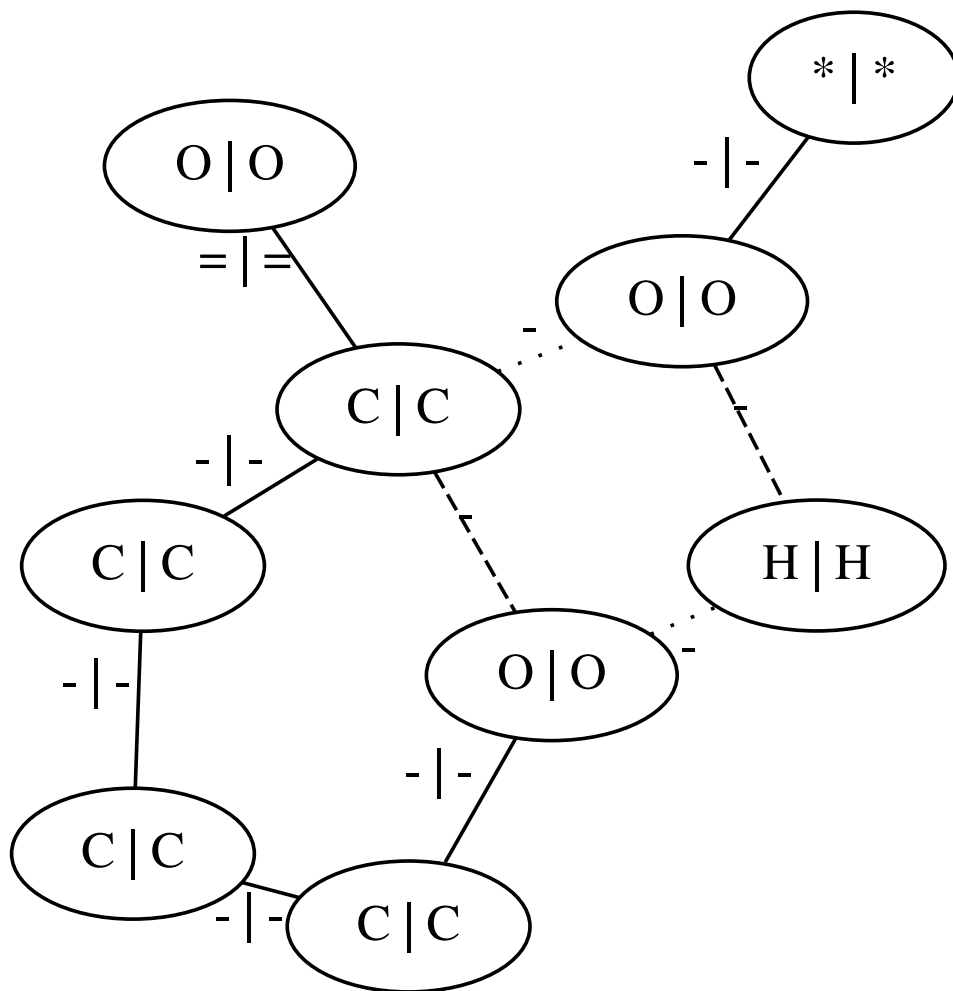


File: out/598_r_153_combined

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

1.0.151 Ring Closure 5 membered, inverse O, O



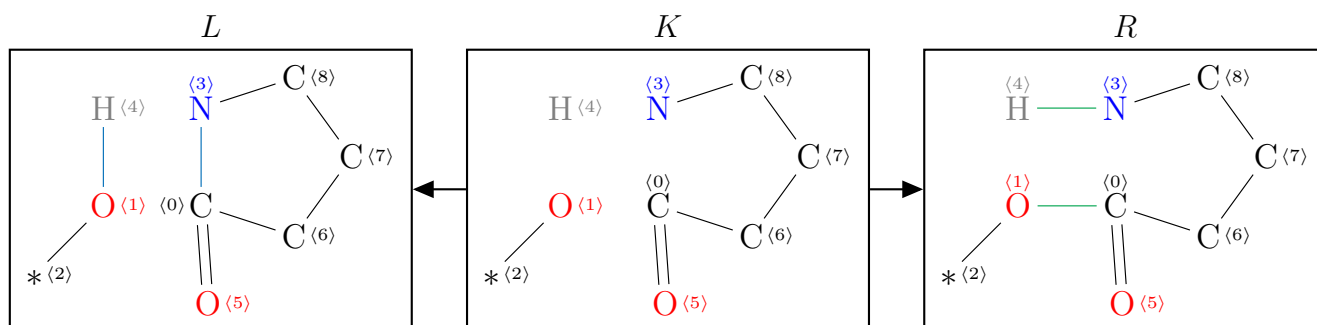


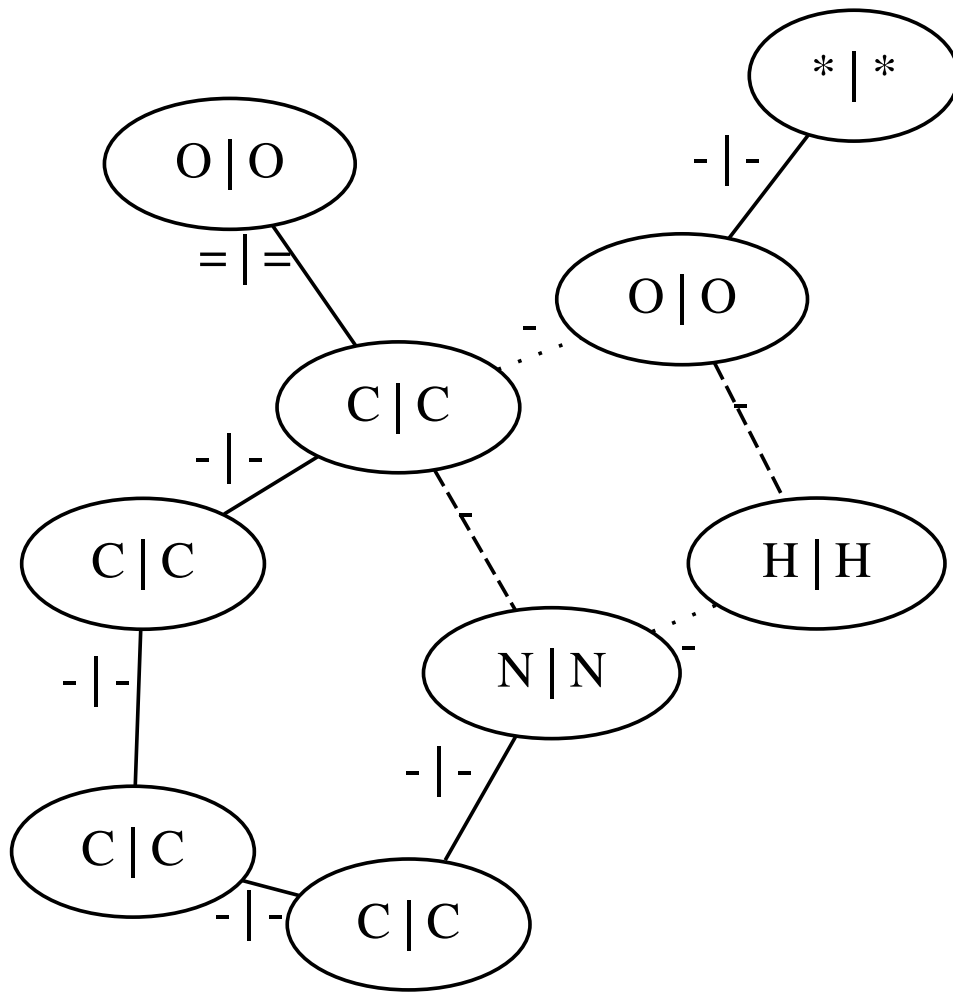
File: out/602_r_154_combined

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

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

1.0.152 Ring Closure 5 membered, inverse O, N





File: out/606_r_155_combined

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

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

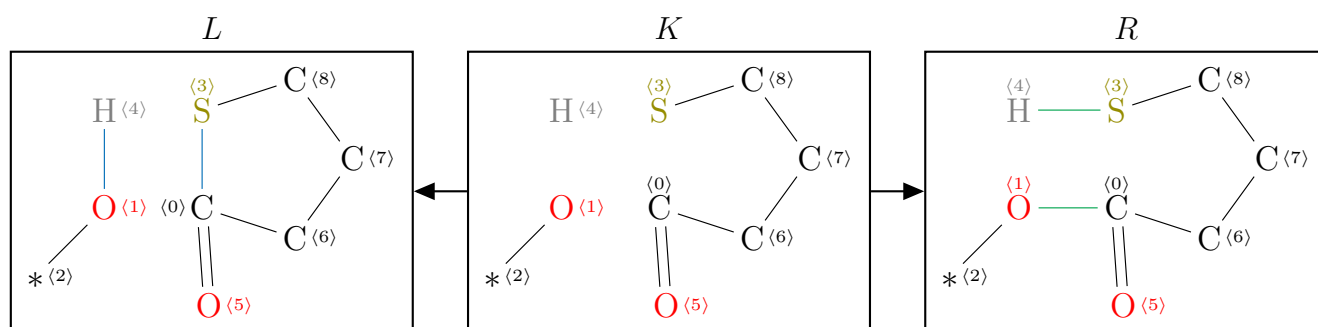
$$\wedge$$

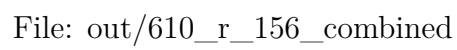
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}\} \leq 1$$

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

1.0.153 Ring Closure 5 membered, inverse O, S

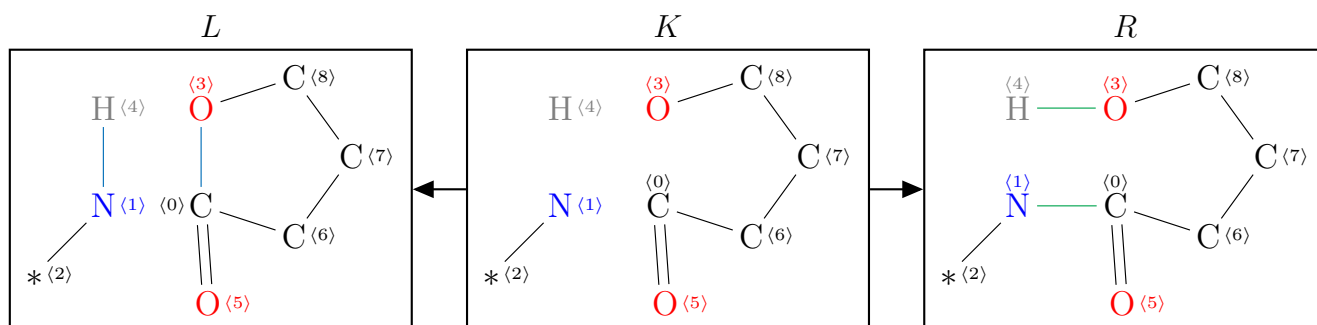


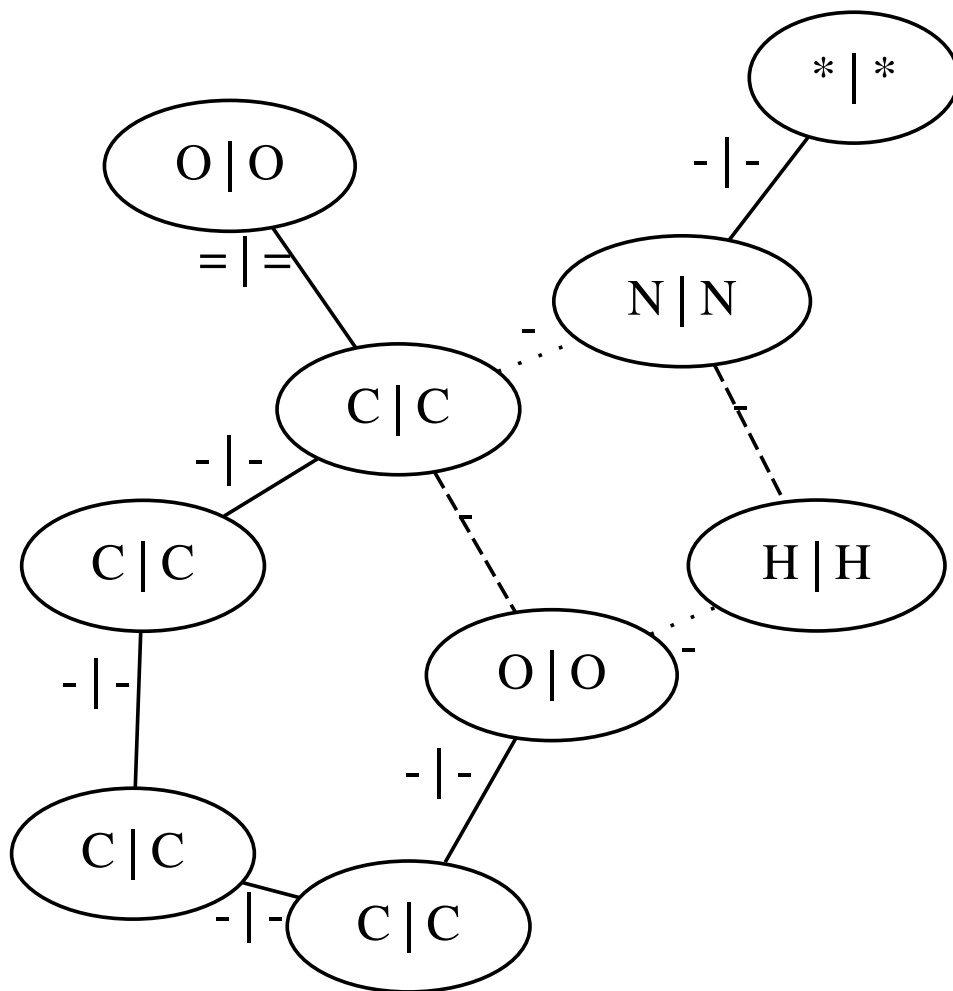


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$$\begin{aligned}
& |\{e \in \text{outEdges}(2) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'C'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'='}\} \\
& \quad \}| = 1
\end{aligned}$$

1.0.154 Ring Closure 5 membered, inverse N, O





File: out/614_r_157_combined

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

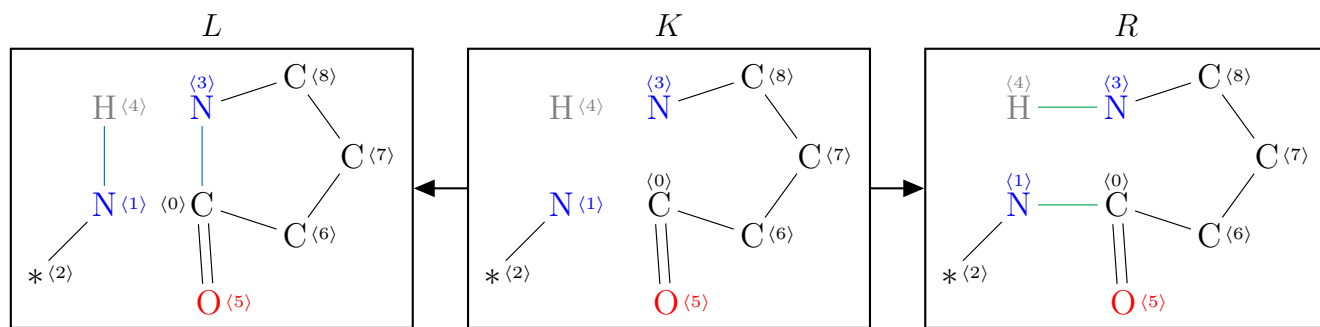
$$\text{label}(\text{target}(e)) \in \{ '0' \}$$

$$\wedge$$

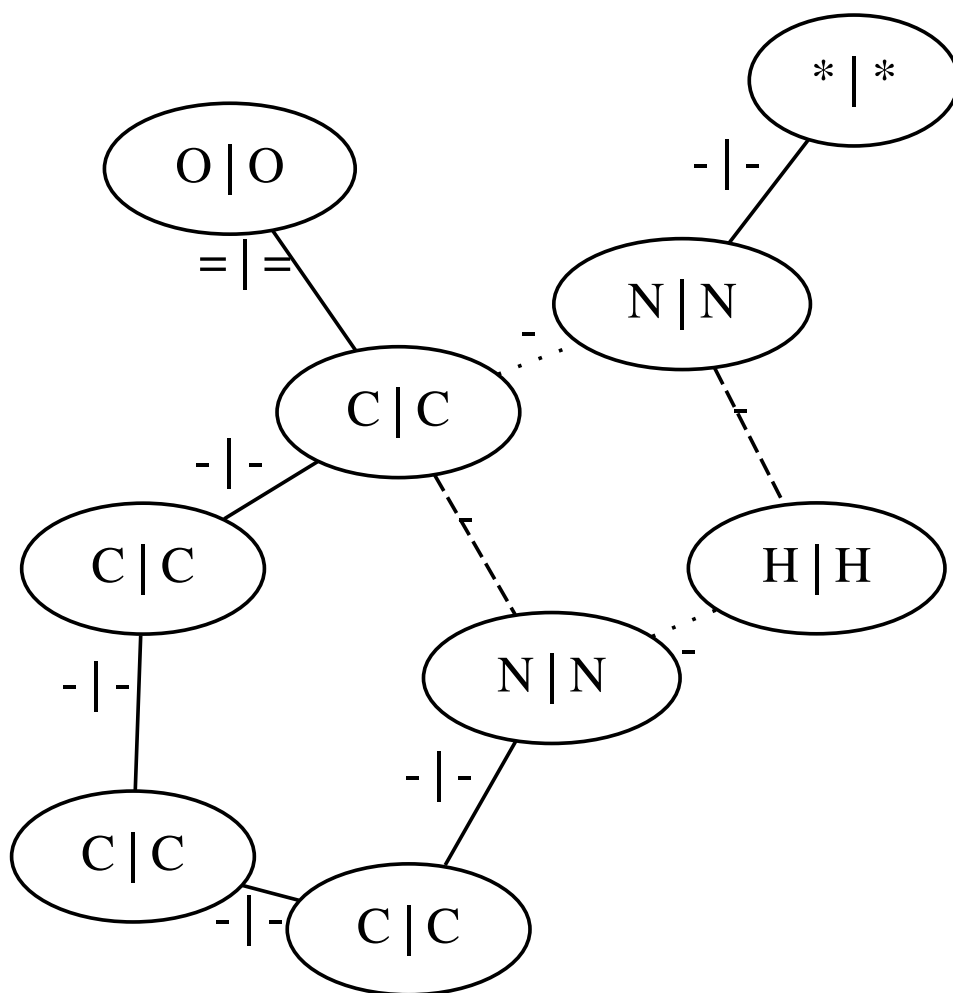
$$\text{label}(e) \in \{ '-' \}$$

$$\}| \leq 1$$

1.0.155 Ring Closure 5 membered, inverse N, N



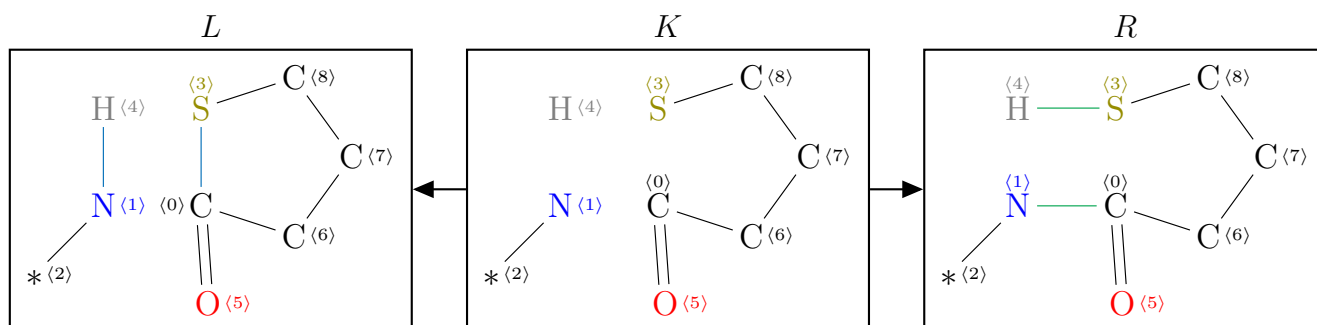
Files: out/617_r_158_10300110_{L, K, R}

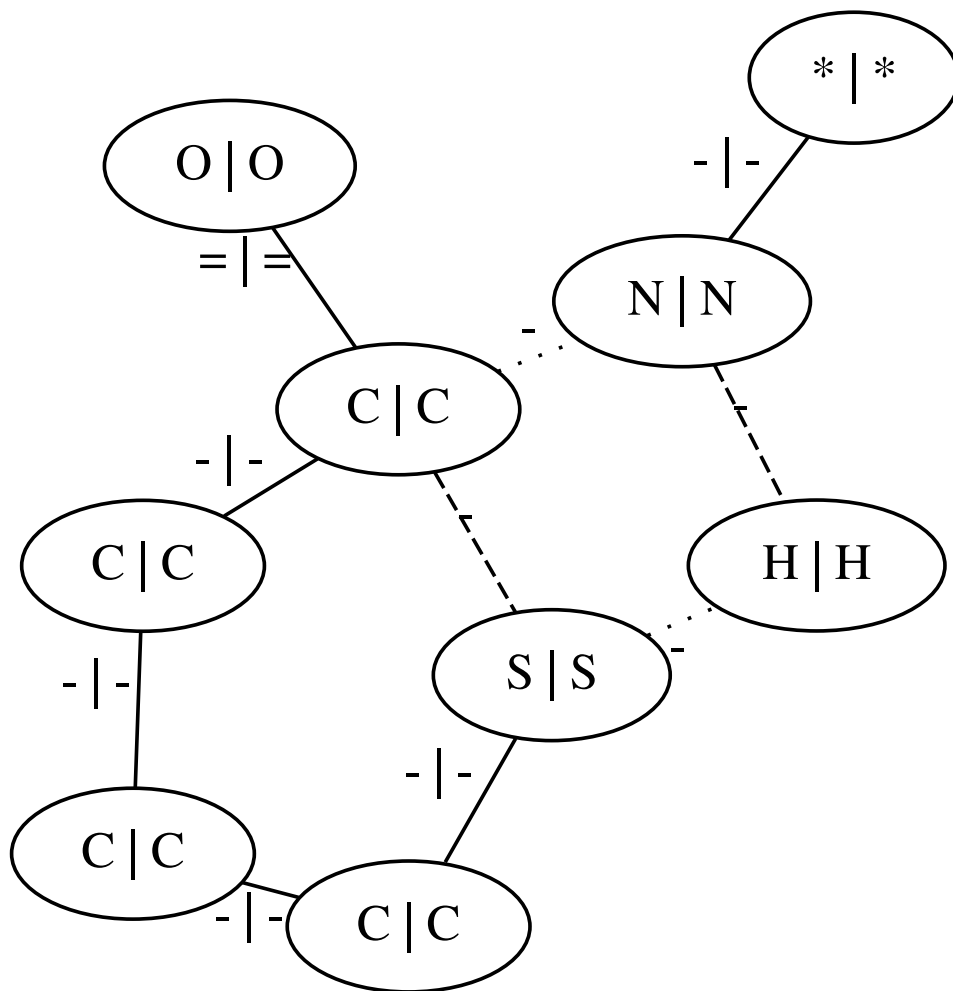


File: out/618_r_158_combined

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

1.0.156 Ring Closure 5 membered, inverse N, S

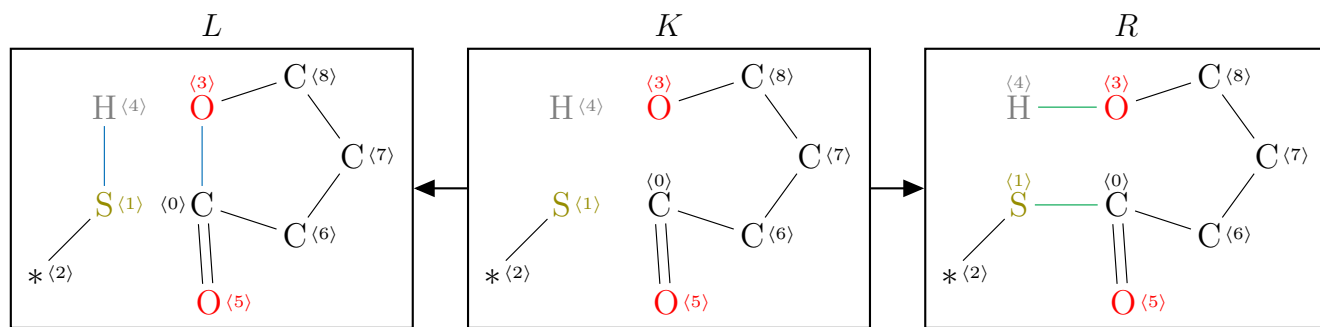




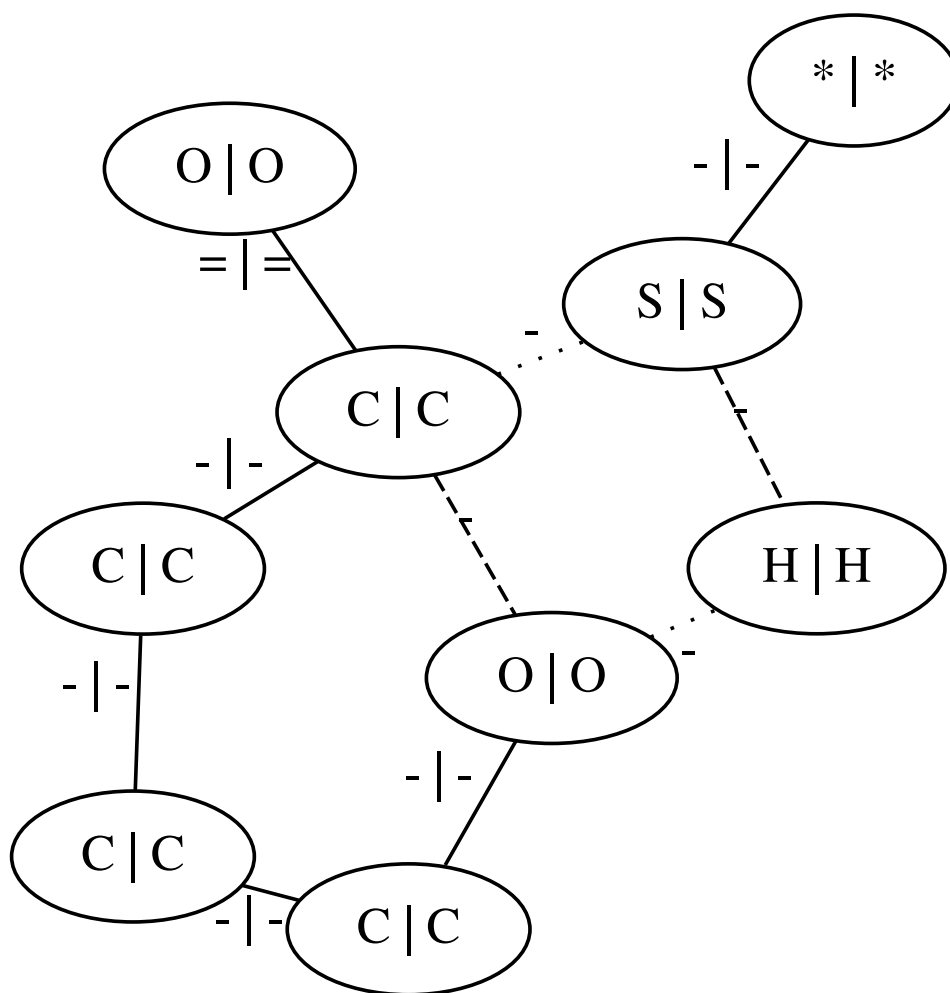
File: out/622_r_159_combined

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

1.0.157 Ring Closure 5 membered, inverse S, O



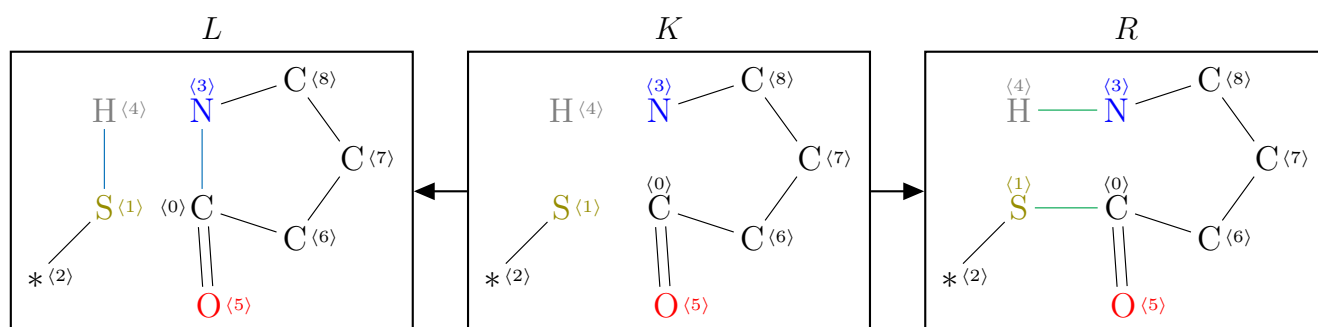
Files: out/625_r_160_10300110_{L, K, R}

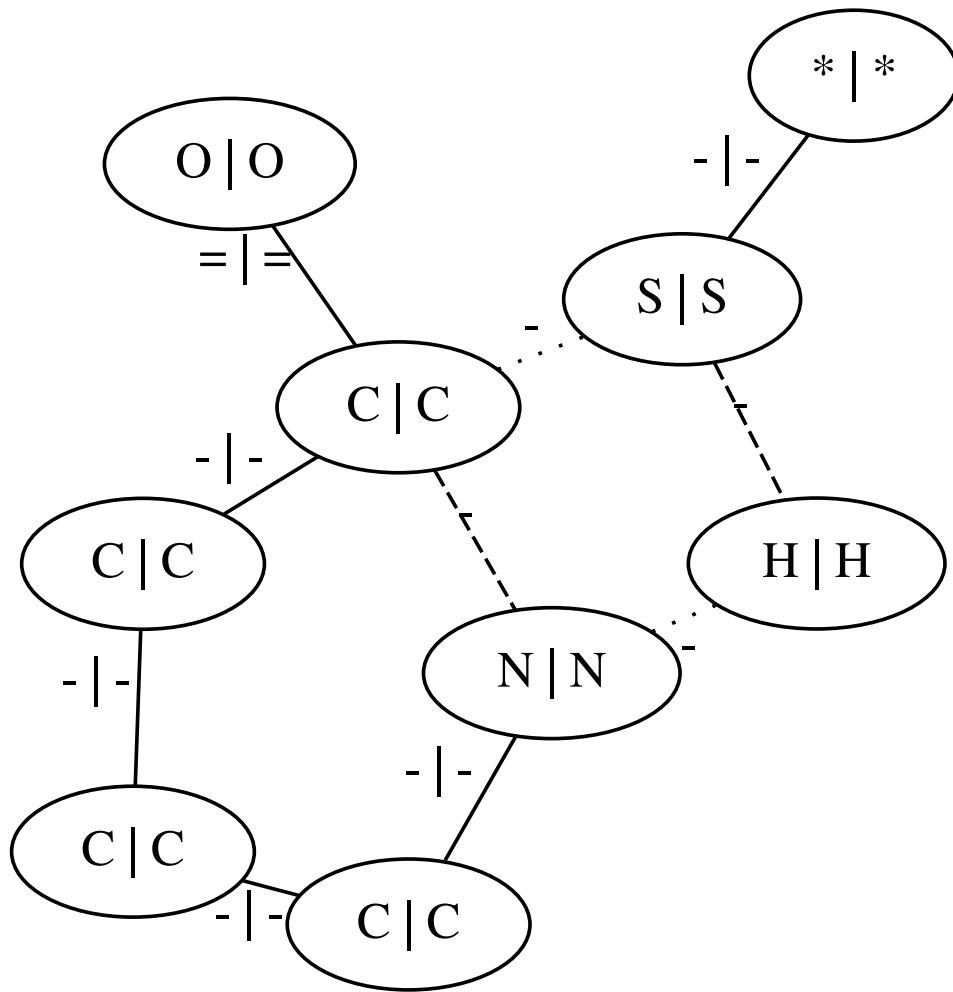


File: out/626_r_160_combined

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

1.0.158 Ring Closure 5 membered, inverse S, N

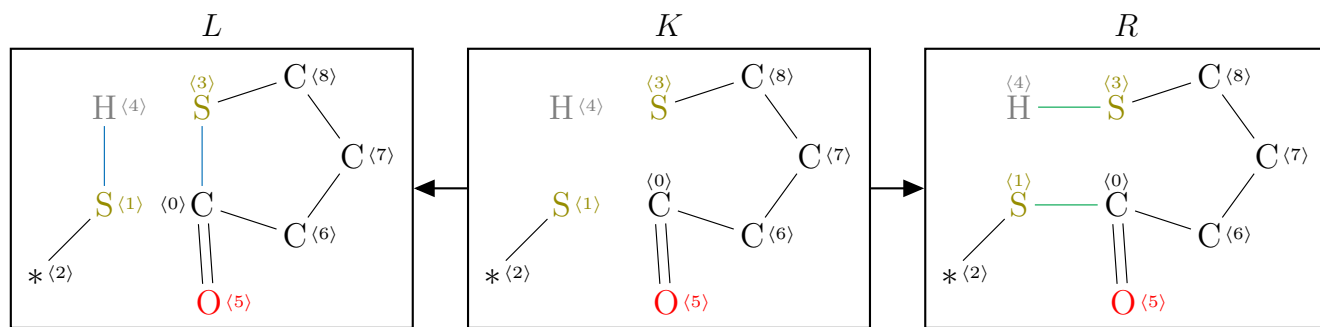




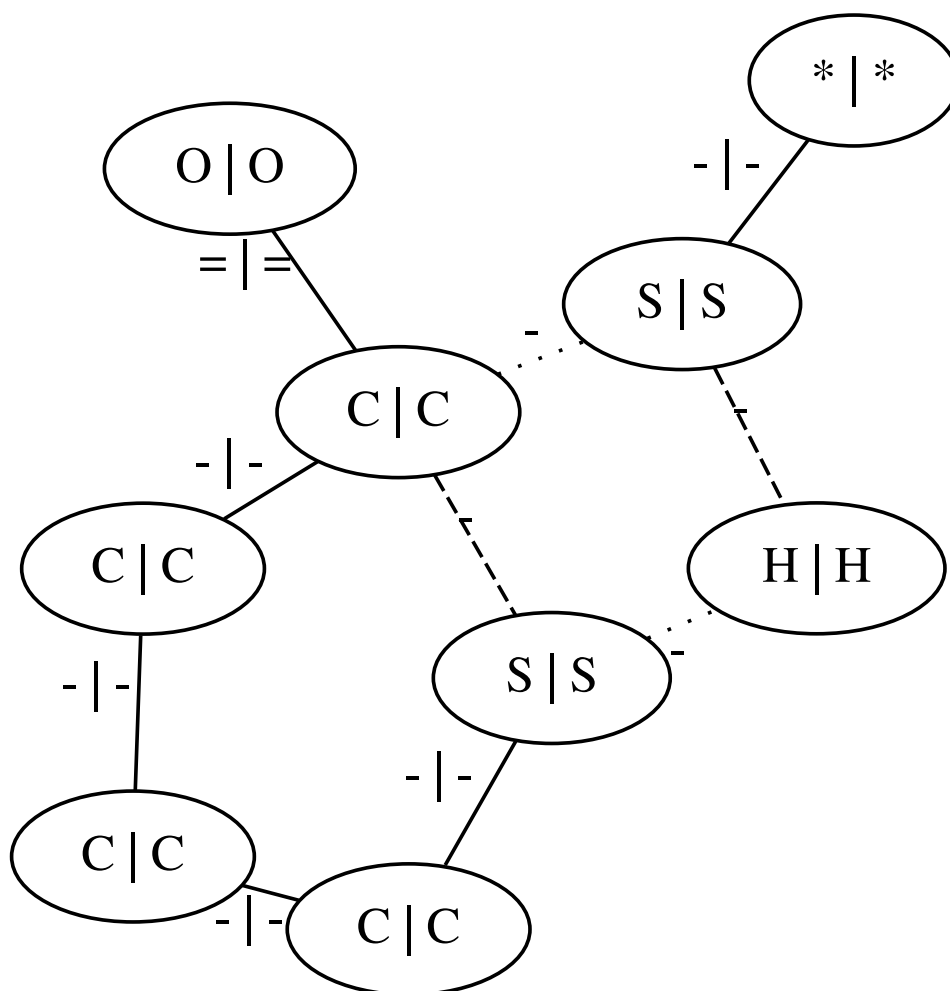
File: out/630_r_161_combined

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

1.0.159 Ring Closure 5 membered, inverse S, S



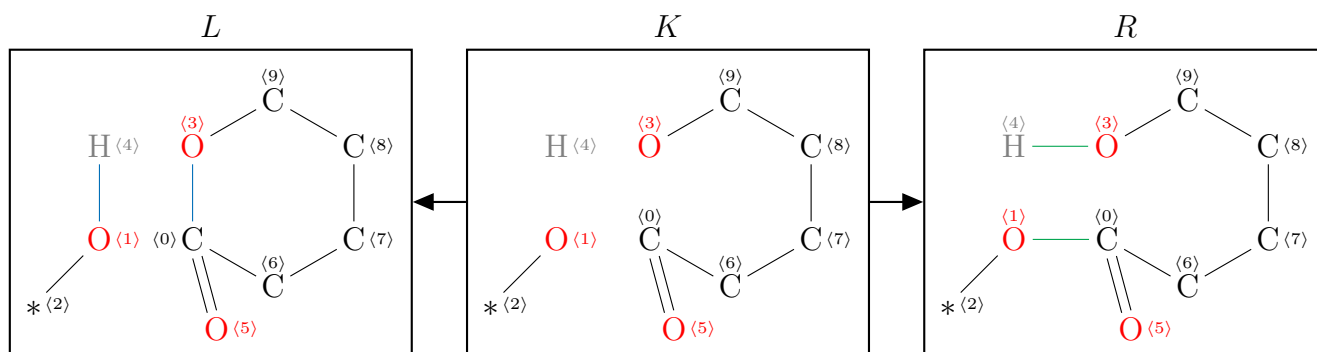
Files: out/633_r_162_10300110_{L, K, R}

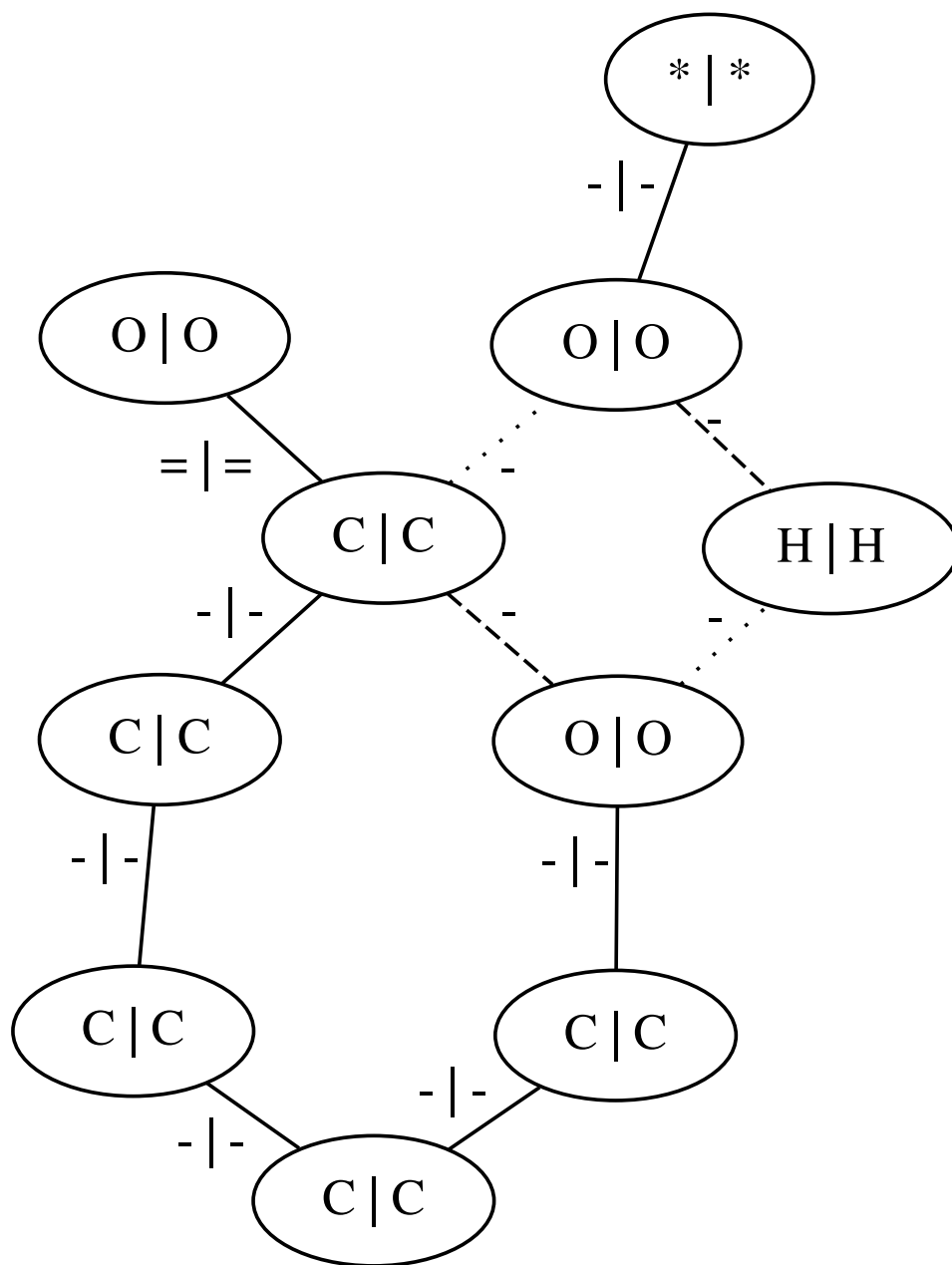


File: out/634_r_162_combined

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

1.0.160 Ring Closure 6 membered, inverse O, O



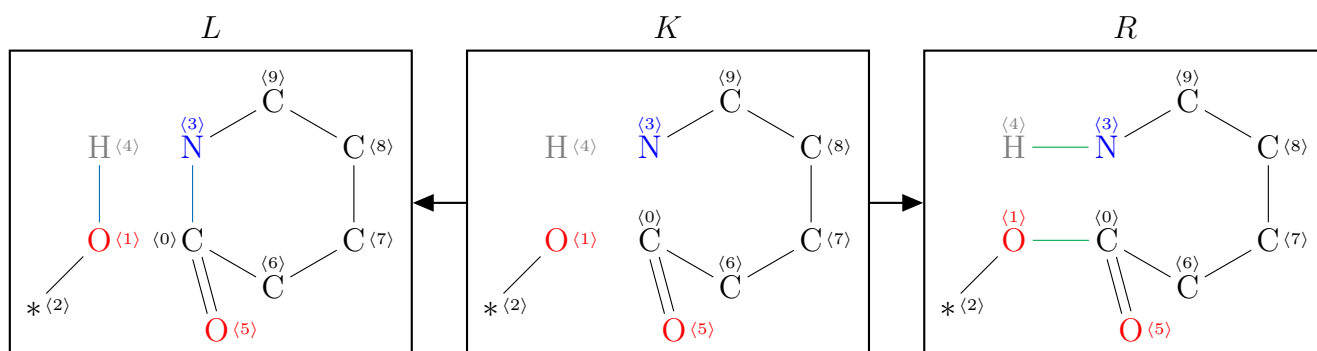


File: out/638_r_163_combined

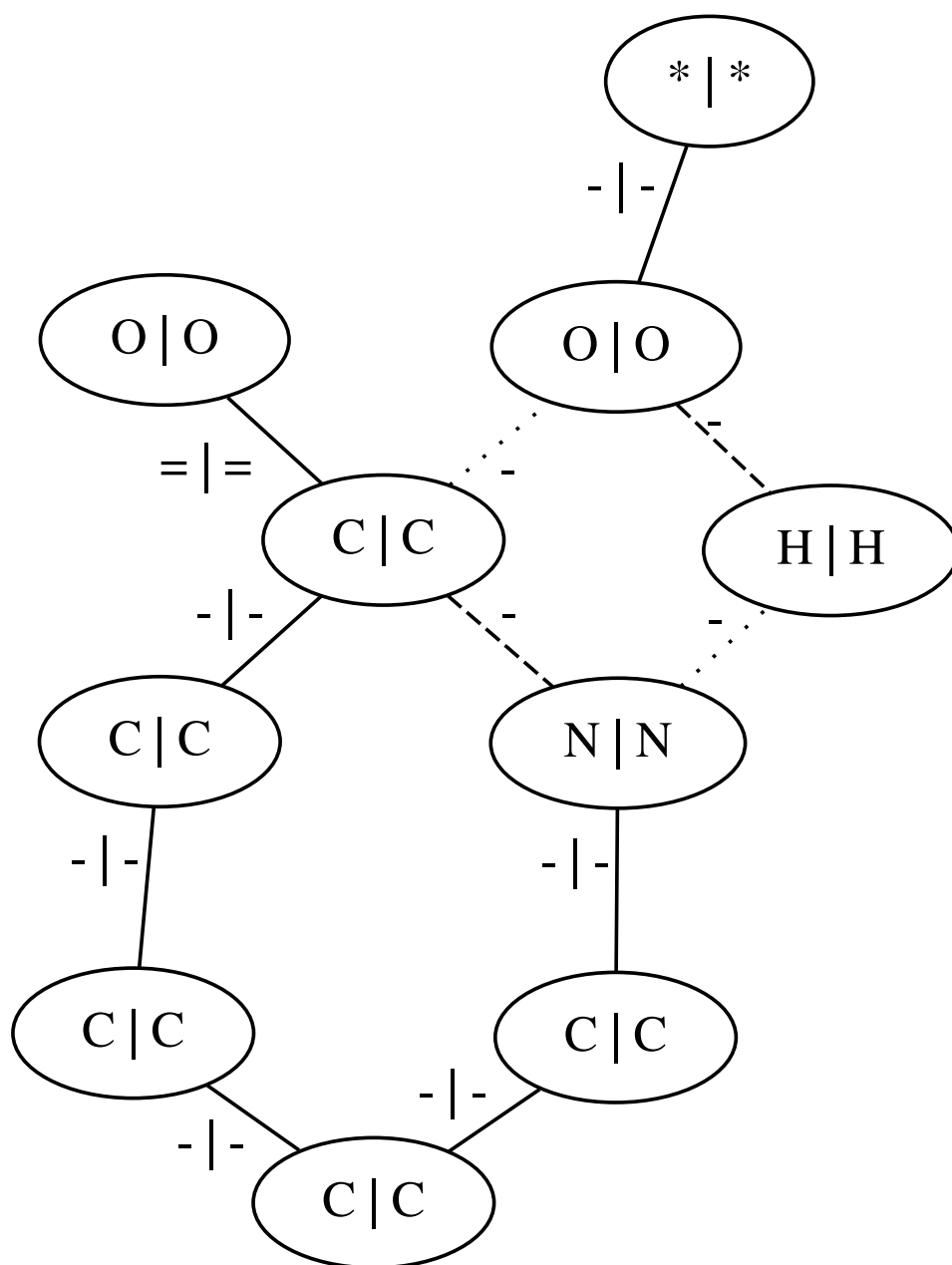
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'O'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid \leq 1
\end{aligned}$$

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

1.0.161 Ring Closure 6 membered, inverse O, N



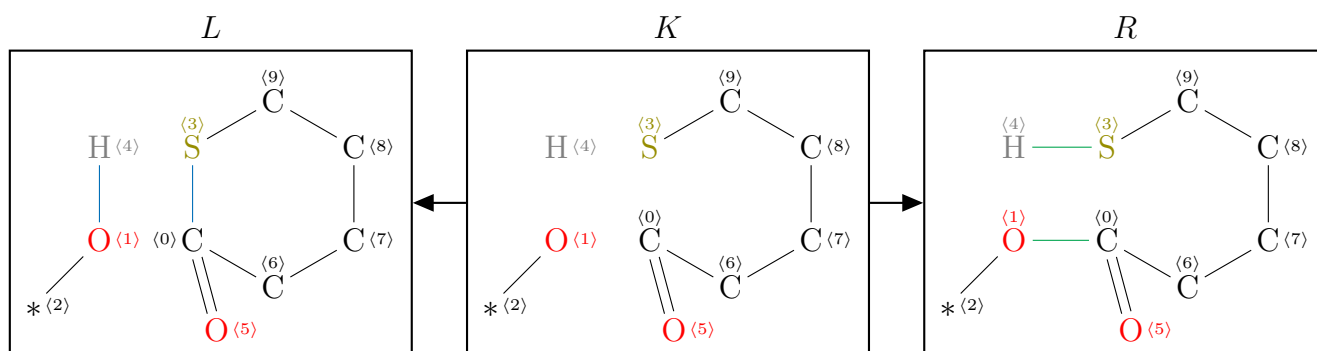
Files: out/641_r_164_10300110_{L, K, R}



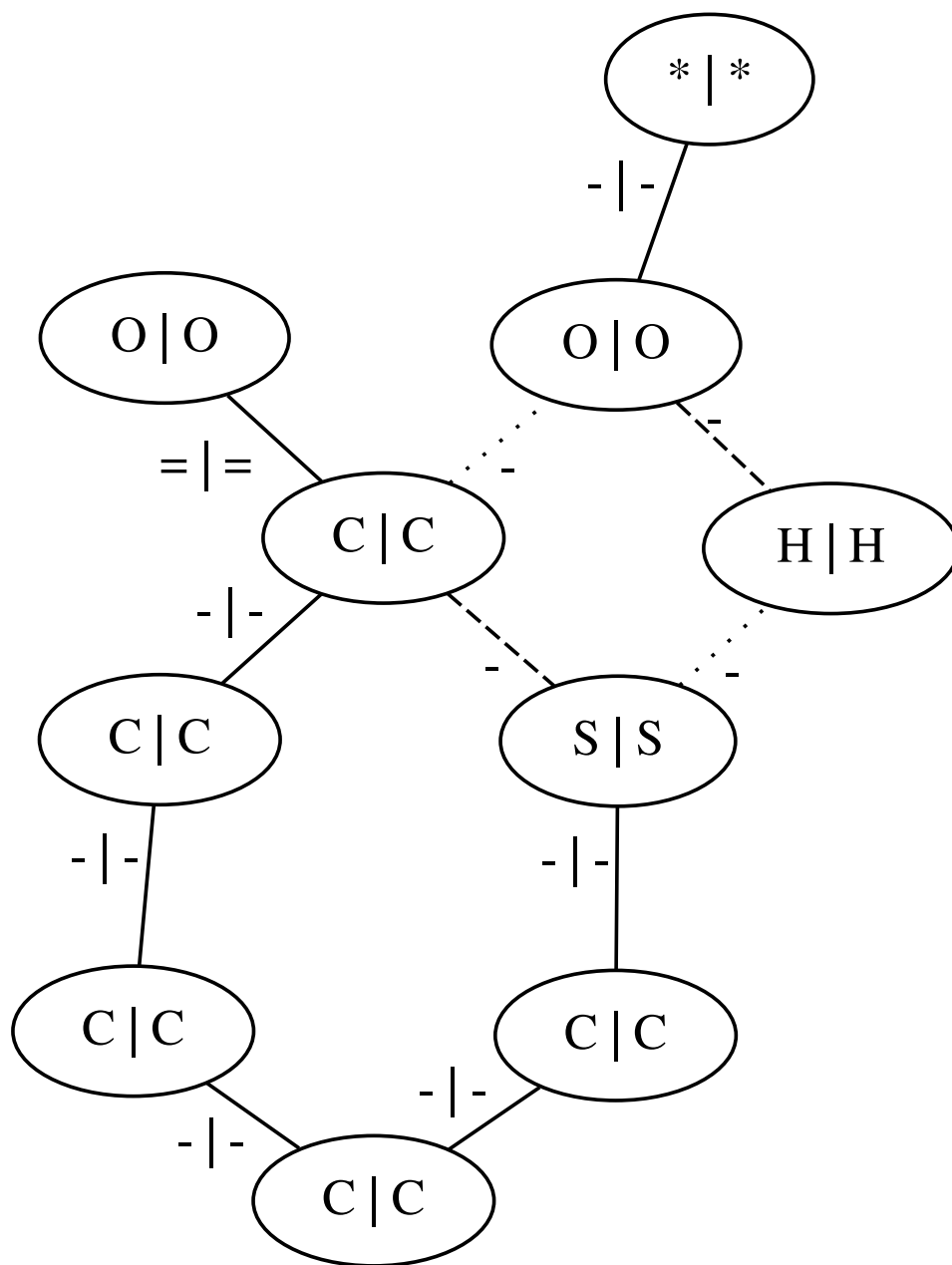
File: out/642_r_164_combined

$$\begin{aligned} & |\{e \in \text{outEdges}(9) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'-'}\} \\ & \quad \}| \leq 1 \end{aligned}$$
$$\begin{aligned} & |\{e \in \text{outEdges}(2) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'C'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'='}\} \\ & \quad \} | = 1 \end{aligned}$$

1.0.162 Ring Closure 6 membered, inverse O, S



Files: out/645_r_165_10300110_{L, K, R}

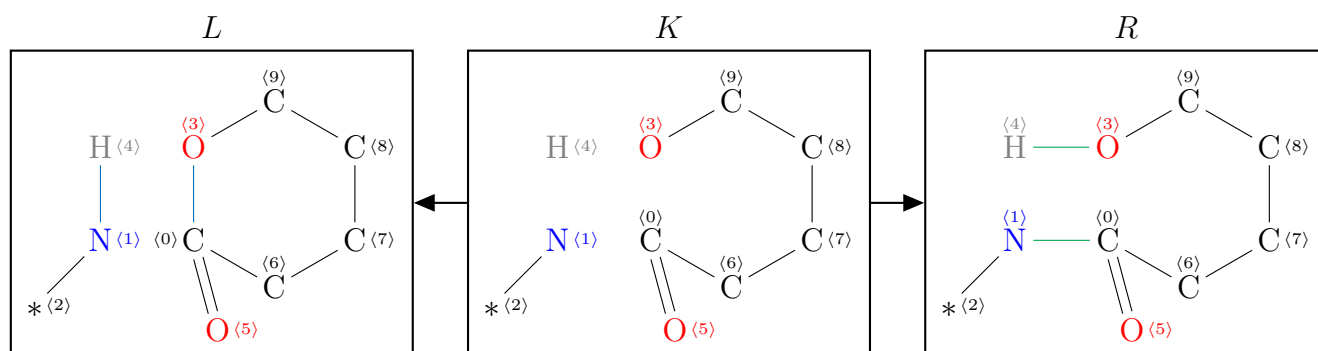


File: out/646_r_165_combined

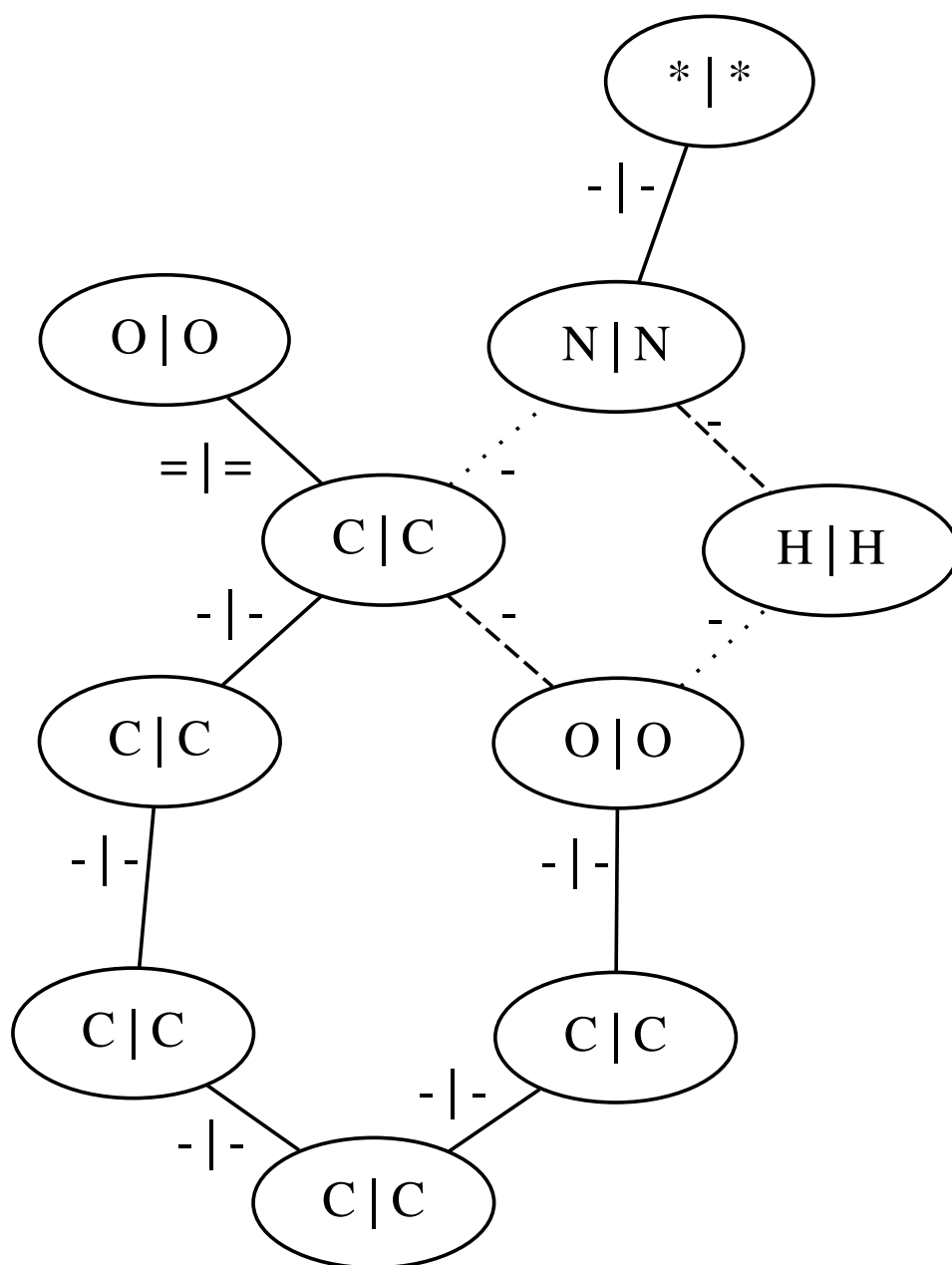
$$\begin{aligned}
& |\{e \in \text{outEdges}(9) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid \leq 1
\end{aligned}$$

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

1.0.163 Ring Closure 6 membered, inverse N, O



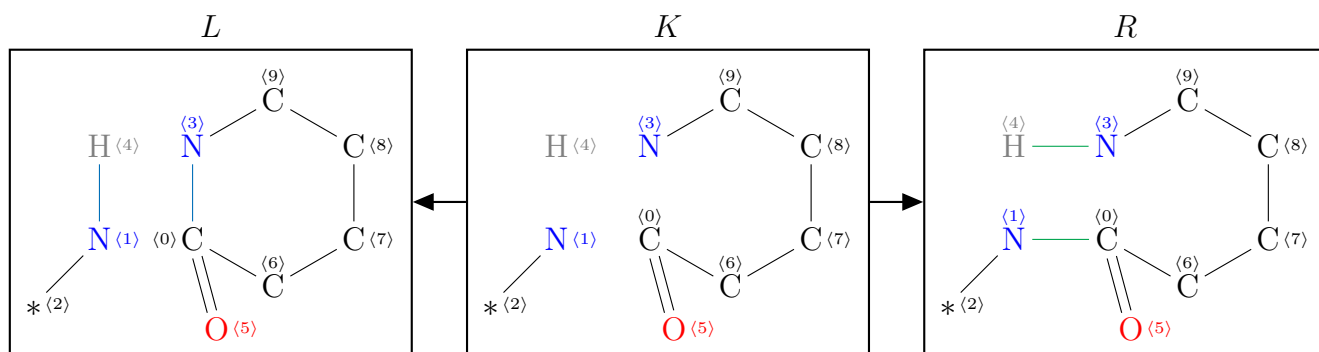
Files: out/649_r_166_10300110_{L, K, R}

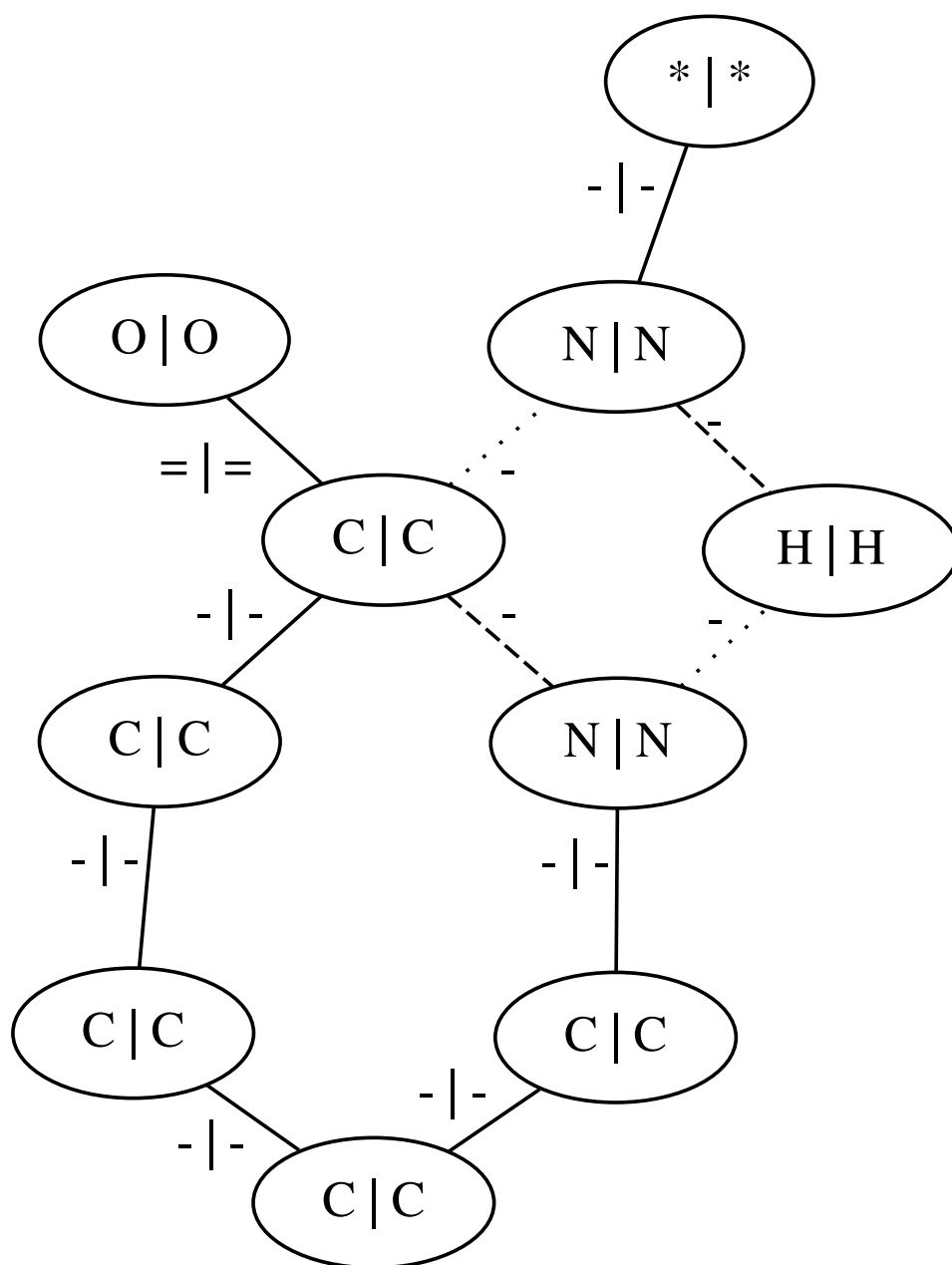


File: out/650_r_166_combined

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

1.0.164 Ring Closure 6 membered, inverse N, N

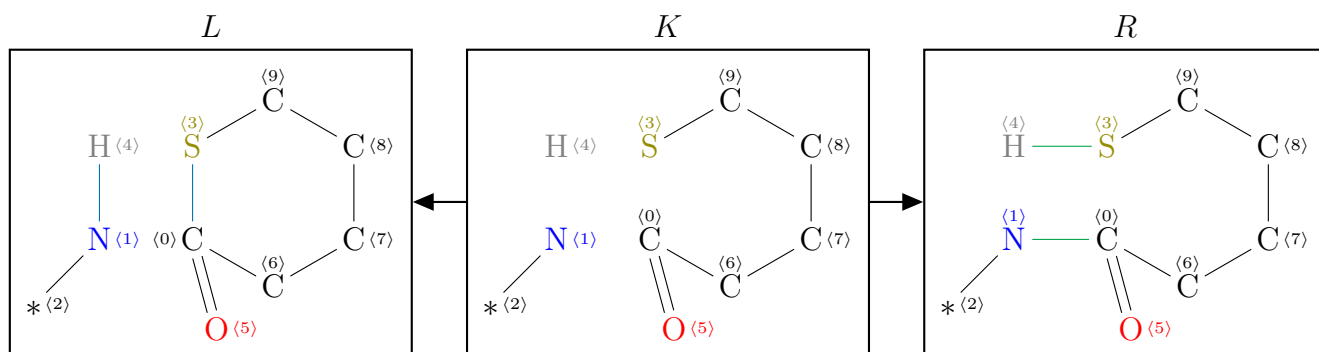


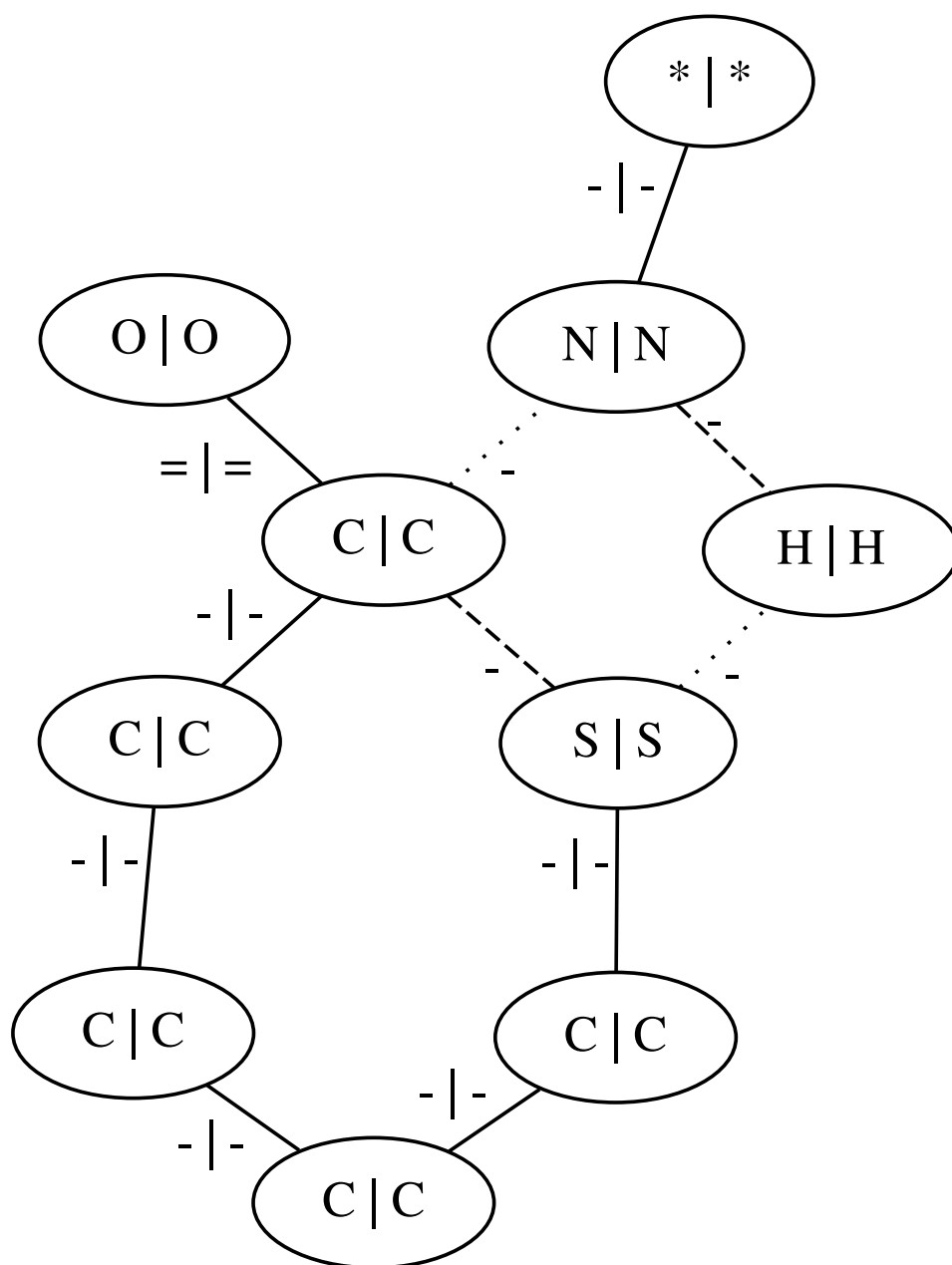


File: out/654_r_167_combined

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

1.0.165 Ring Closure 6 membered, inverse N, S

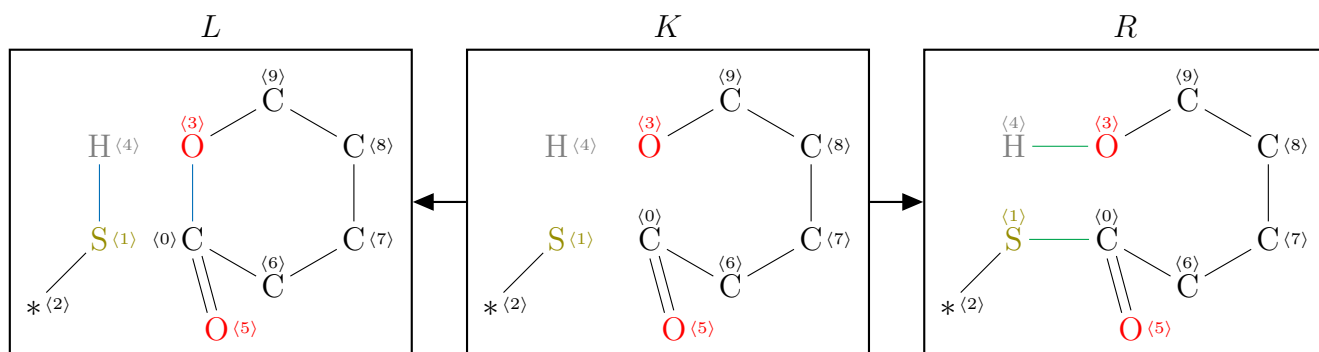




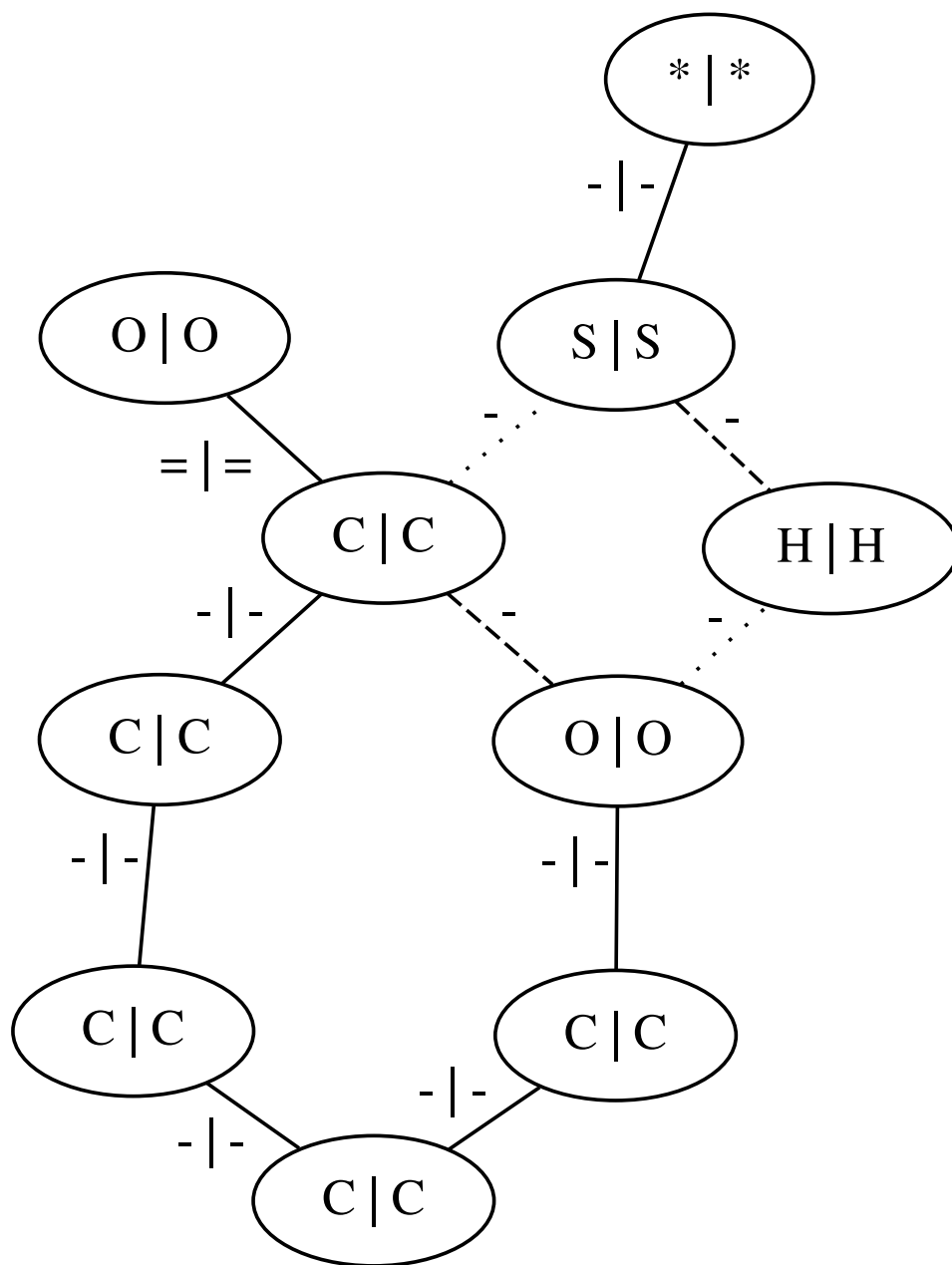
File: out/658_r_168_combined

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

1.0.166 Ring Closure 6 membered, inverse S, O



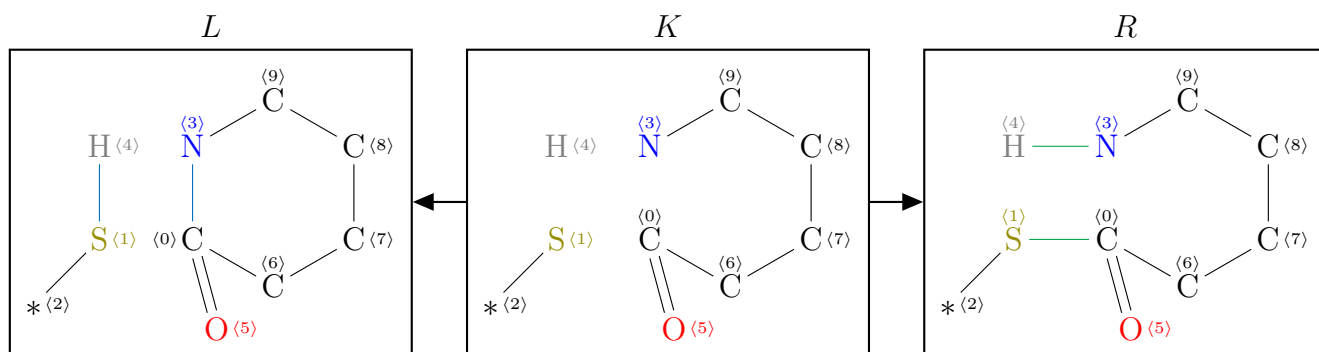
Files: out/661_r_169_10300110_{L, K, R}



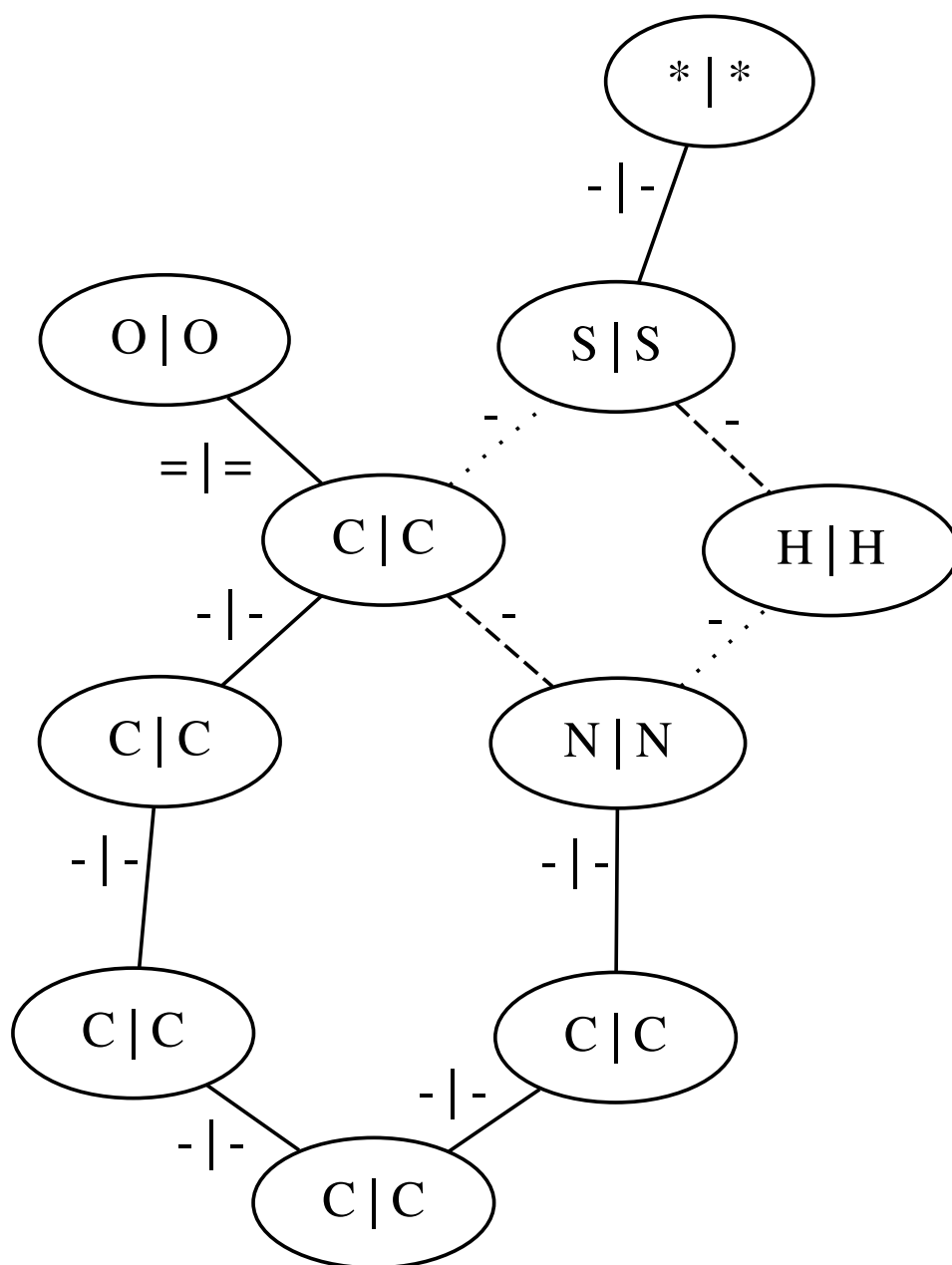
File: out/662_r_169_combined

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

1.0.167 Ring Closure 6 membered, inverse S, N



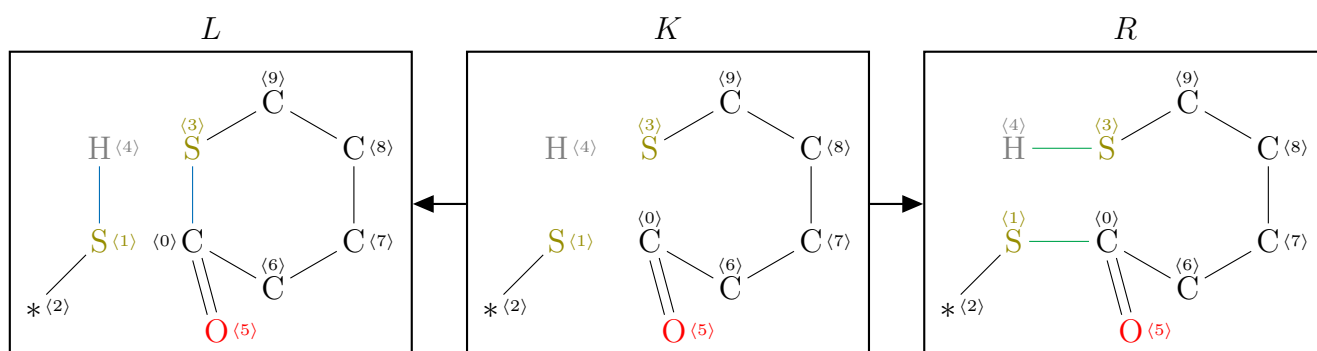
Files: out/665_r_170_10300110_{L, K, R}

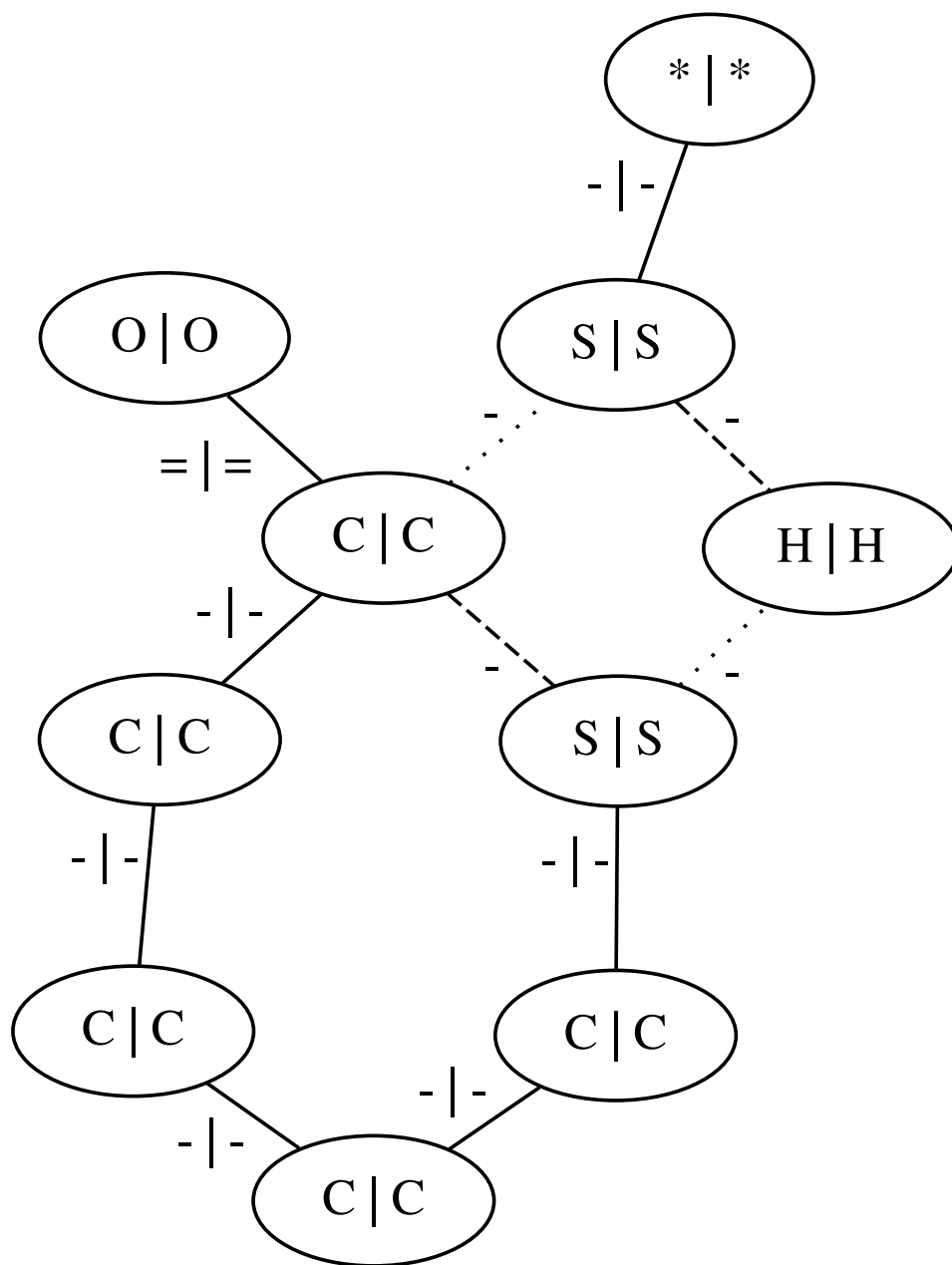


File: out/666_r_170_combined

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

1.0.168 Ring Closure 6 membered, inverse S, S

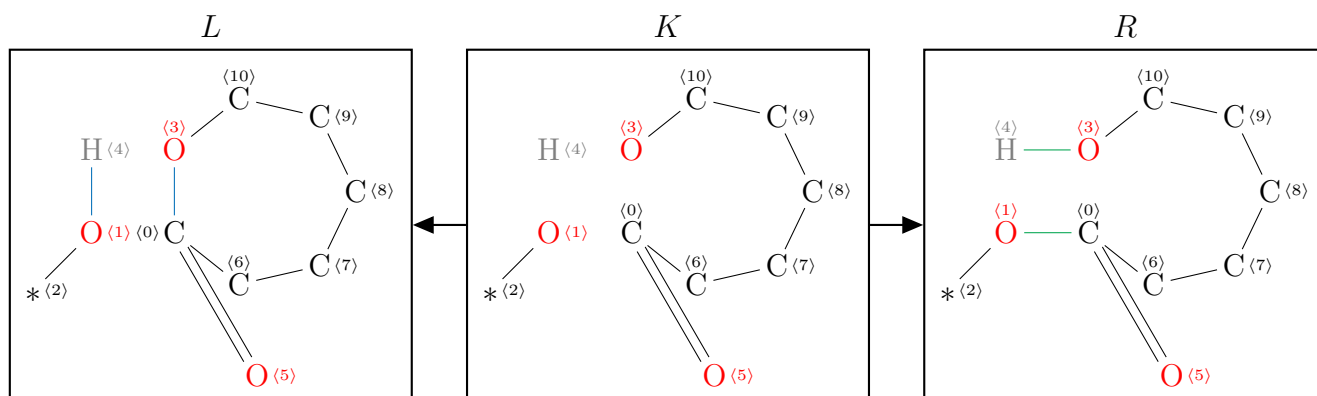




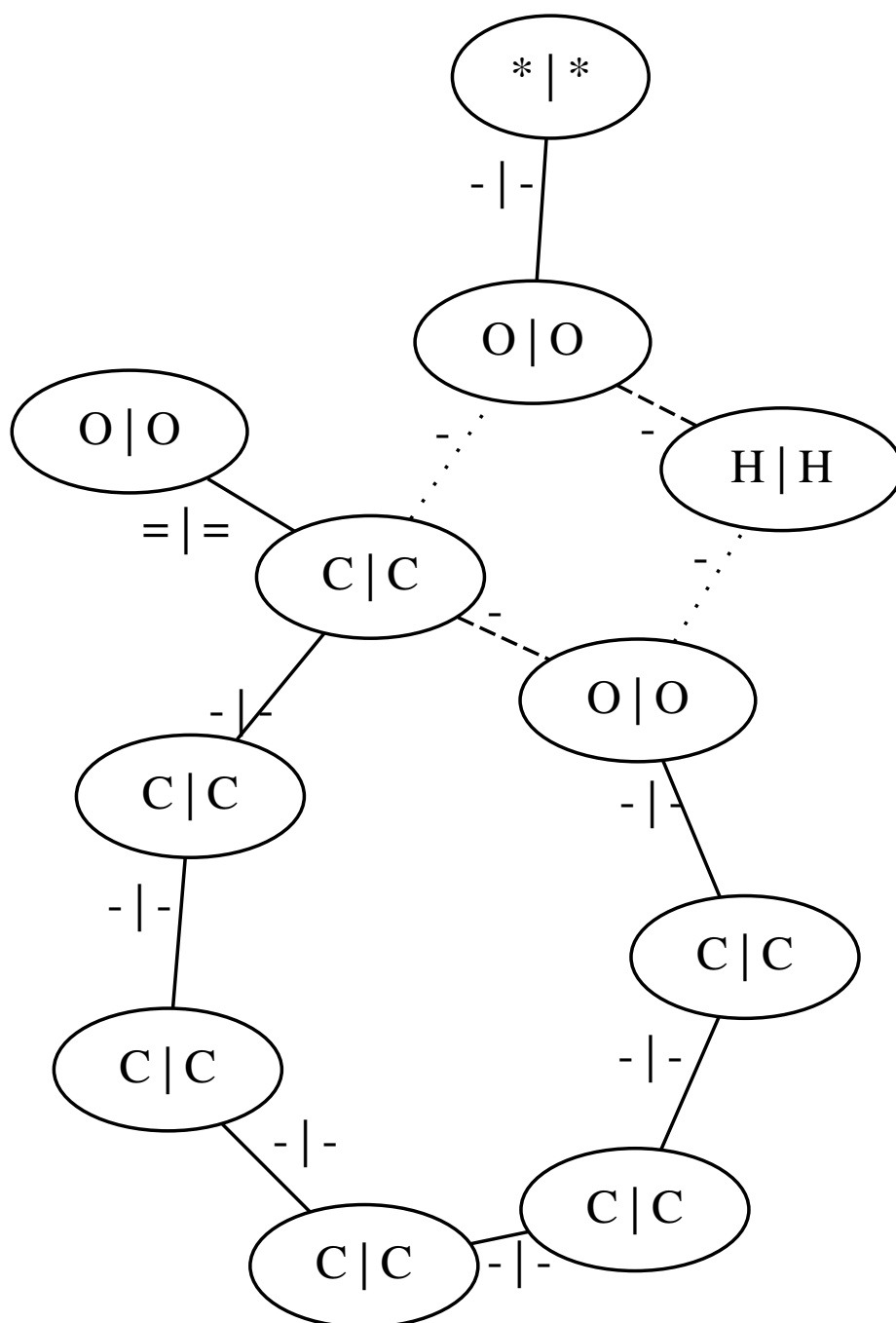
File: out/670_r_171_combined

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

1.0.169 Ring Closure 7 membered, inverse O, O



Files: out/673_r_172_10300110_{L, K, R}

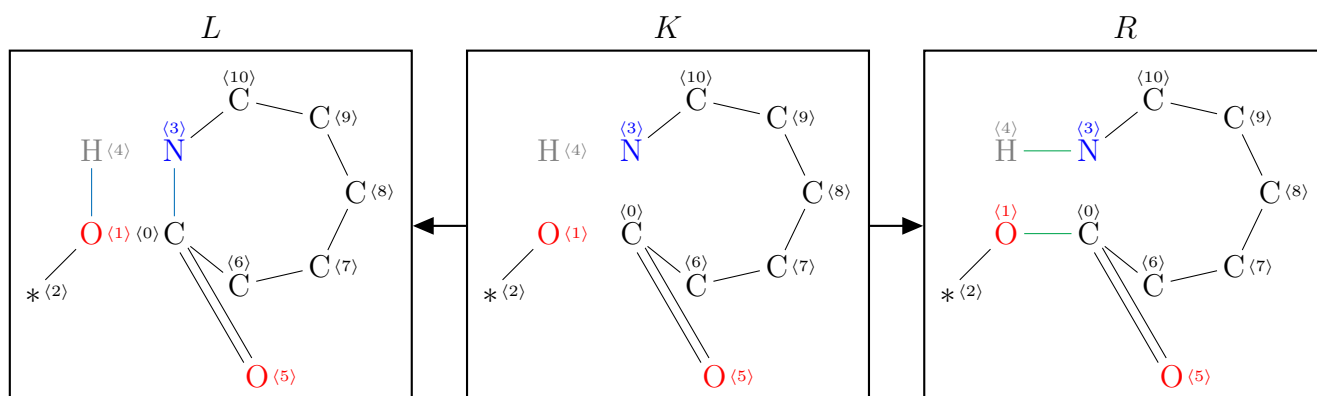


File: out/674_r_172_combined

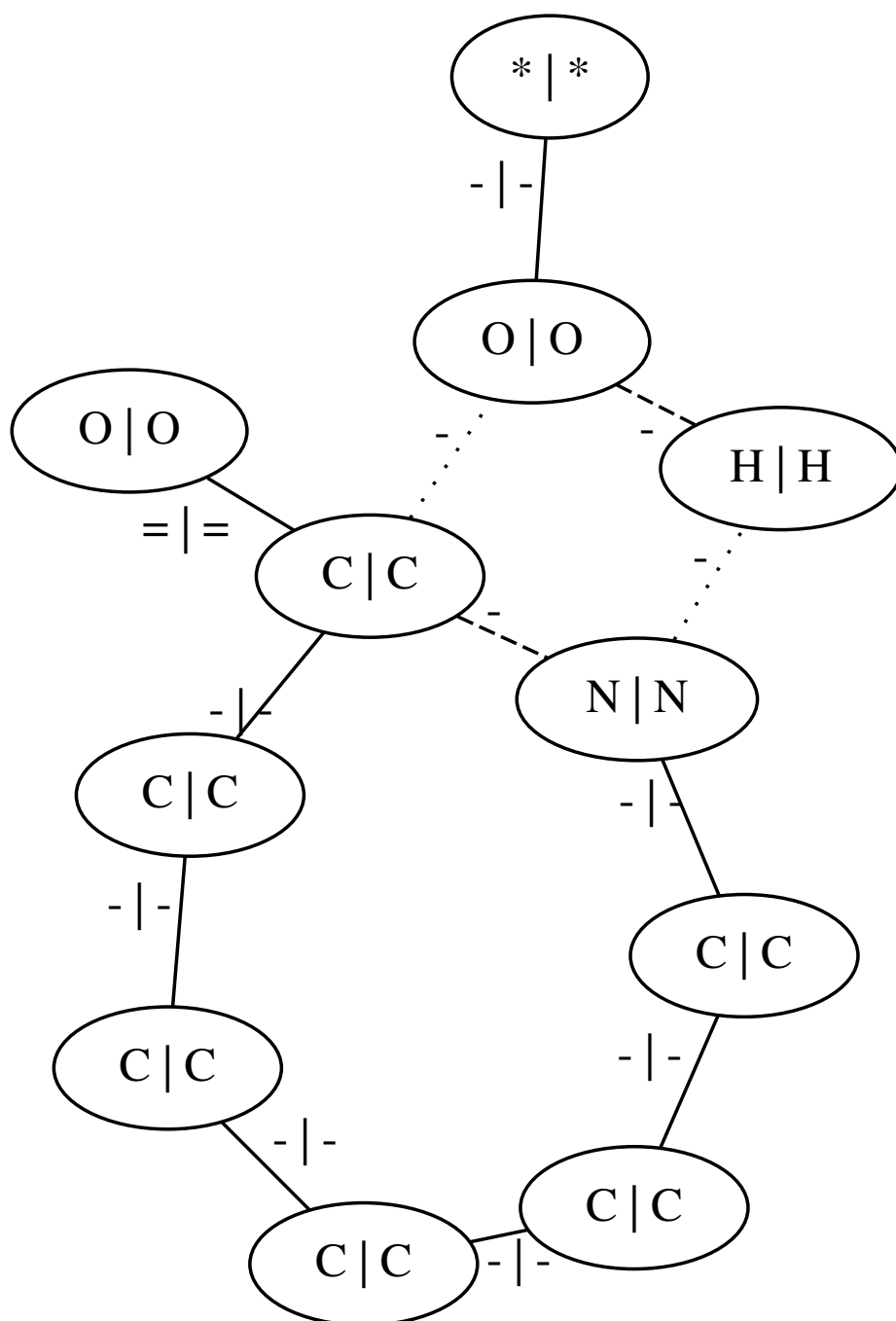
$$\begin{aligned} & |\{e \in \text{outEdges}(10) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'-'}\} \\ & \} | \leq 1 \end{aligned}$$

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

1.0.170 Ring Closure 7 membered, inverse O, N



Files: out/677_r_173_10300110_{L, K, R}

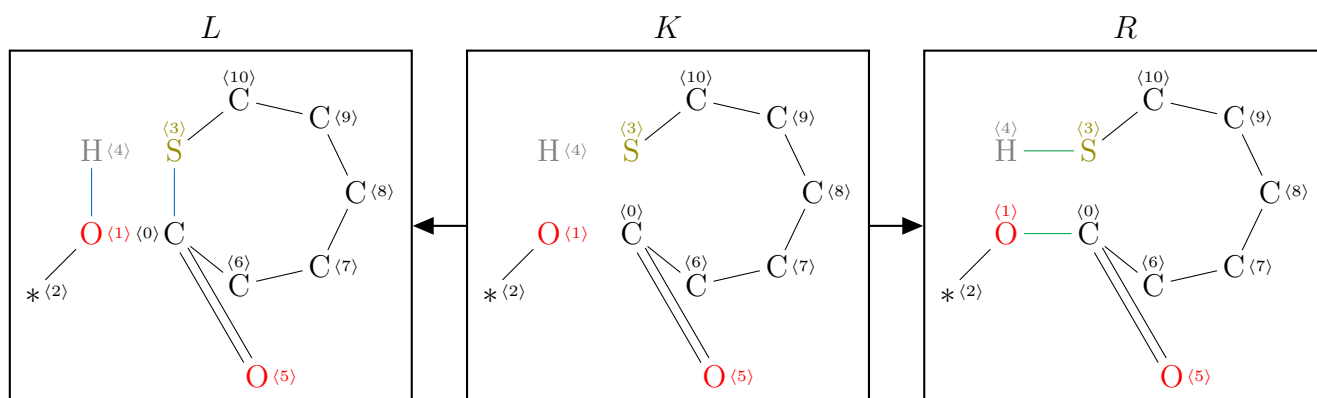


File: out/678_r_173_combined

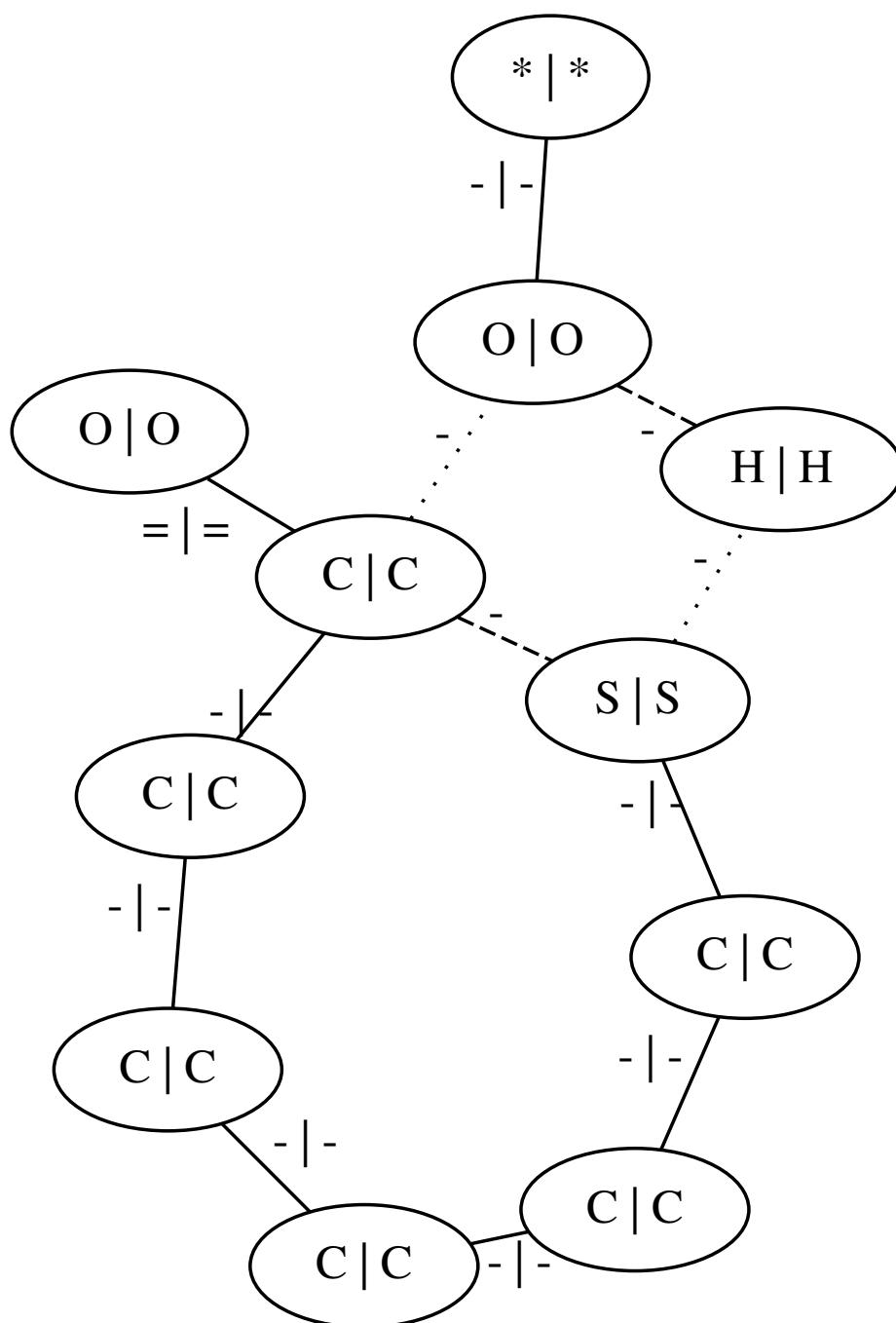
$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| \leq 1
\end{aligned}$$

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

1.0.171 Ring Closure 7 membered, inverse O, S



Files: out/681_r_174_10300110_{L, K, R}

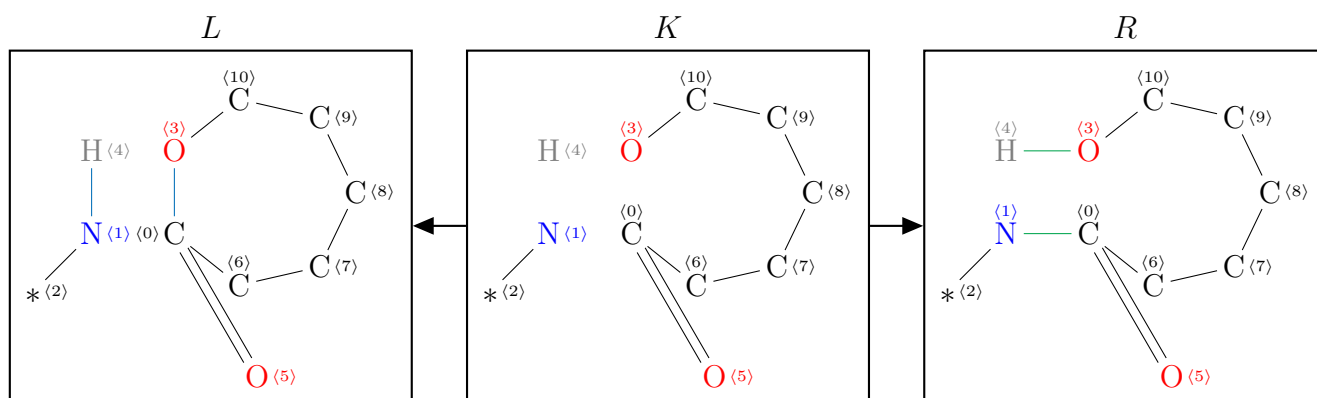


File: out/682_r_174_combined

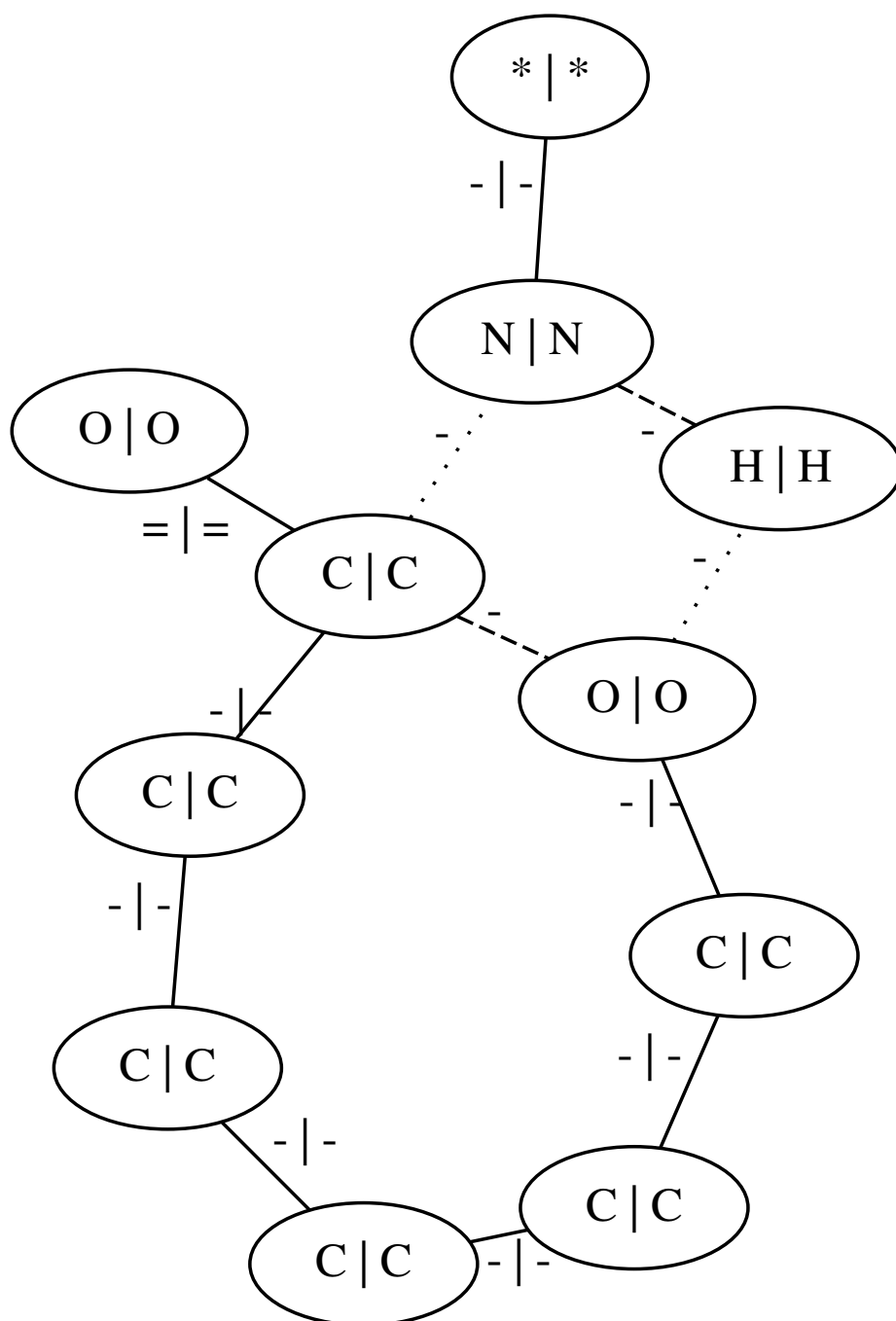
$$\begin{aligned}
& |\{e \in \text{outEdges}(10) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'S'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}\mid \leq 1
\end{aligned}$$

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

1.0.172 Ring Closure 7 membered, inverse N, O



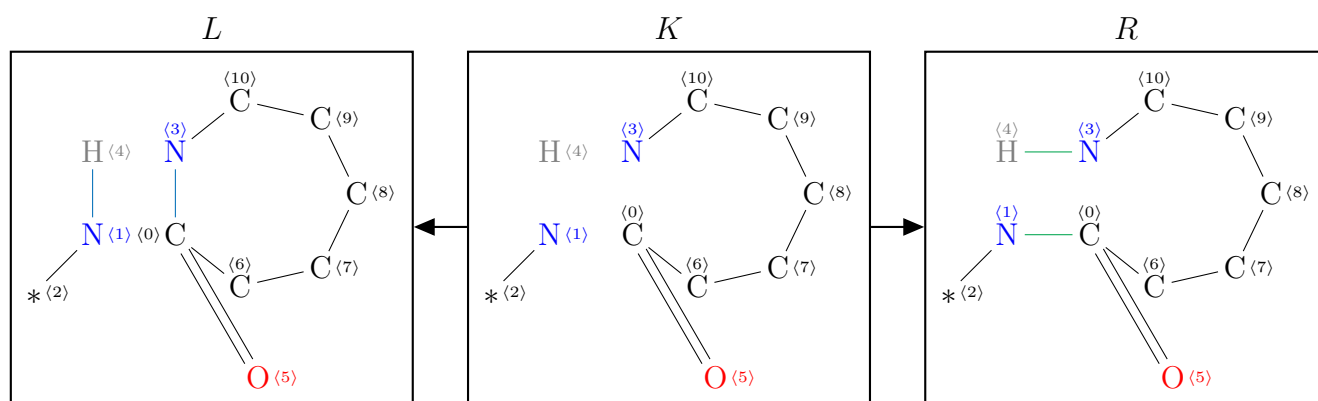
Files: out/685_r_175_10300110_{L, K, R}

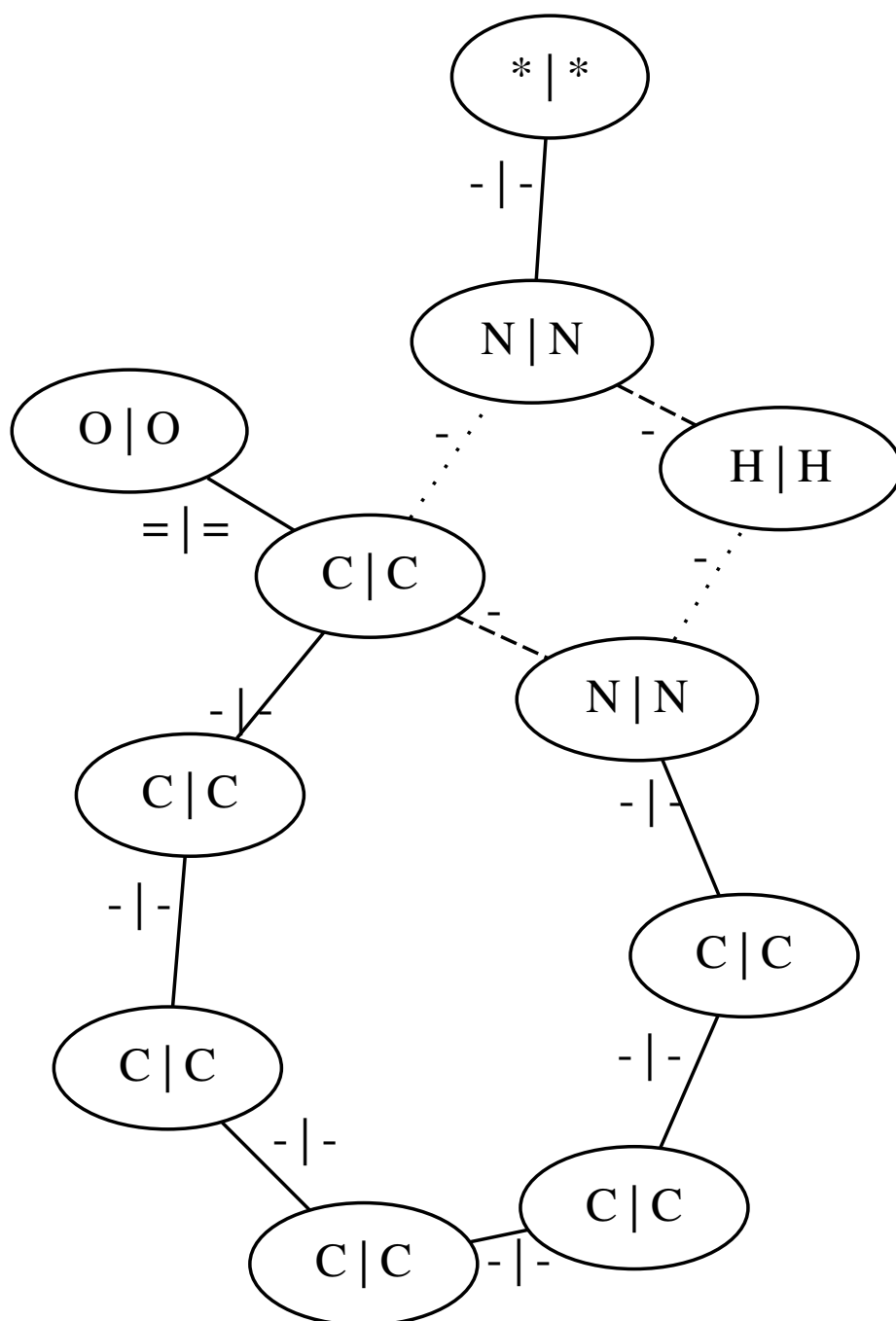


File: out/686_r_175_combined

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

1.0.173 Ring Closure 7 membered, inverse N, N

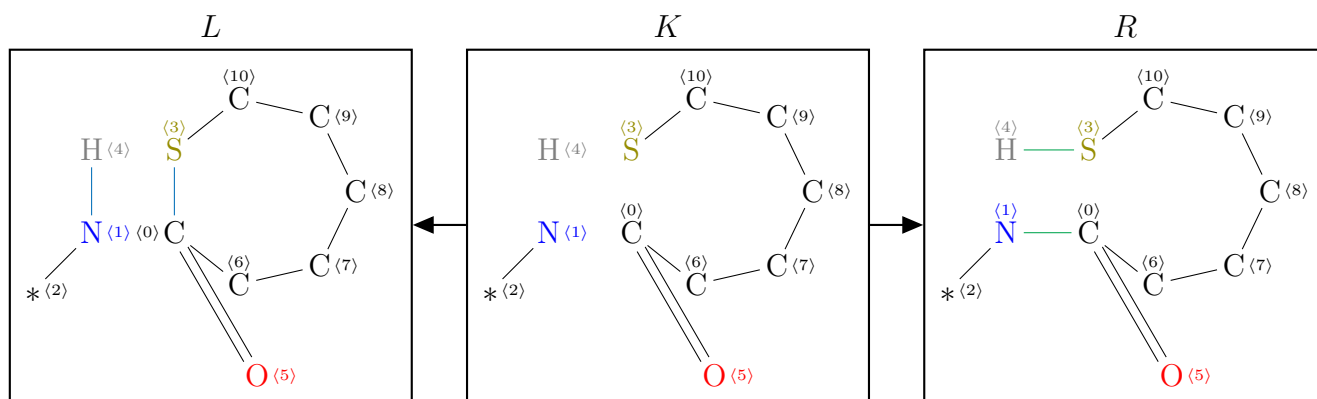




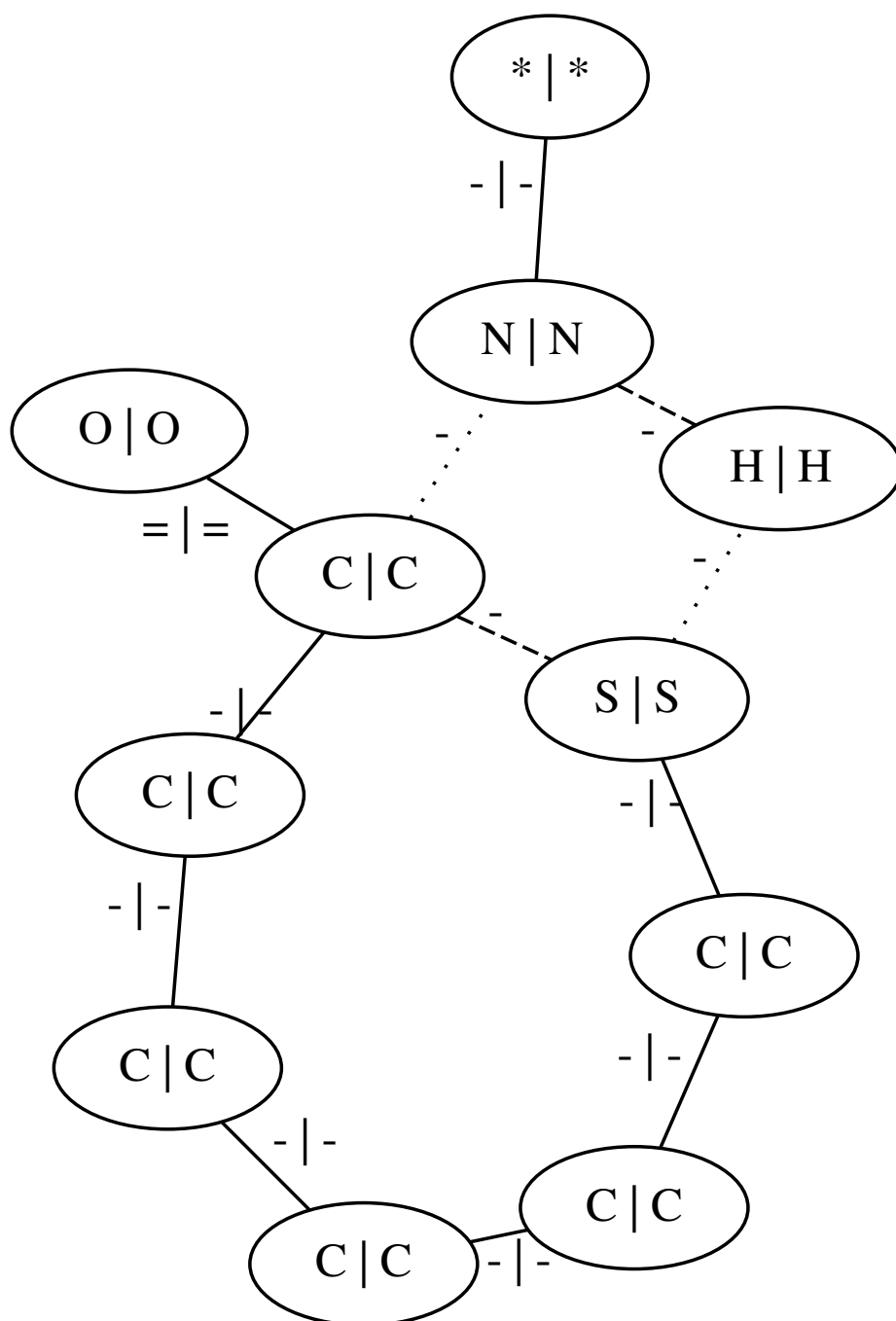
File: out/690_r_176_combined

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

1.0.174 Ring Closure 7 membered, inverse N, S



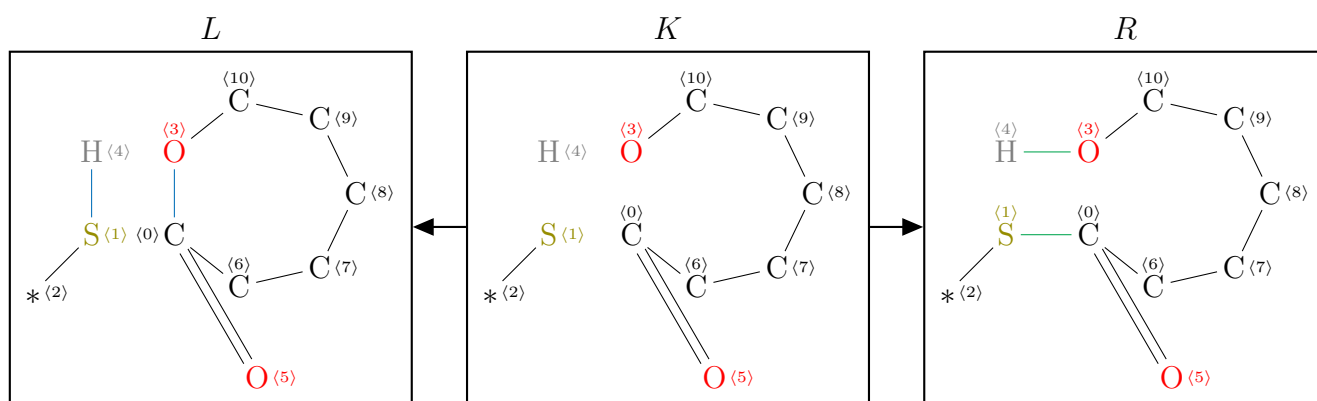
Files: out/693_r_177_10300110_{L, K, R}

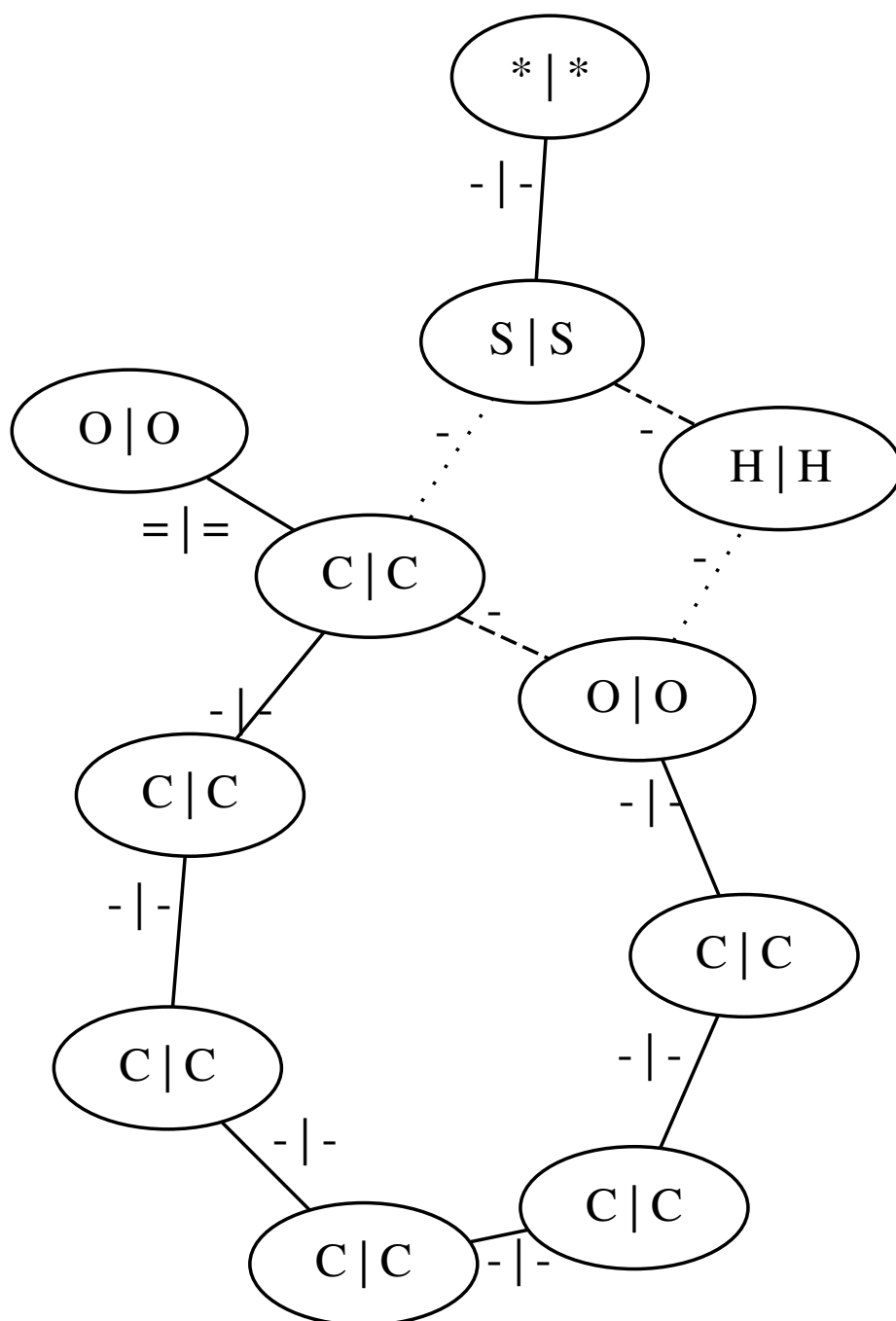


File: out/694_r_177_combined

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

1.0.175 Ring Closure 7 membered, inverse S, O

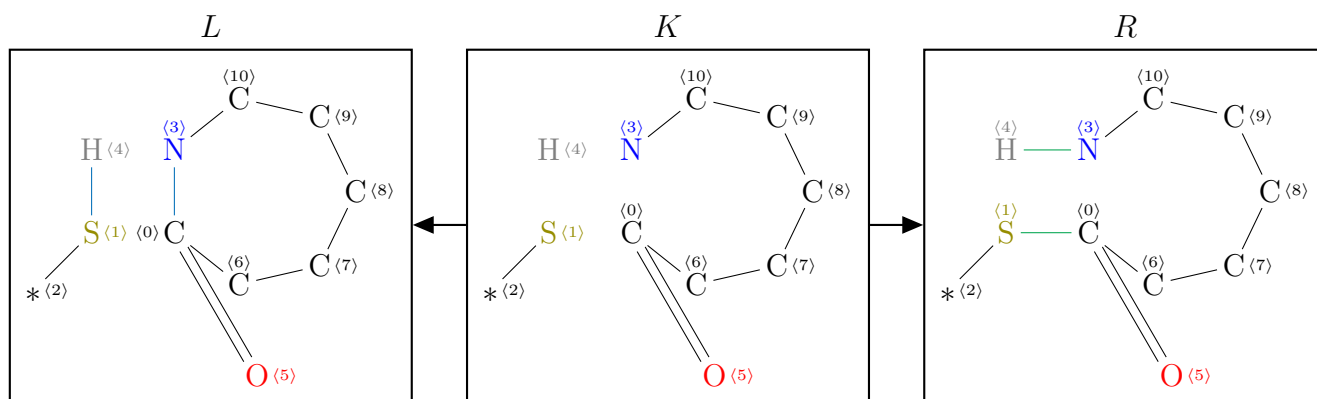




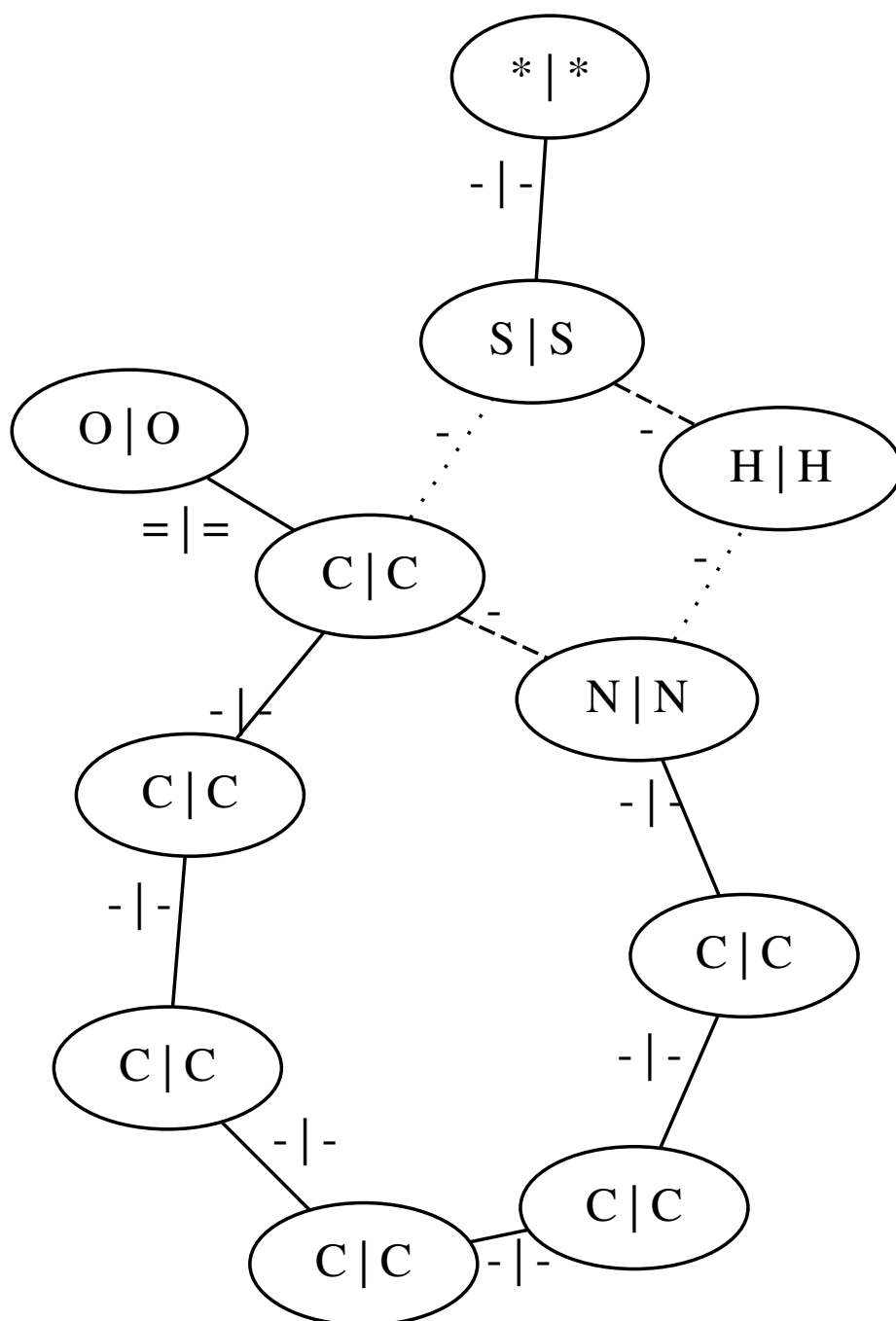
File: out/698_r_178_combined

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

1.0.176 Ring Closure 7 membered, inverse S, N



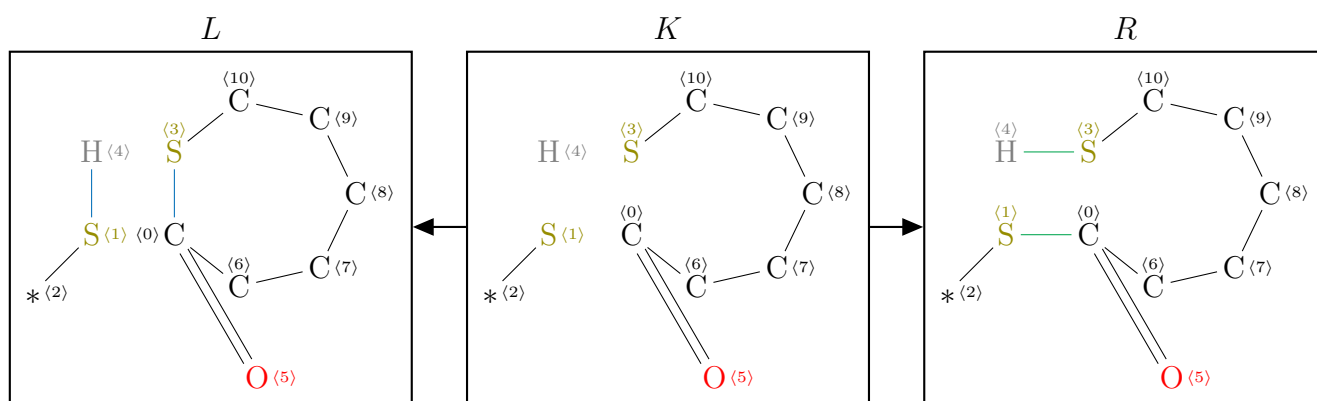
Files: out/701_r_179_10300110_{L, K, R}

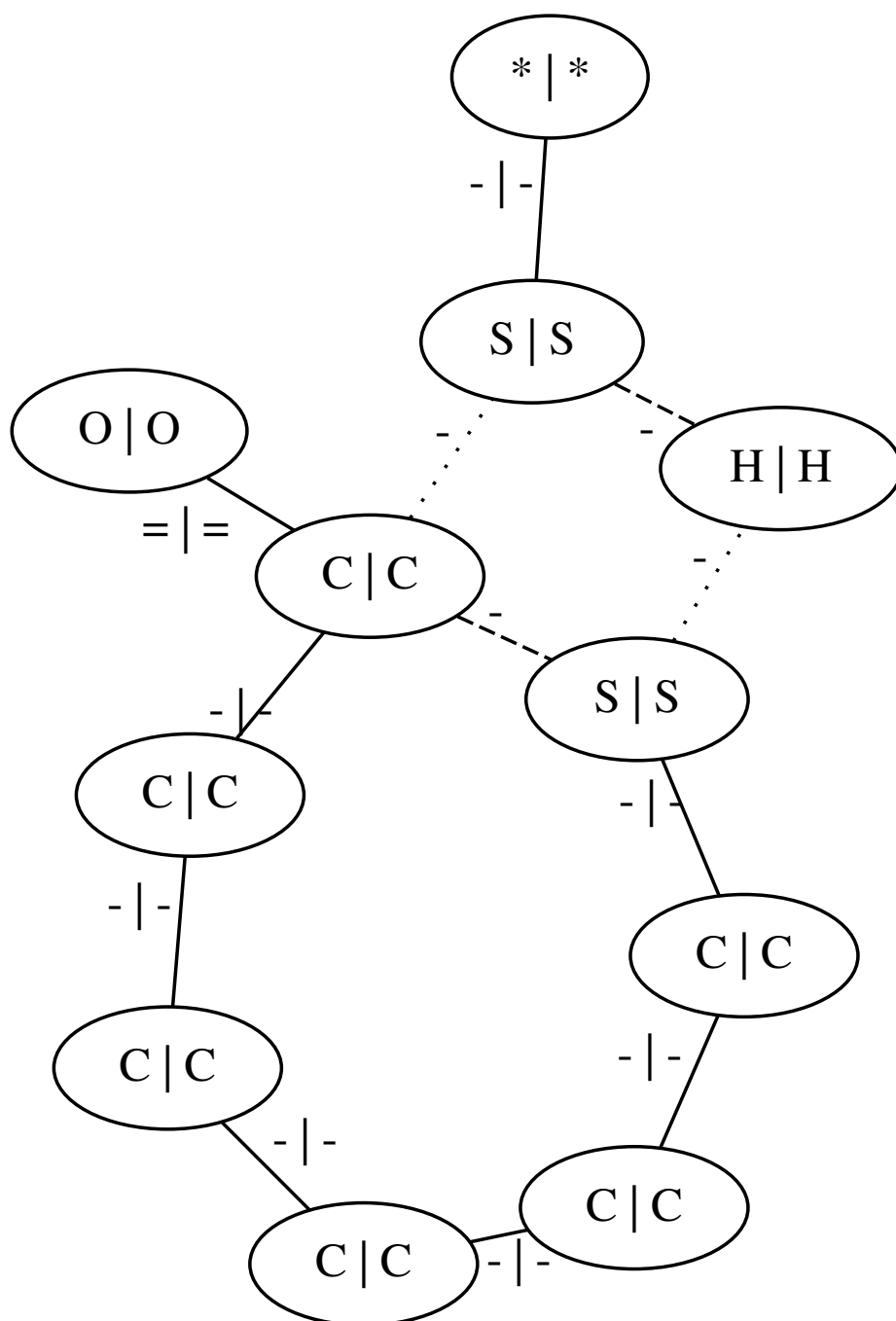


File: out/702_r_179_combined

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

1.0.177 Ring Closure 7 membered, inverse S, S

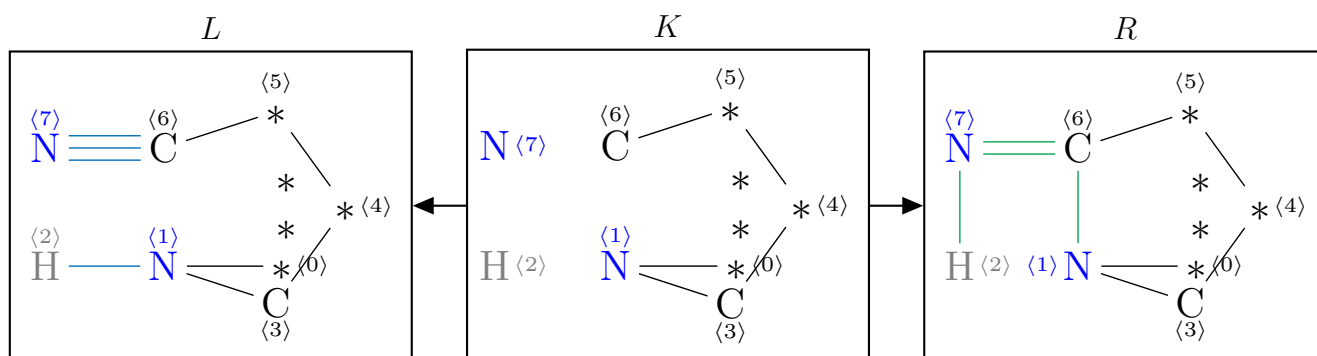




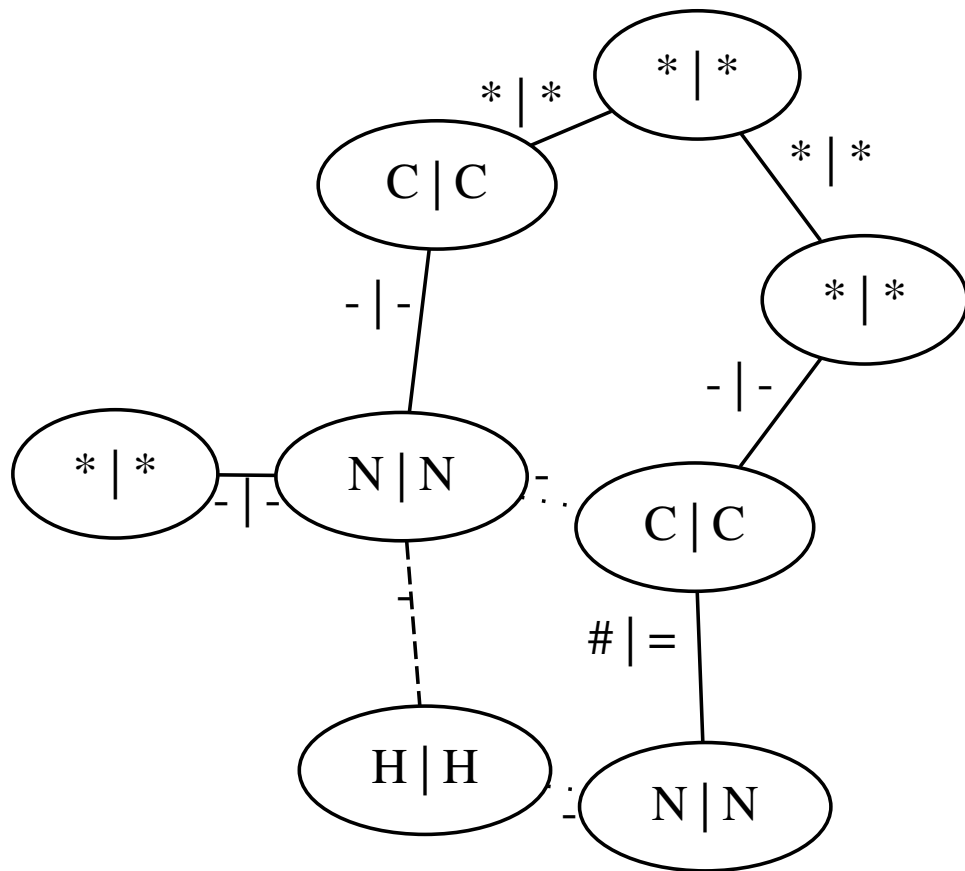
File: out/706_r_180_combined

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

1.0.178 Amine Nitrile Ring Closure 5



Files: out/709_r_181_10300110_{L, K, R}



File: out/710_r_181_combined

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

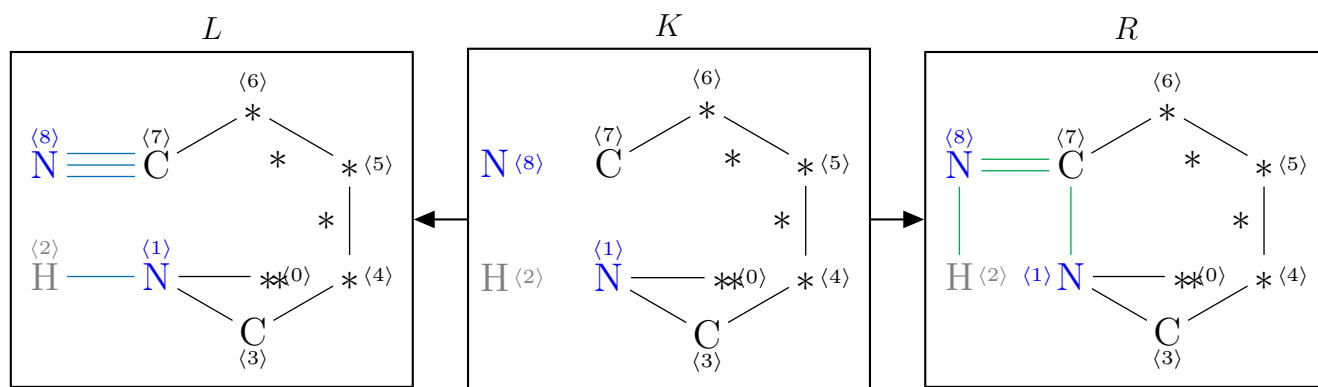
$$\text{label}(\text{target}(e)) \in \{\text{'O'}, \text{'N'}\}$$

$$\wedge$$

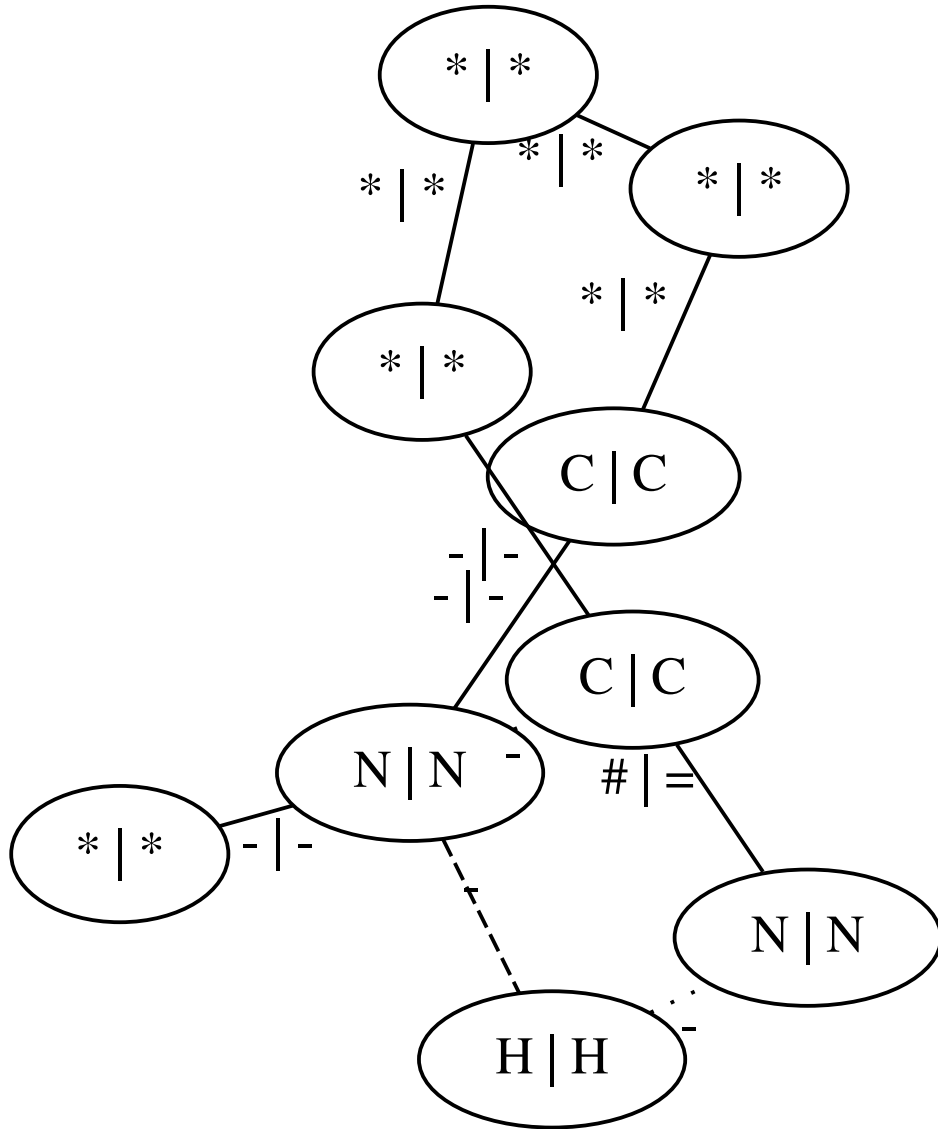
$$\text{label}(e) \in \{\text{'='}, \text{'-'}\}$$

$$\} = 1$$

1.0.179 Amine Nitrile Ring Closure 6



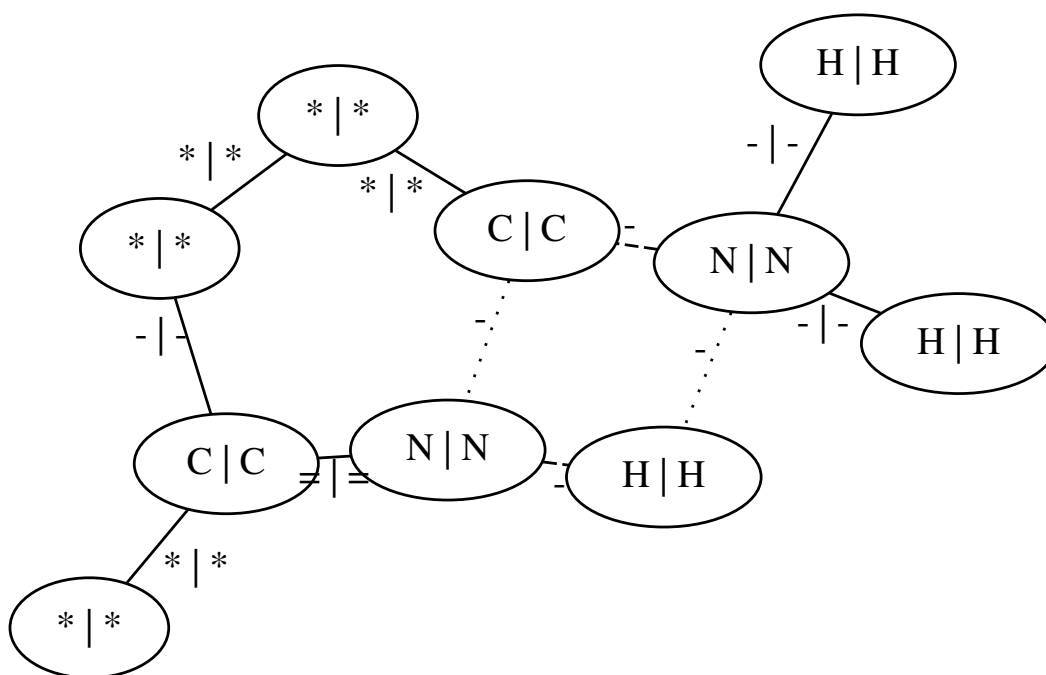
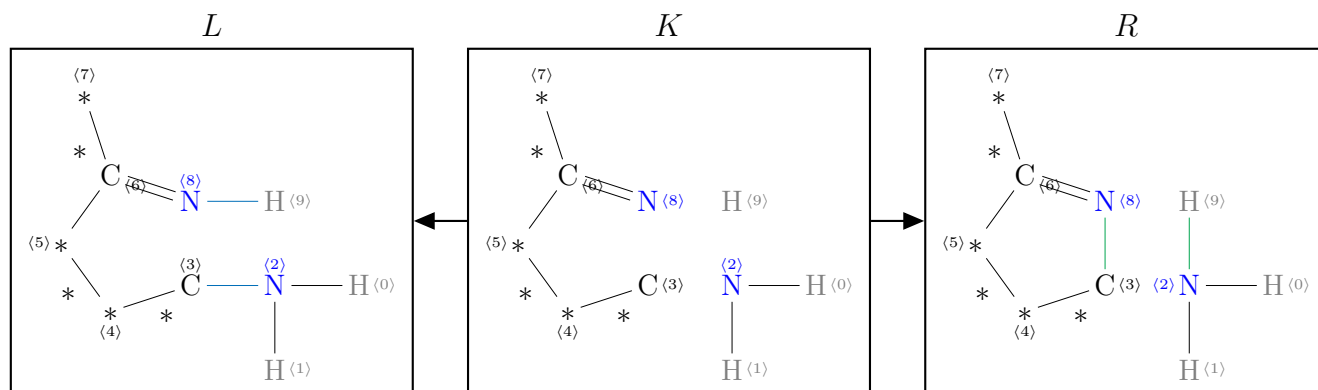
Files: out/713_r_182_10300110_{L, K, R}



File: out/714_r_182_combined

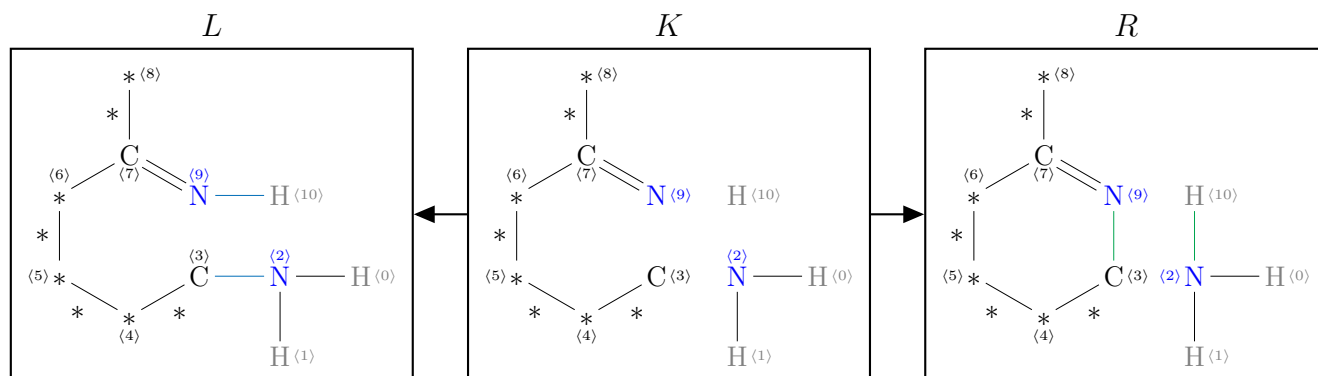
$|\{e \in \text{outEdges}(0) \mid$
 $\text{label}(\text{target}(e)) \in \{'0', 'N'\}$
 \wedge
 $\text{label}(e) \in \{ '=', '- \}$
 $\} = 1$

1.0.180 Amine Imine Ring Closure 5

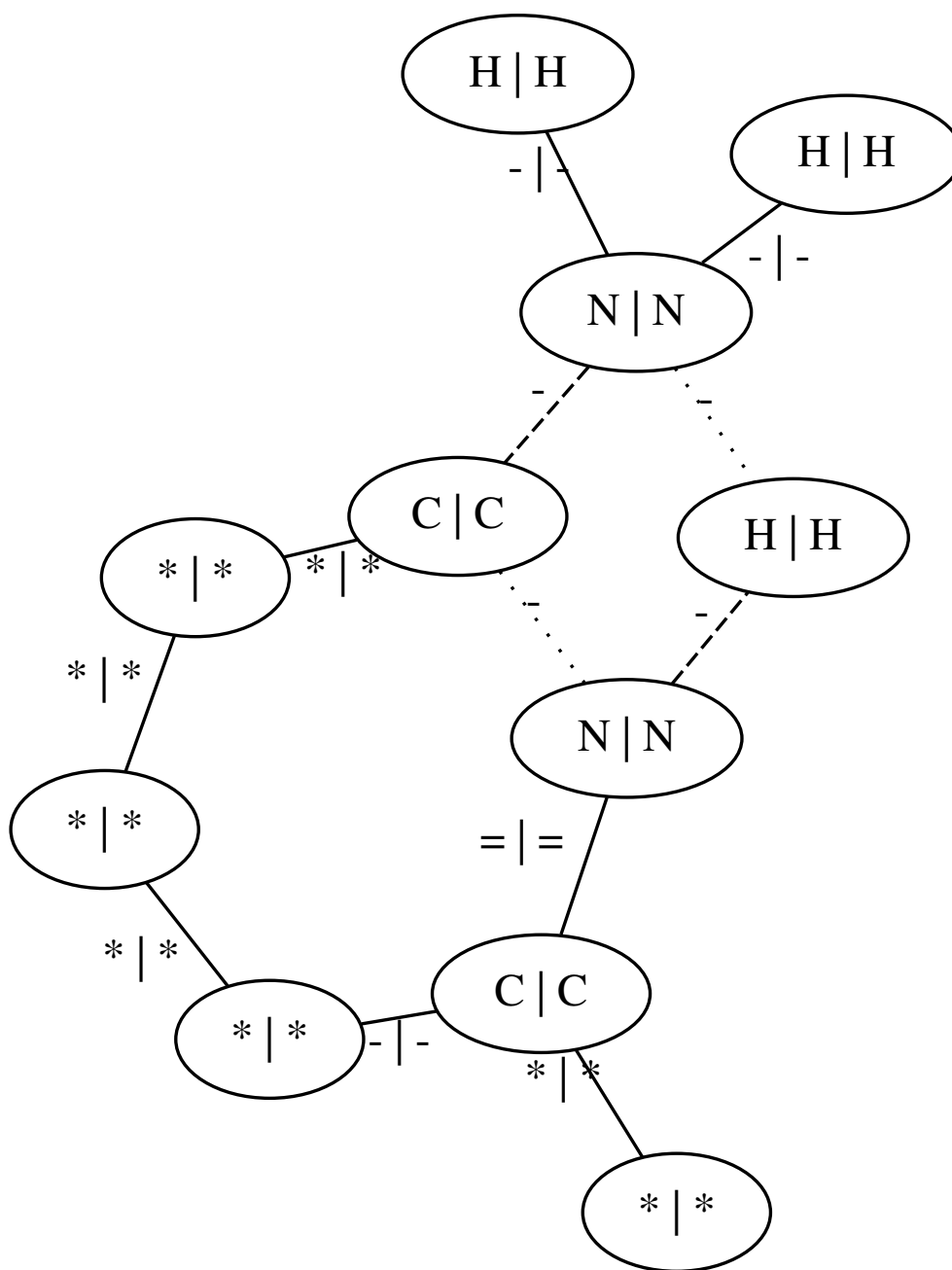


File: out/718_r_183_combined

1.0.181 Amine Imine Ring Closure 6

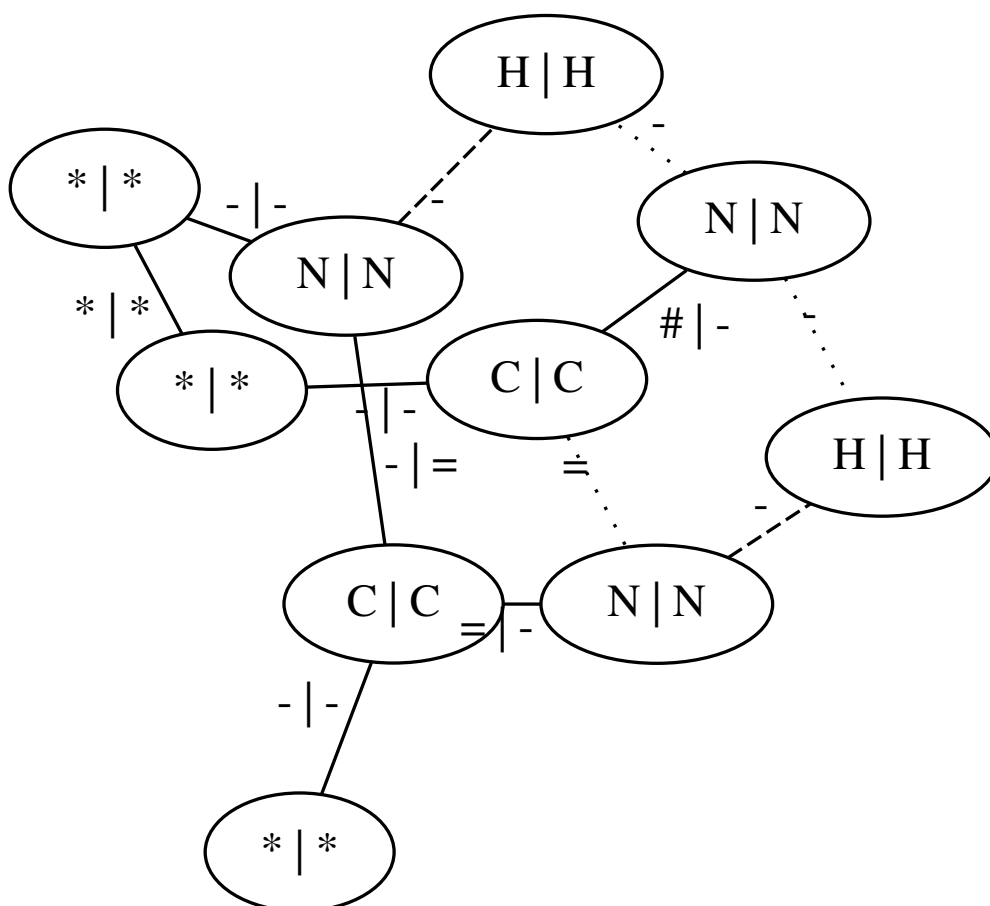
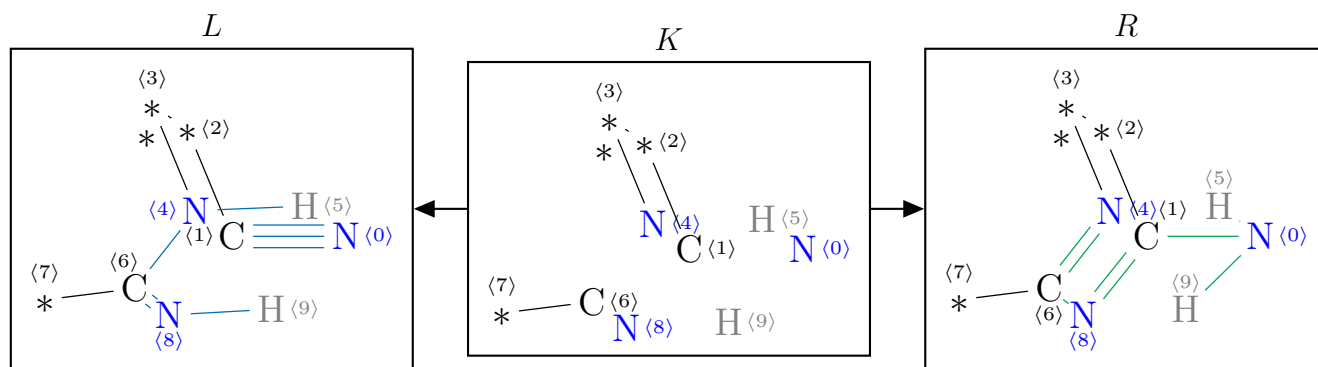


Files: out/721_r_184_10300110_{L, K, R}



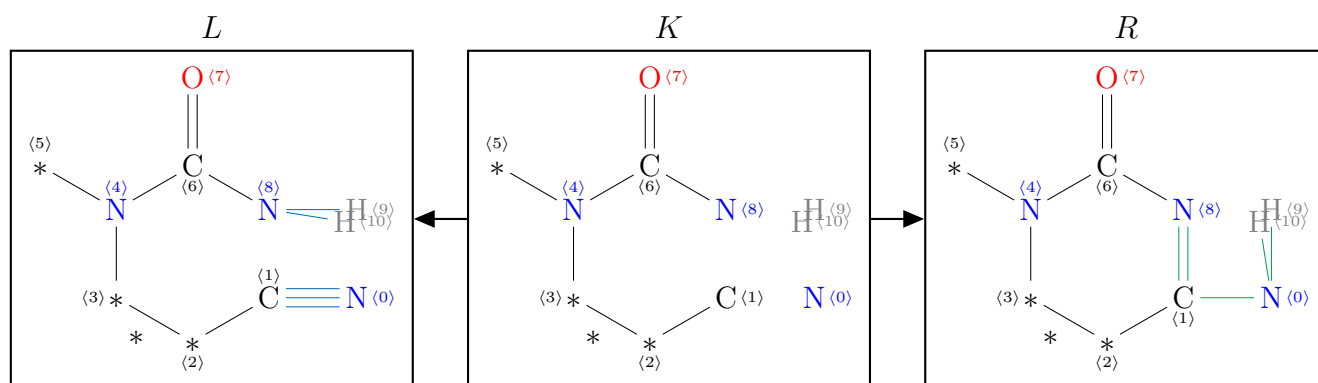
File: out/722_r_184_combined

1.0.182 Amidine Nitrile Ring Closure 6

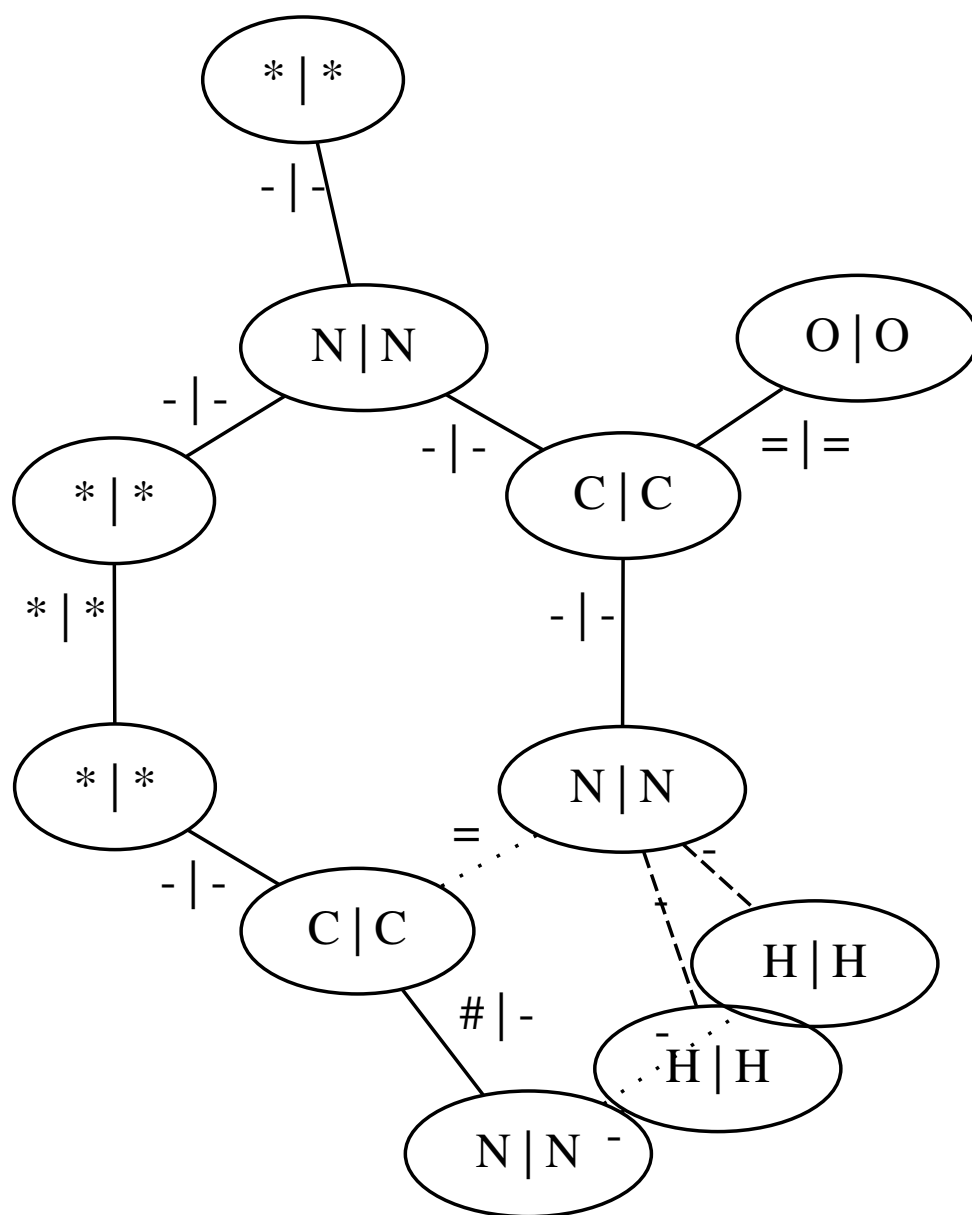


File: out/726_r_185_combined

1.0.183 Amide Nitrile Ring Closure 6

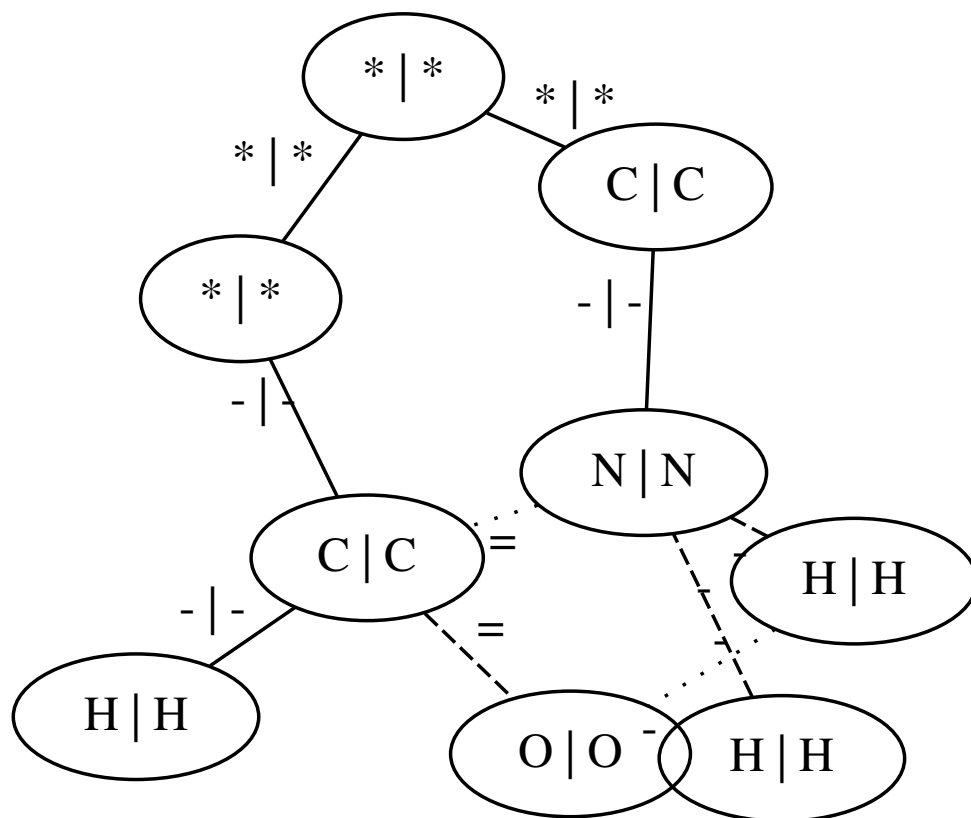
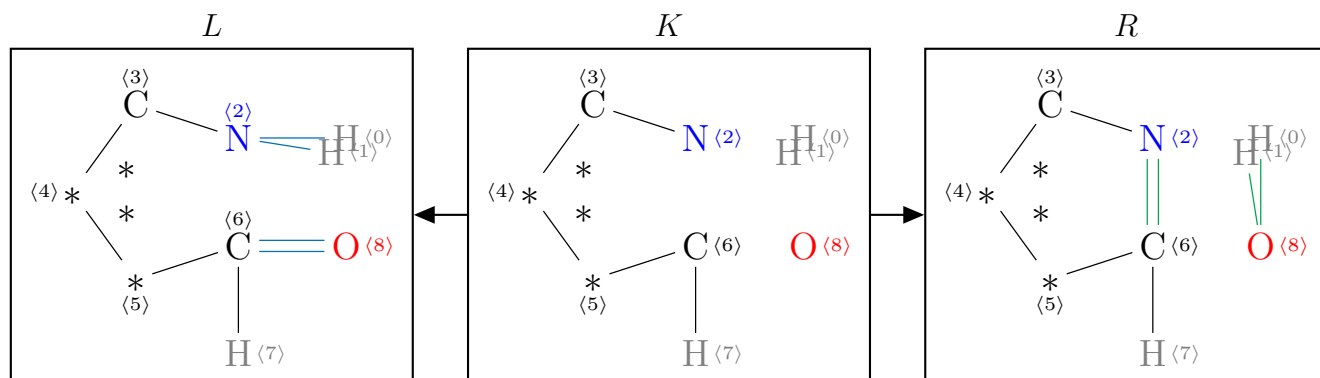


Files: out/729_r_186_10300110_{L, K, R}



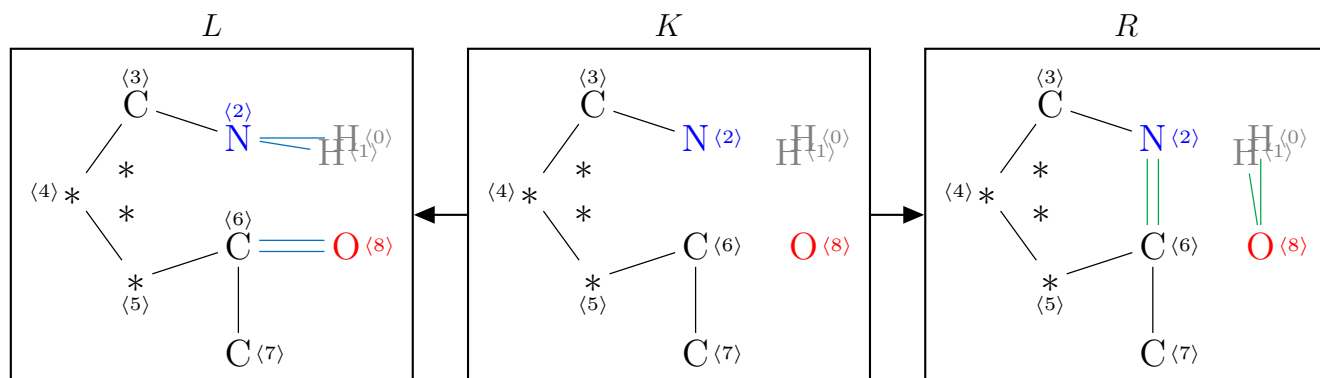
File: out/730_r_186_combined

1.0.184 Amine Carbonyl Ring Closure, H, 5

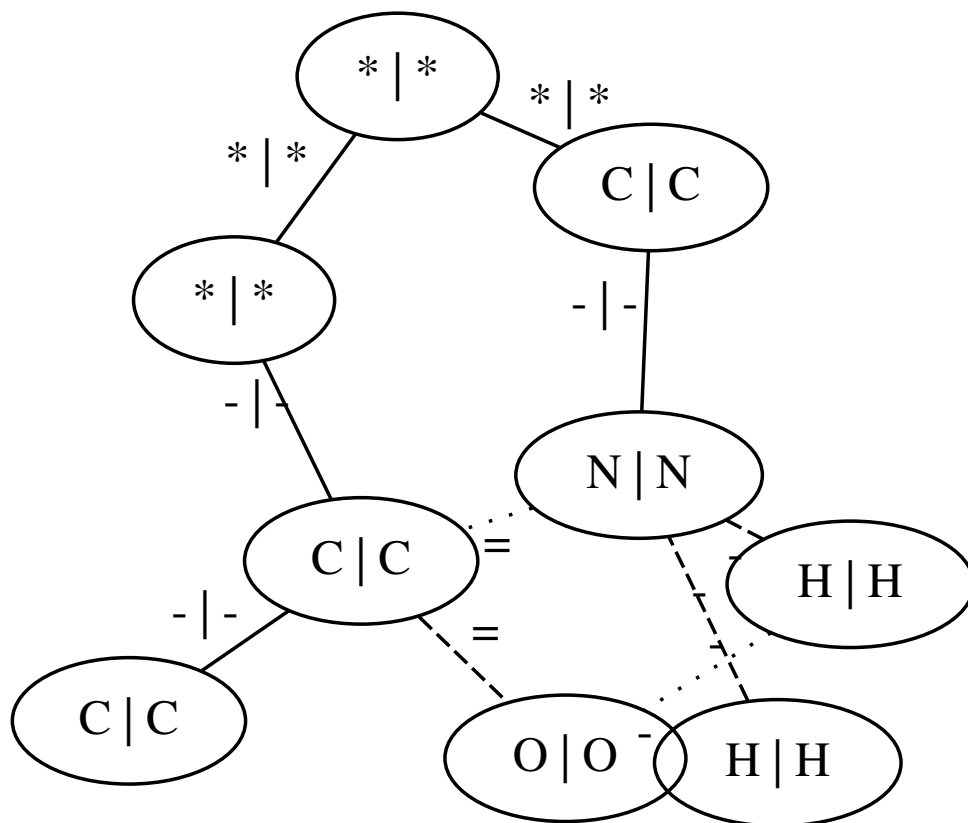


File: out/734_r_187_combined

1.0.185 Amine Carbonyl Ring Closure, C, 5

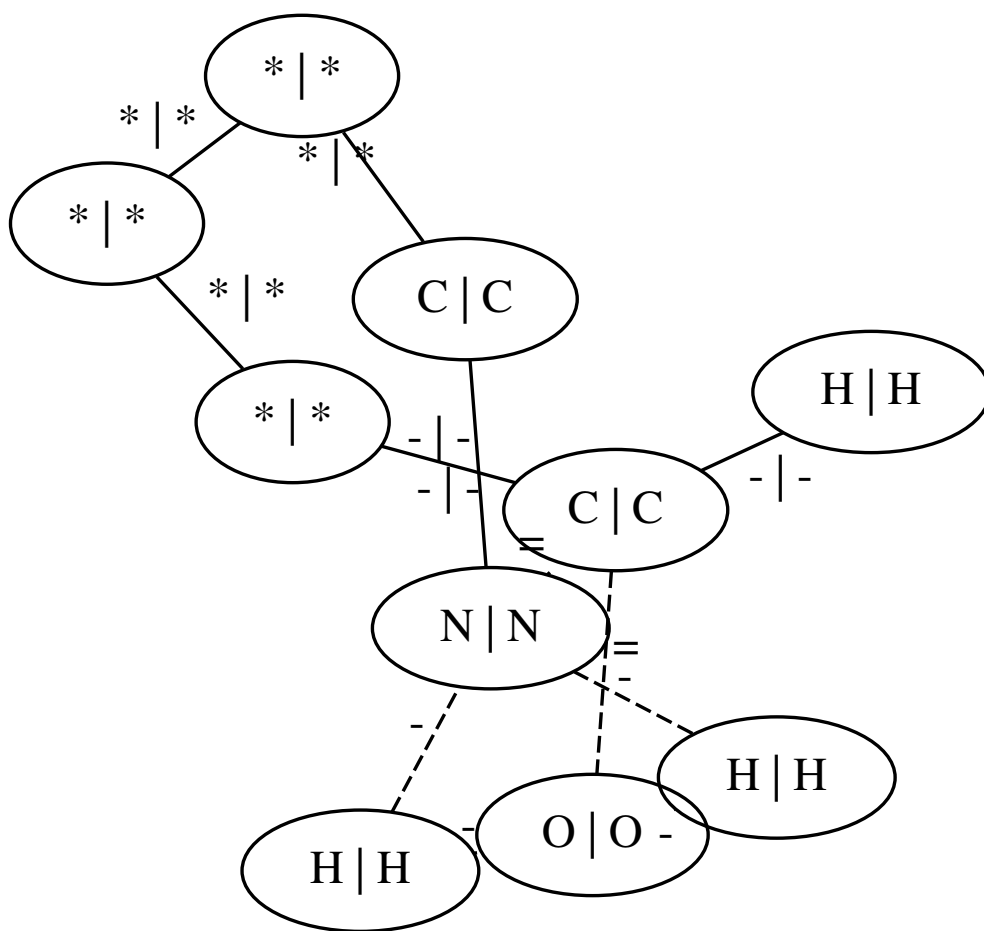
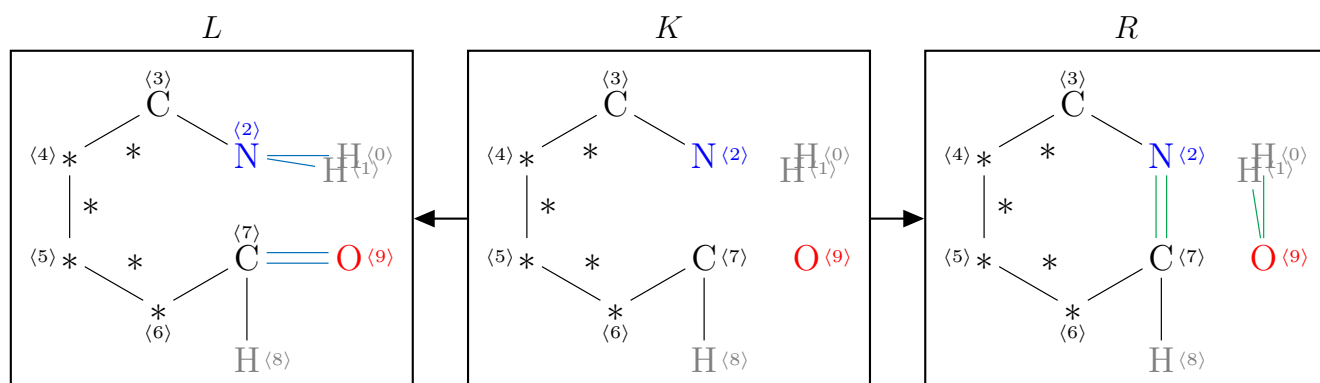


Files: out/737_r_188_10300110_{L, K, R}



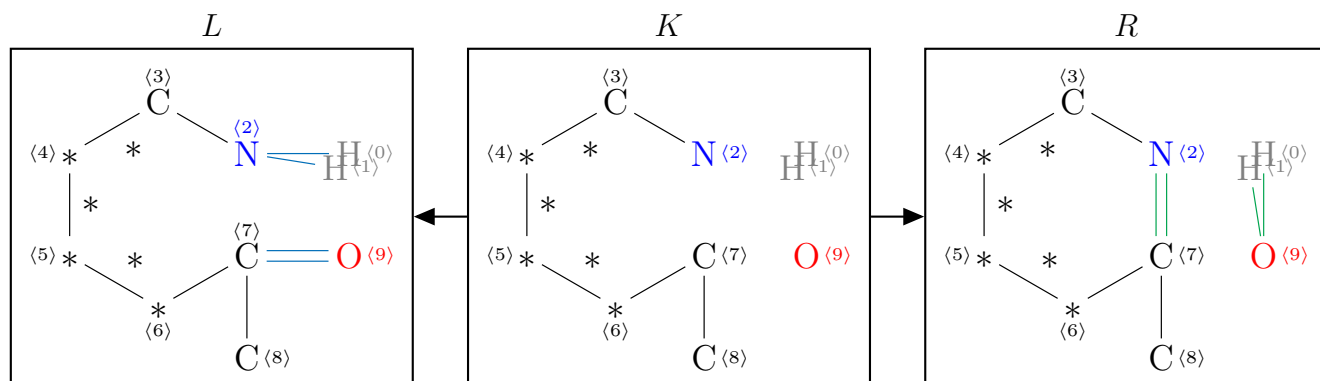
File: out/738_r_188_combined

1.0.186 Amine Carbonyl Ring Closure, H, 6

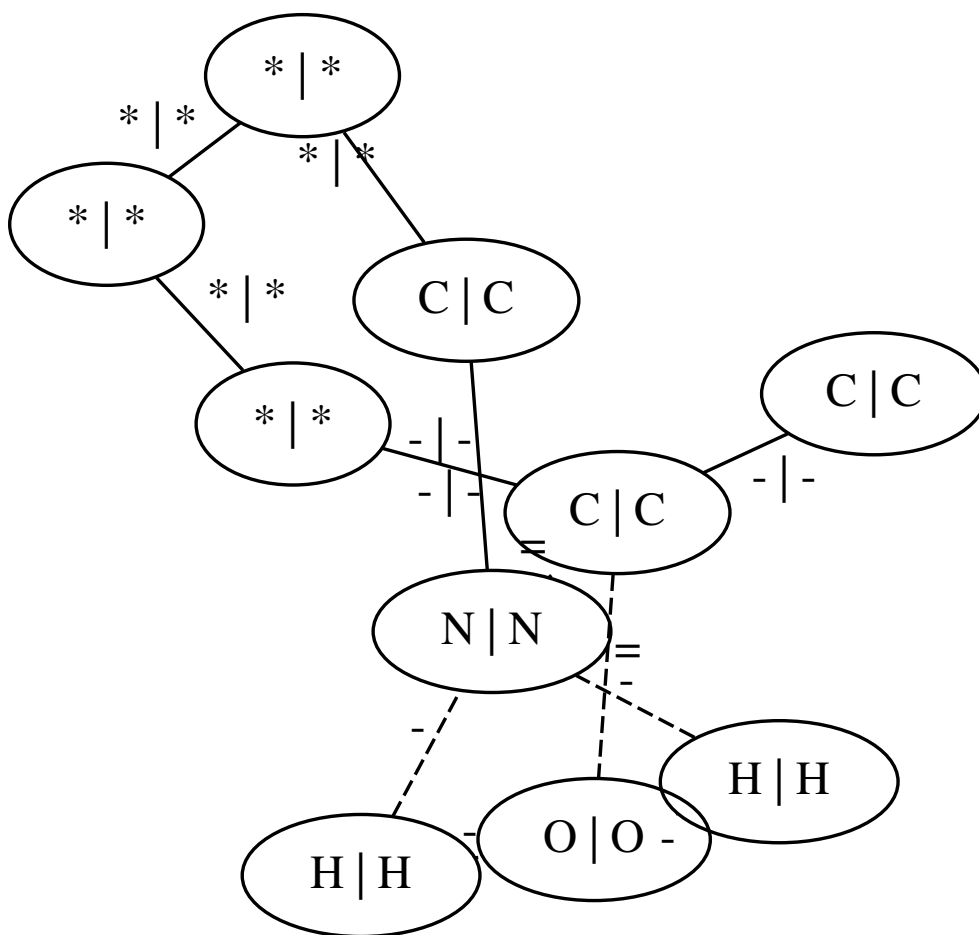


File: out/742_r_189_combined

1.0.187 Amine Carbonyl Ring Closure, C, 6

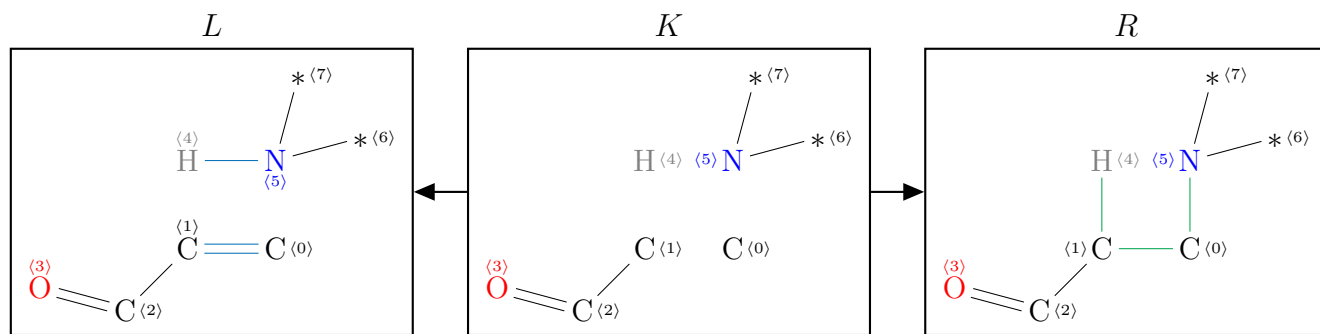


Files: out/745_r_190_10300110_{L, K, R}

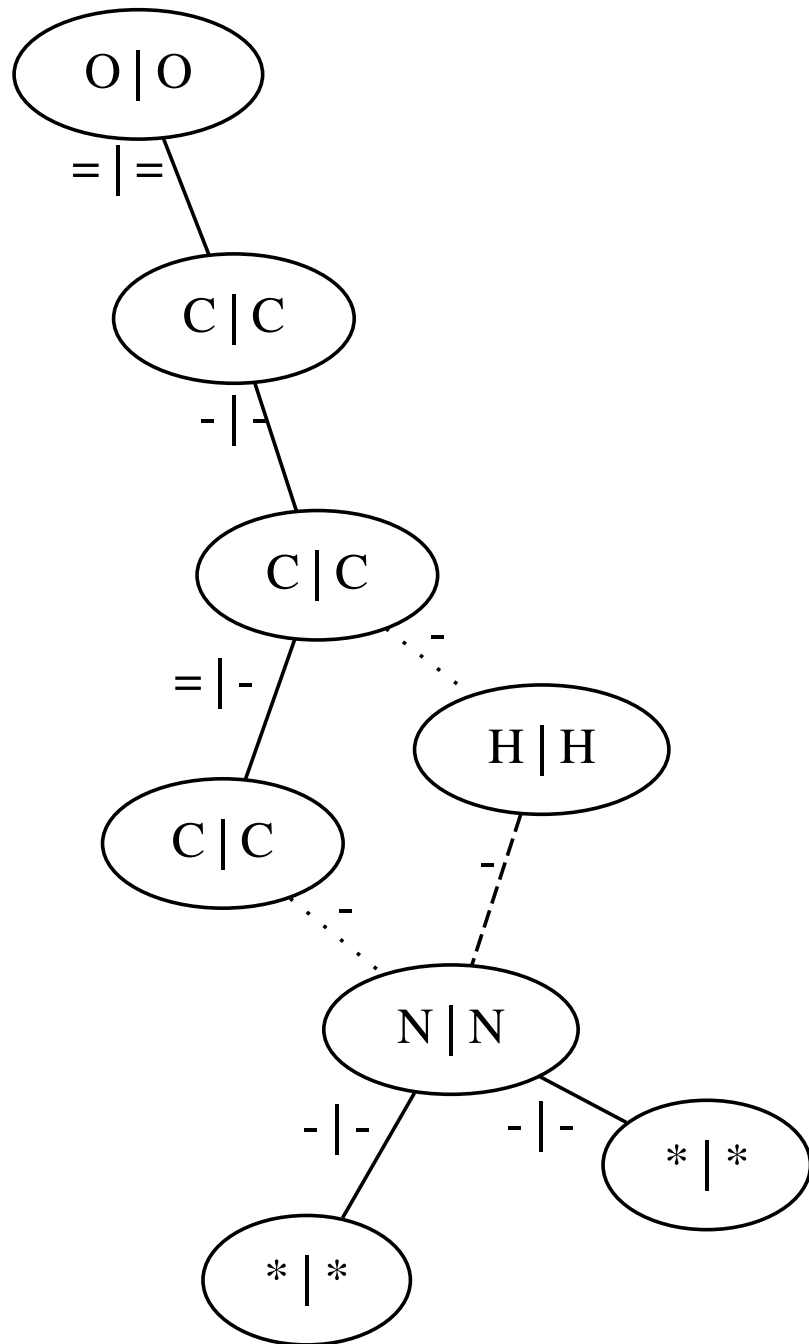


File: out/746_r_190_combined

1.0.188 Michael Addition 0,0,



Files: out/749_r_191_10300110_{L, K, R}



File: out/750_r_191_combined

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

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

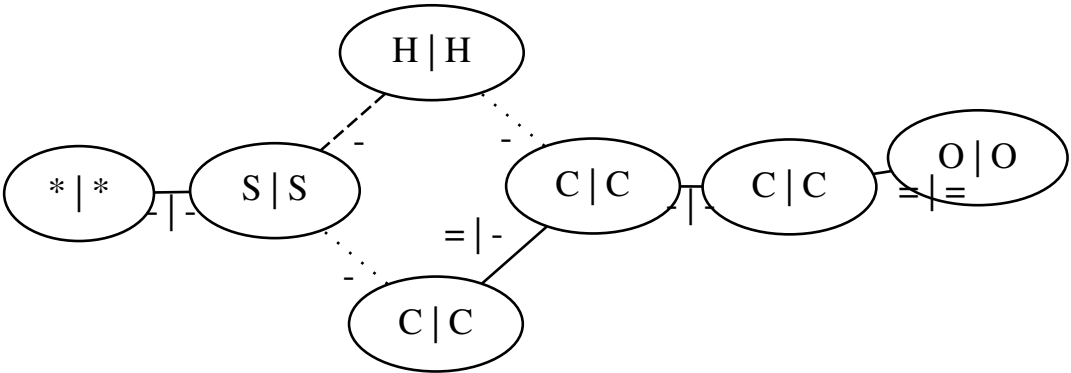
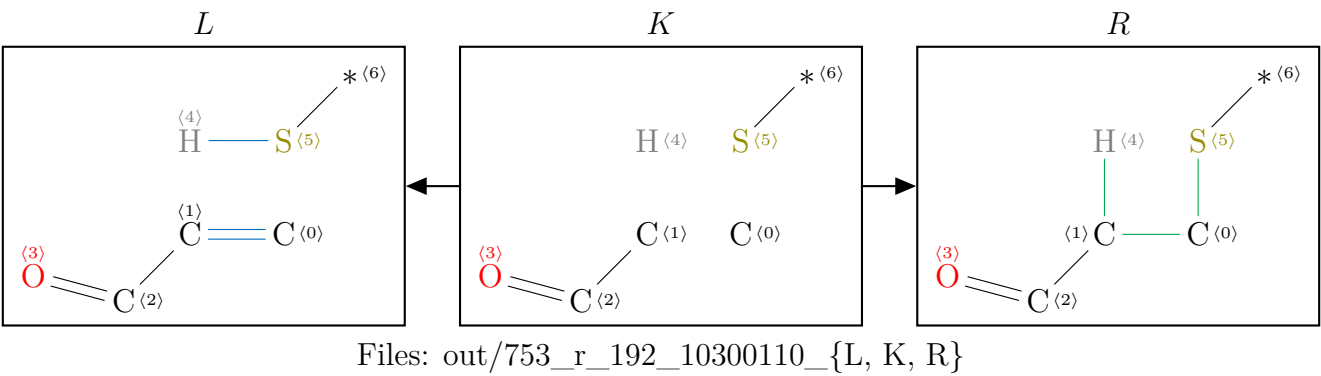
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\mid = 0
\end{aligned}$$

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

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

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

1.0.189 Michael Addition 0,1,



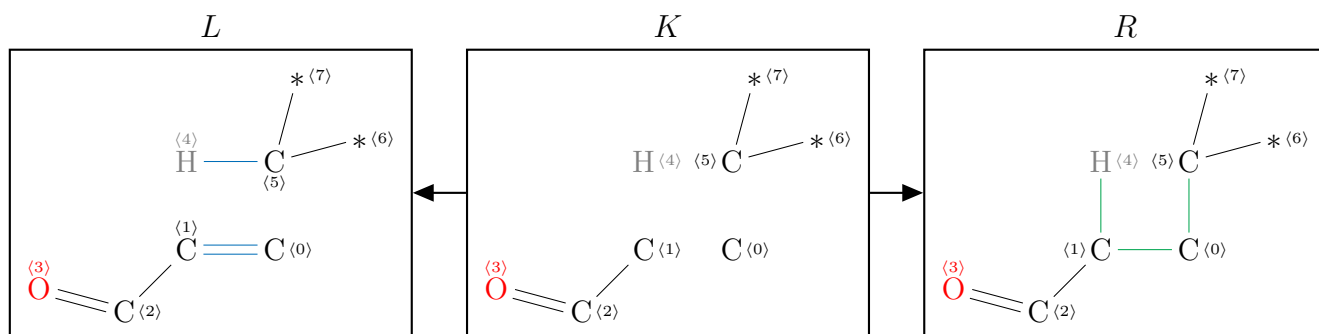
File: out/754_r_192_combined

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

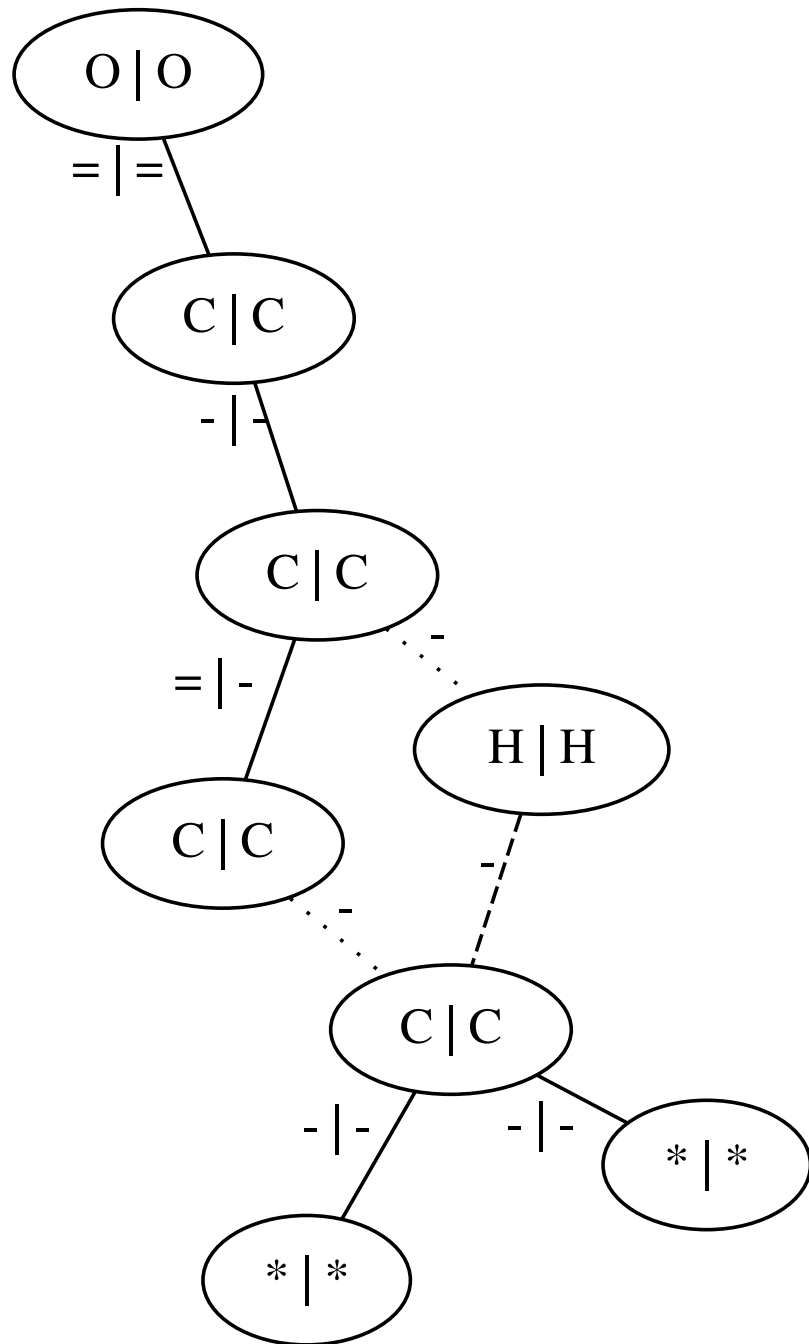
$$\begin{aligned} &|\{e \in \text{outEdges}(1) \mid \\ &\quad \text{label}(\text{target}(e)) \in \{‘0’\} \\ &\quad \wedge \\ &\quad \text{label}(e) \in \{‘-’\} \\ &\}\mid = 0 \end{aligned}$$

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

1.0.190 Michael Addition 0,2,



Files: out/757_r_193_10300110_{L, K, R}



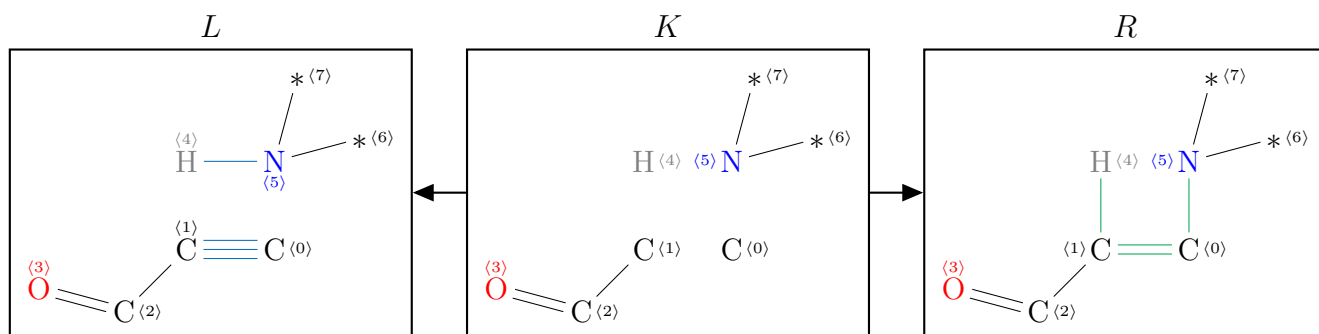
File: out/758_r_193_combined

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

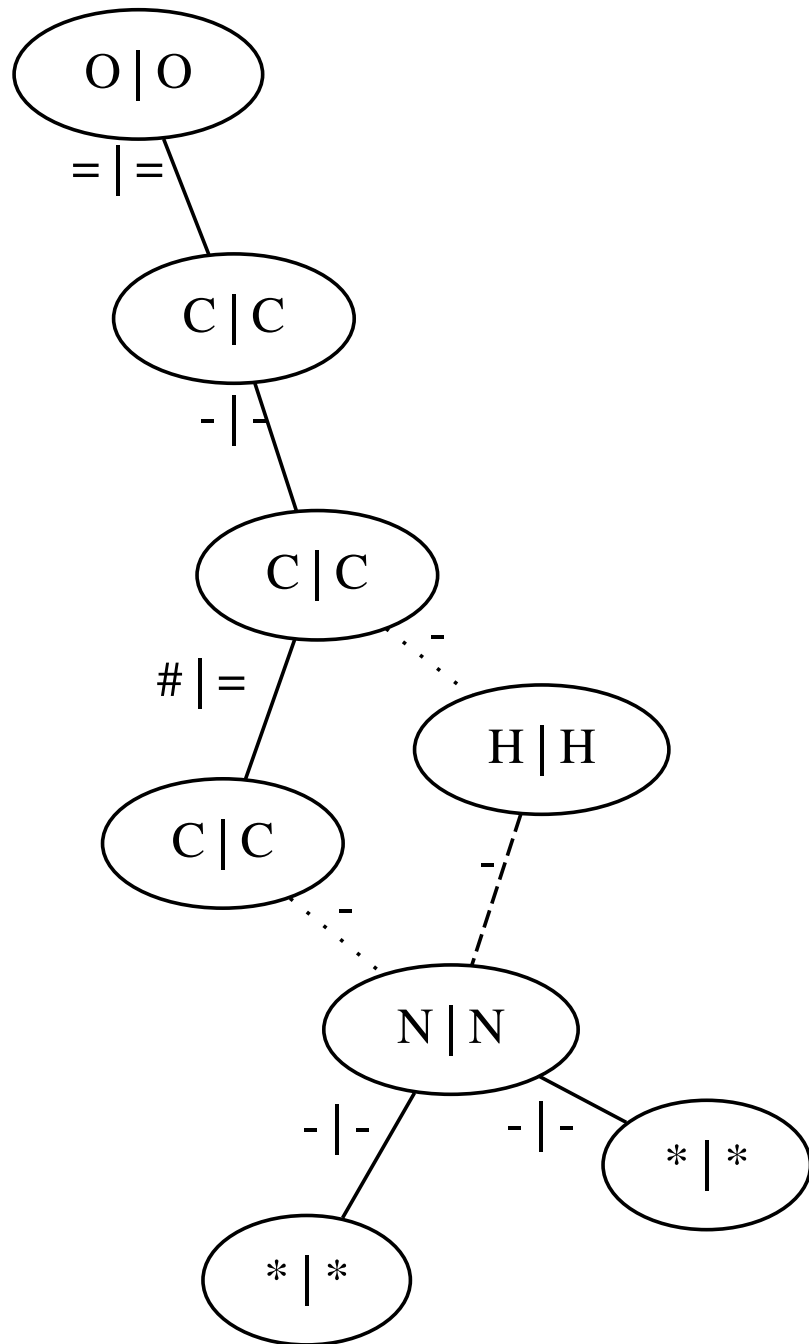
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.191 Michael Addition 1,0,



Files: out/761_r_194_10300110_{L, K, R}



File: out/762_r_194_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

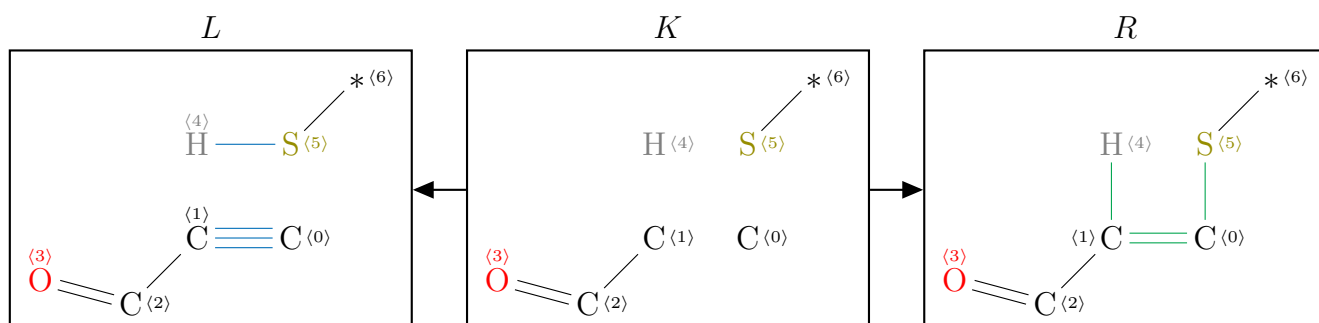
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

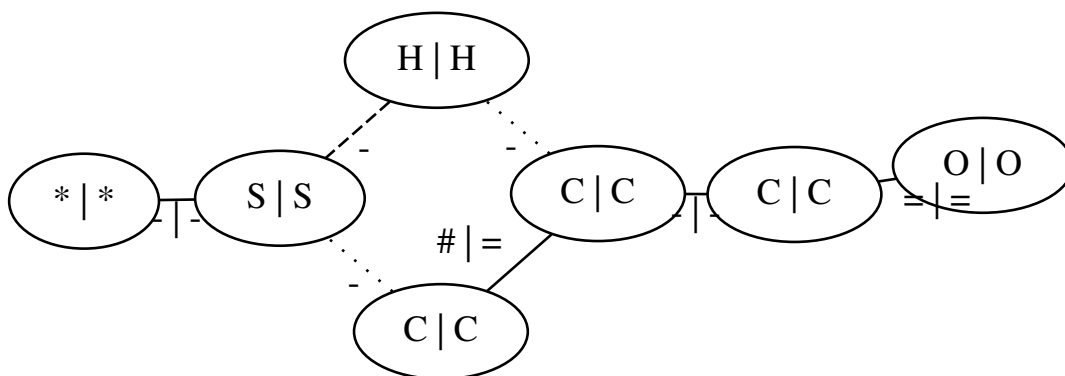
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

1.0.192 Michael Addition 1,1,



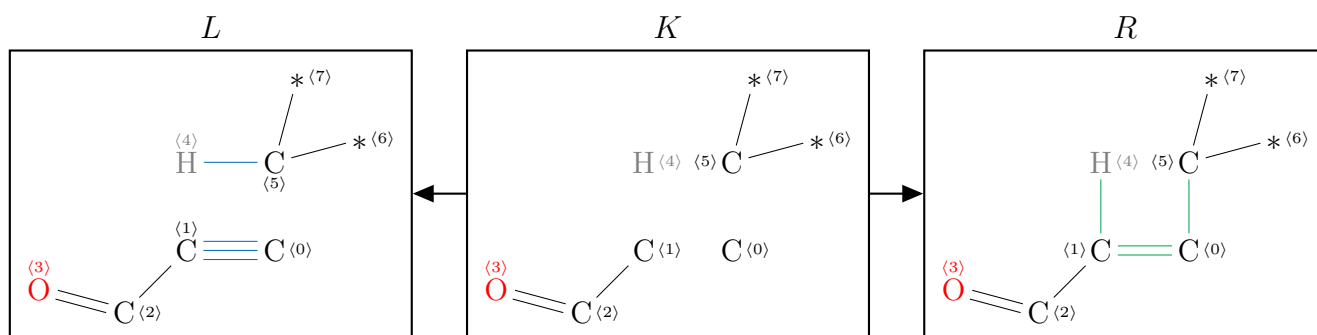
Files: out/765_r_195_10300110_{L, K, R}



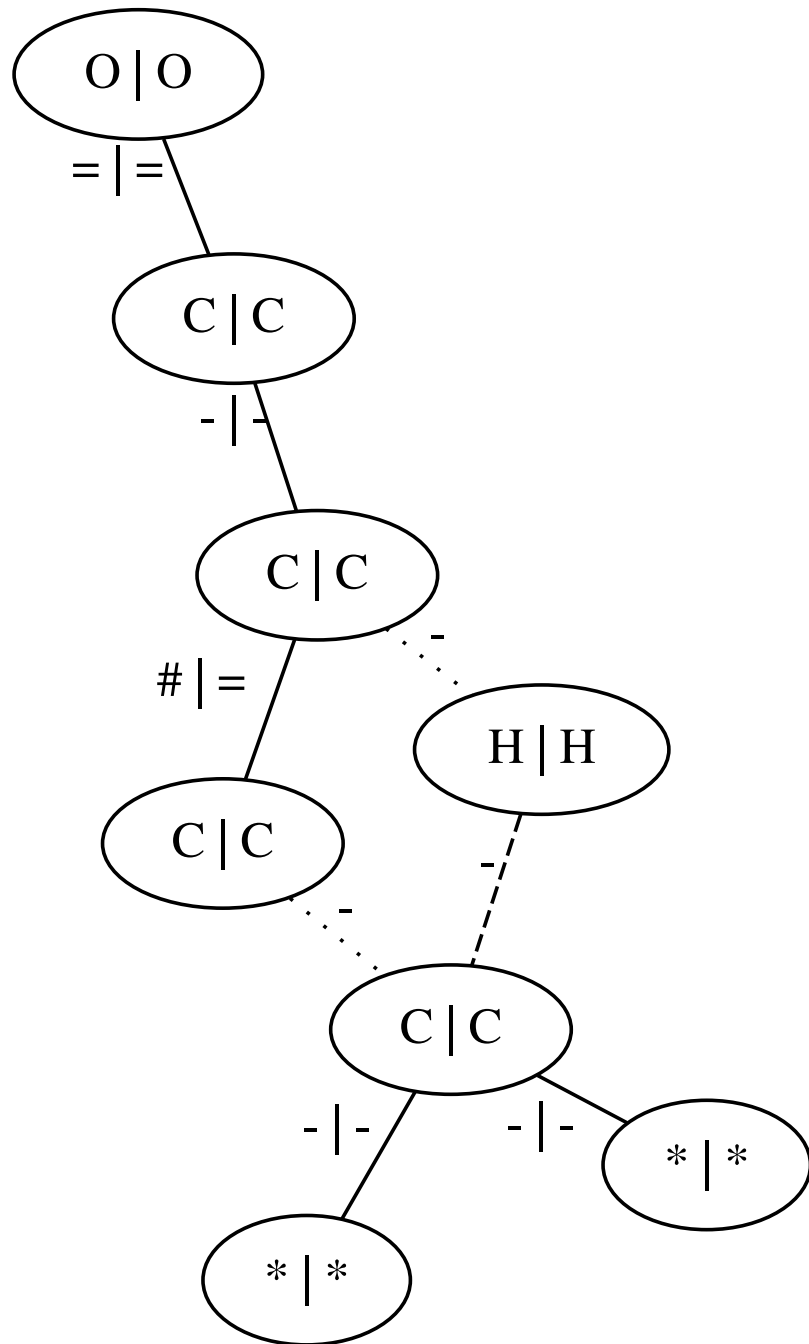
File: out/766_r_195_combined

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

1.0.193 Michael Addition 1,2,



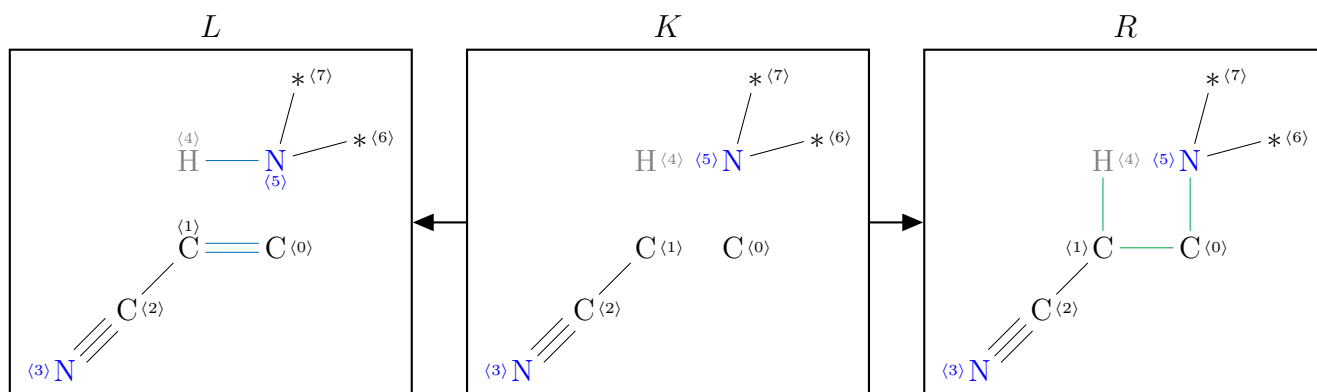
Files: out/769_r_196_10300110_{L, K, R}



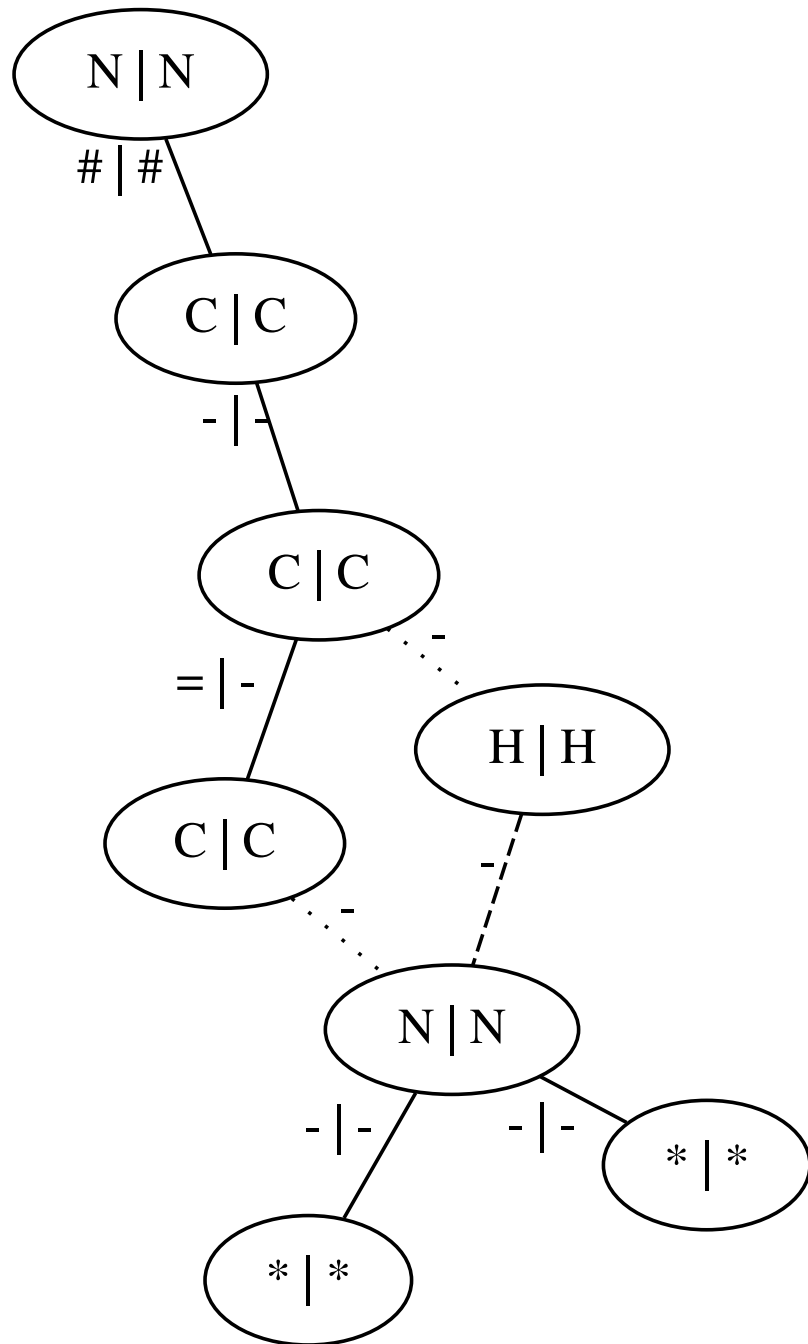
File: out/770_r_196_combined

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

1.0.194 Michael Addition 2,0,



Files: out/773_r_197_10300110_{L, K, R}



File: out/774_r_197_combined

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

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

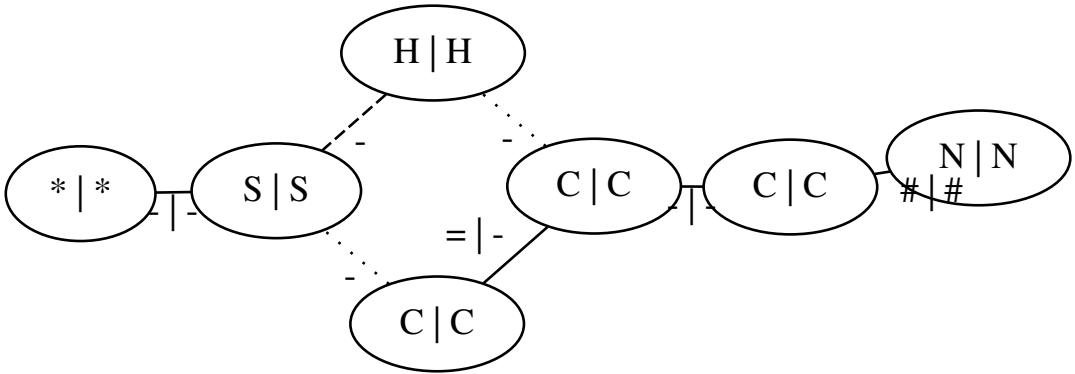
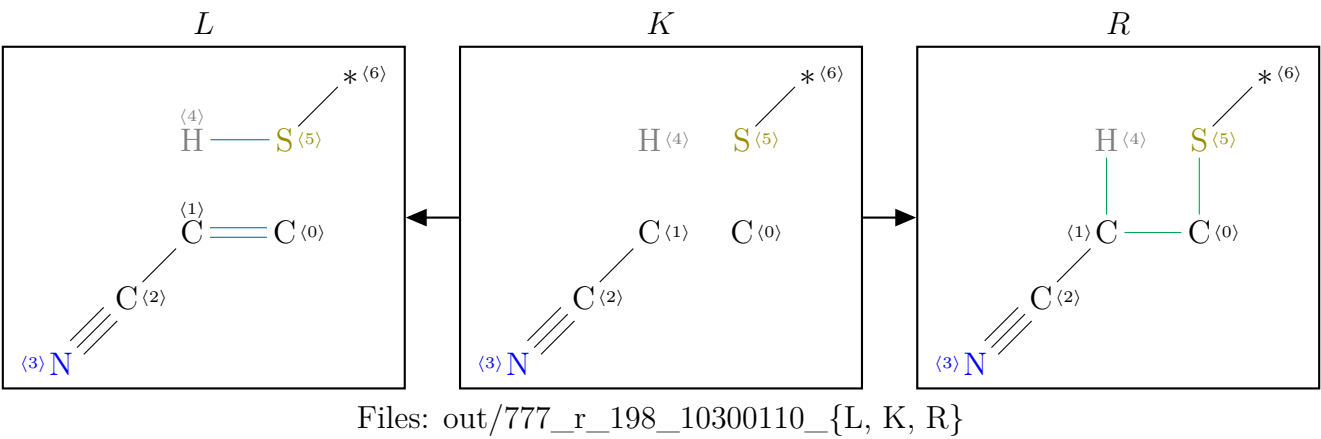
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\} = 0
\end{aligned}$$

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

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

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

1.0.195 Michael Addition 2,1,



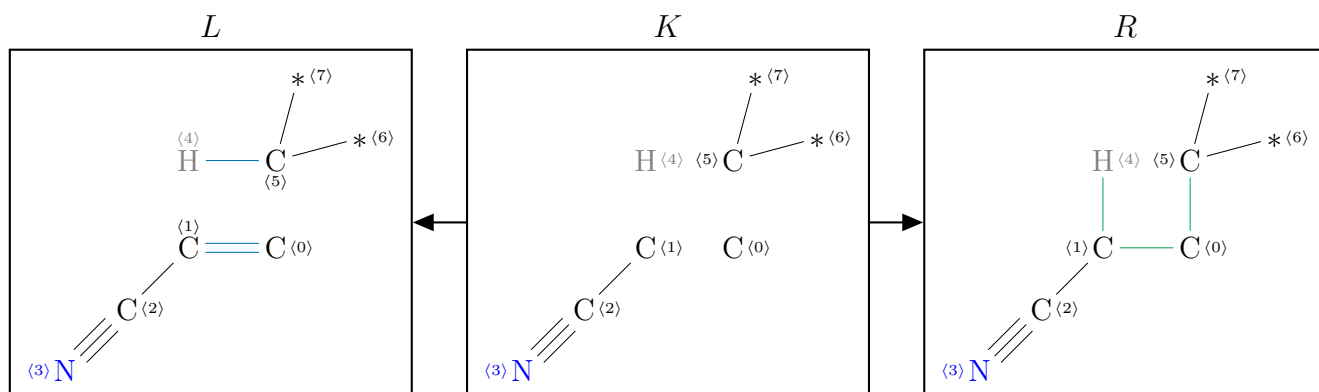
File: out/778_r_198_combined

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

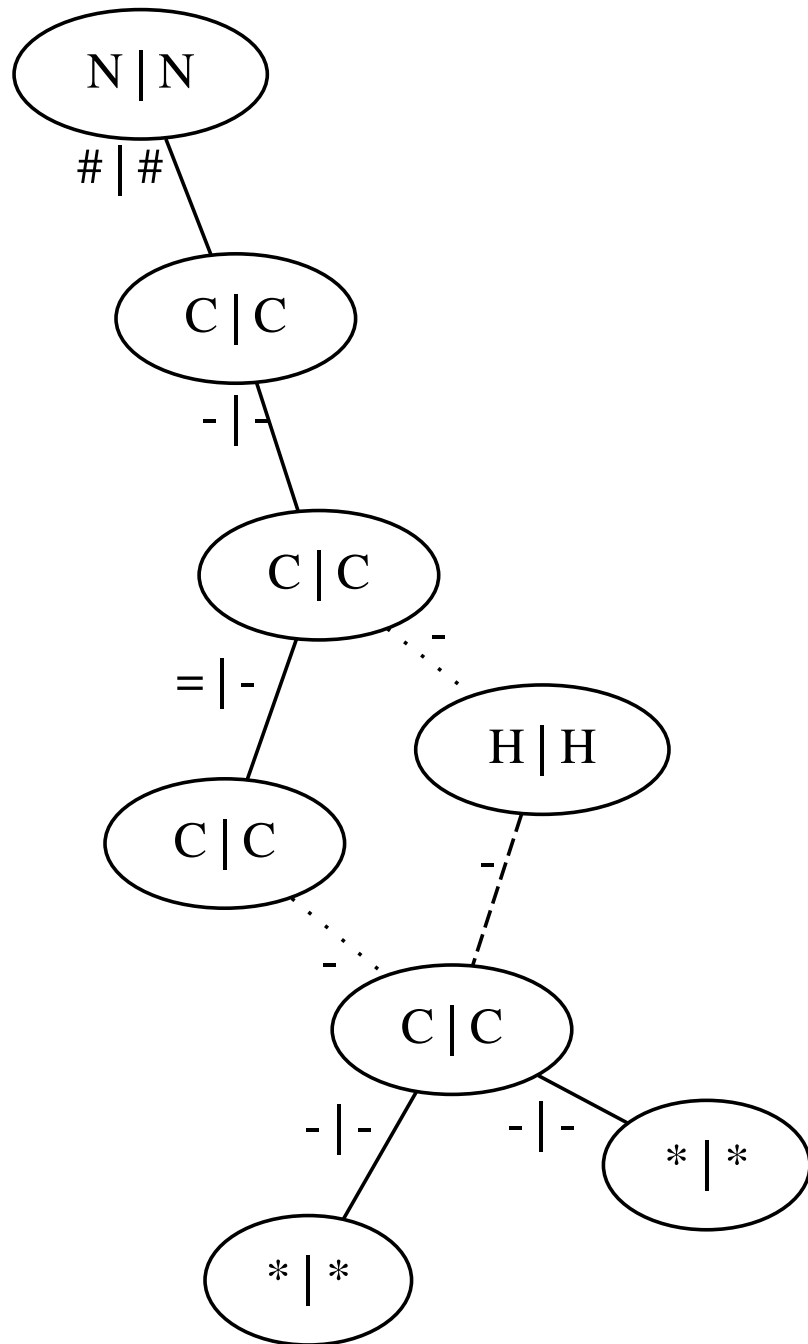
$$\begin{aligned} &|\{e \in \text{outEdges}(1) \mid \\ &\quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ &\quad \wedge \\ &\quad \text{label}(e) \in \{\text{'-'}\} \\ &\quad \}| = 0 \end{aligned}$$

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

1.0.196 Michael Addition 2,2,



Files: out/781_r_199_10300110_{L, K, R}



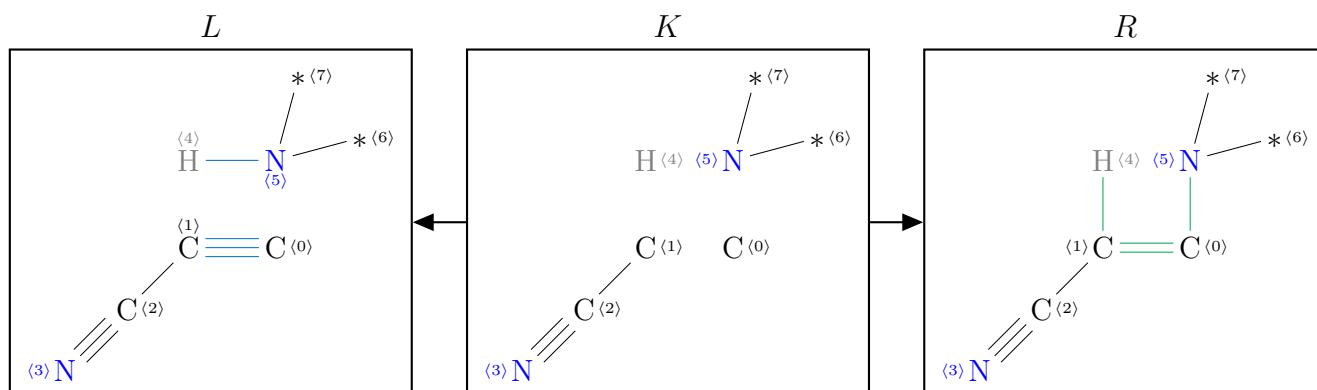
File: out/782_r_199_combined

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

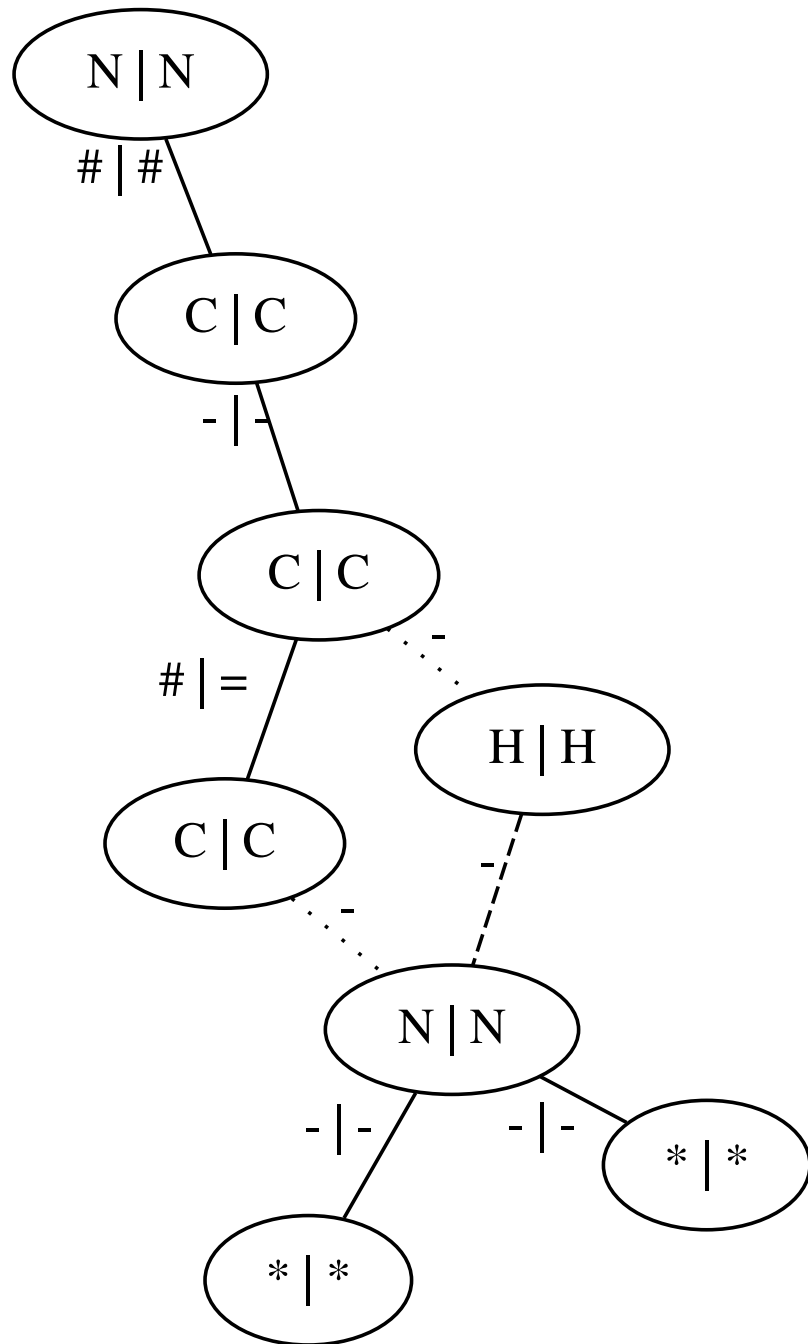
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{'-\'} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.197 Michael Addition 3,0,



Files: out/785_r_200_10300110_{L, K, R}



File: out/786_r_200_combined

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

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

$$\wedge$$

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

$$\}| = 0$$

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

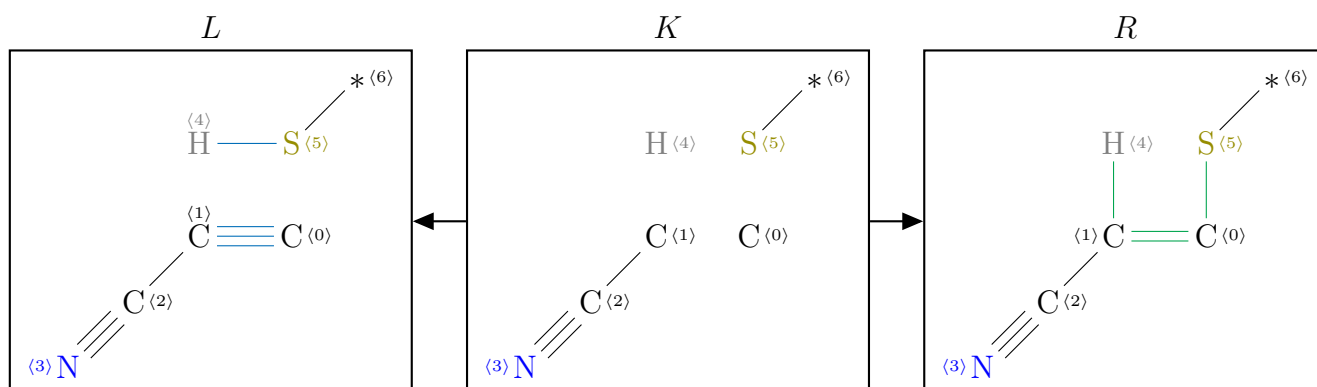
$$\text{label}(\text{target}(e)) \in \{\text{'S'}, \text{'O'}, \text{'N'}\}$$

$$\wedge$$

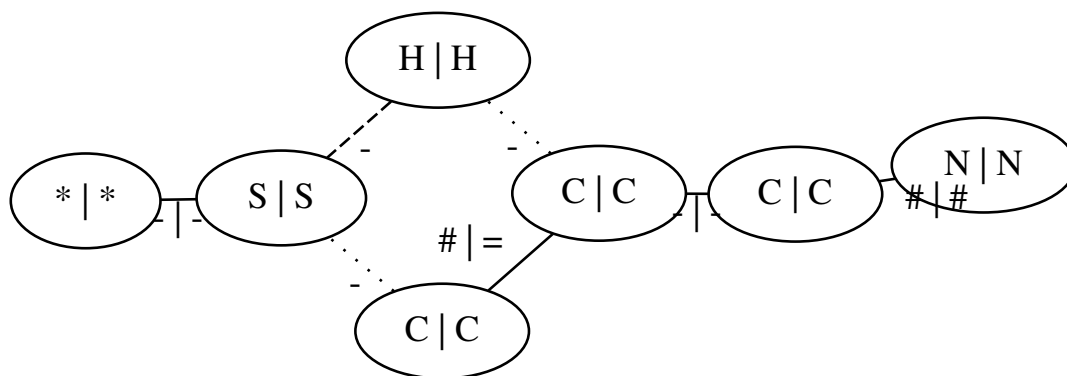
$$\text{label}(e) \in \{\text{'-'}\}$$

$$\}| = 0$$

1.0.198 Michael Addition 3,1,



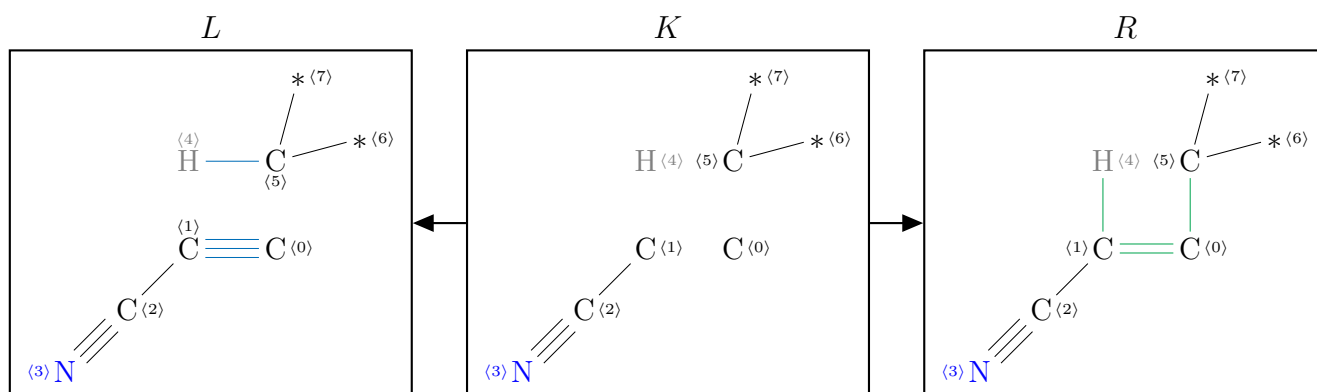
Files: out/789_r_201_10300110_{L, K, R}



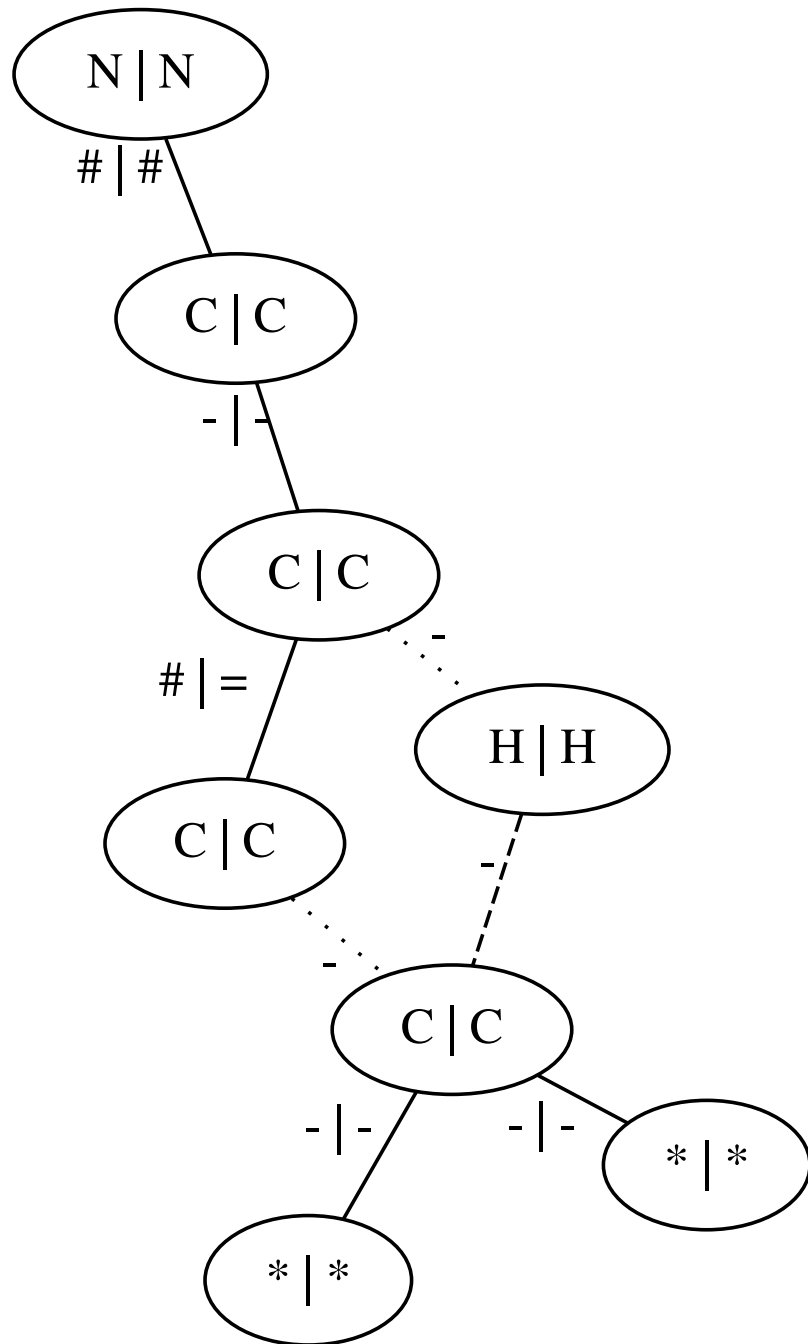
File: out/790_r_201_combined

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

1.0.199 Michael Addition 3,2,



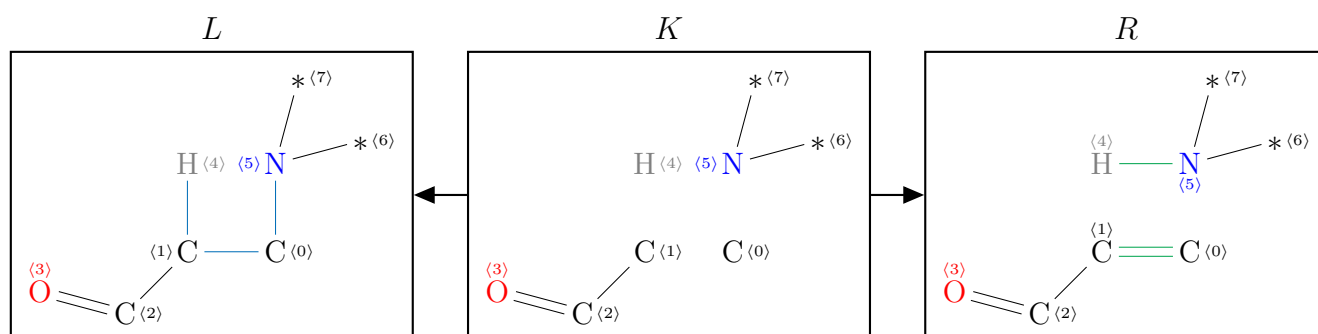
Files: out/793_r_202_10300110_{L, K, R}



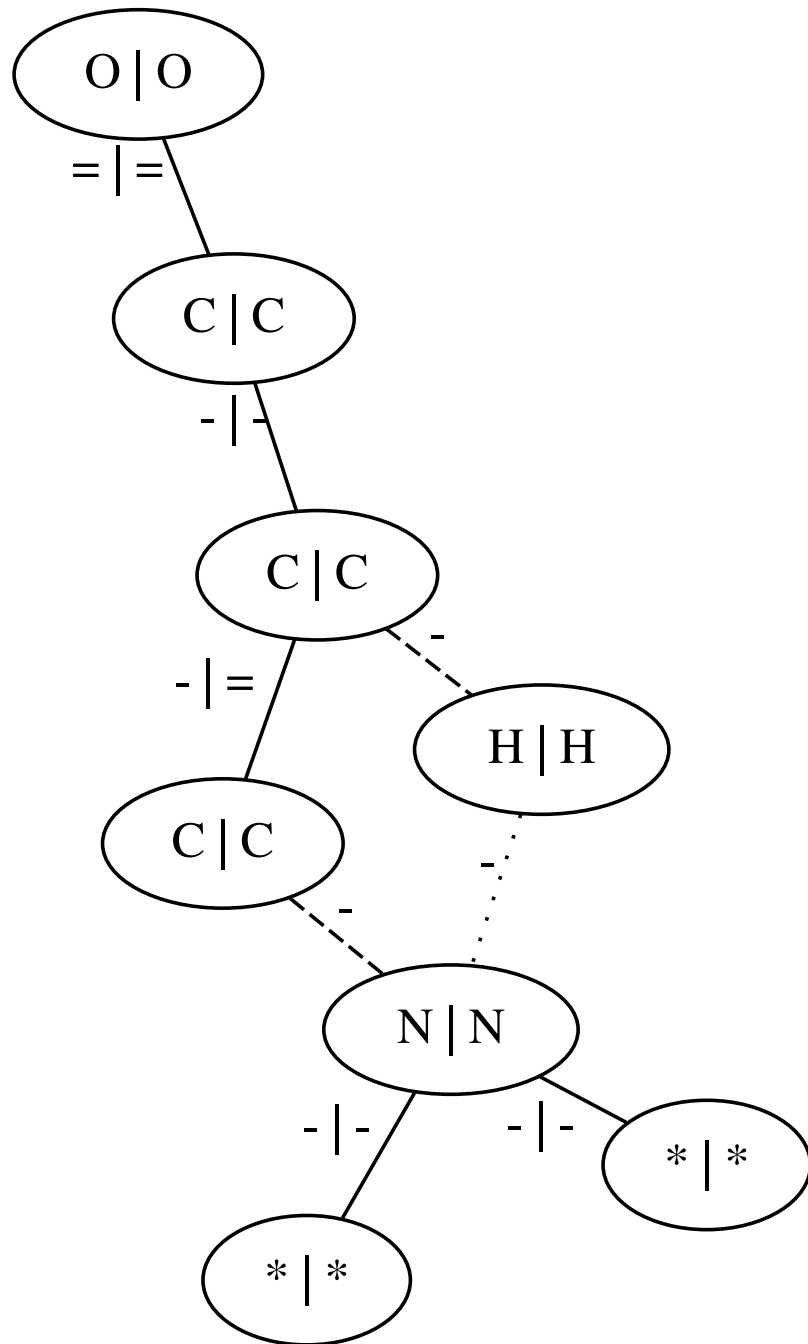
File: out/794_r_202_combined

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

1.0.200 Michael Addition 0,0, (reverse)



Files: out/797_r_203_10300110_{L, K, R}



File: out/798_r_203_combined

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

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

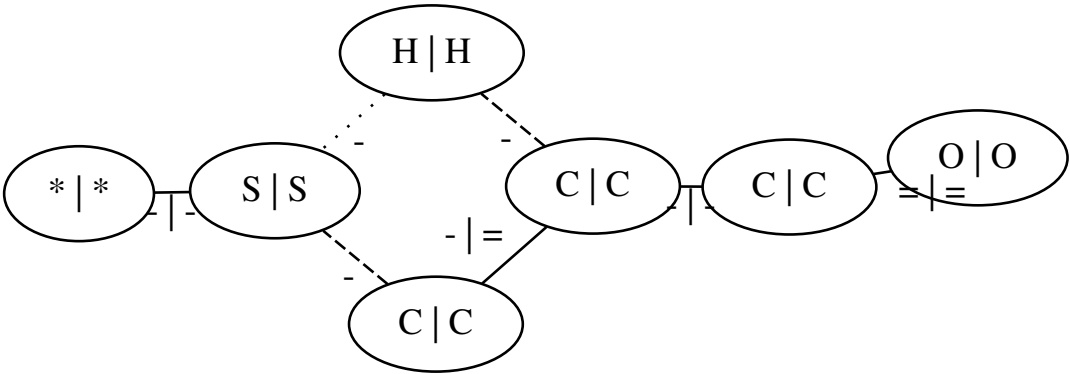
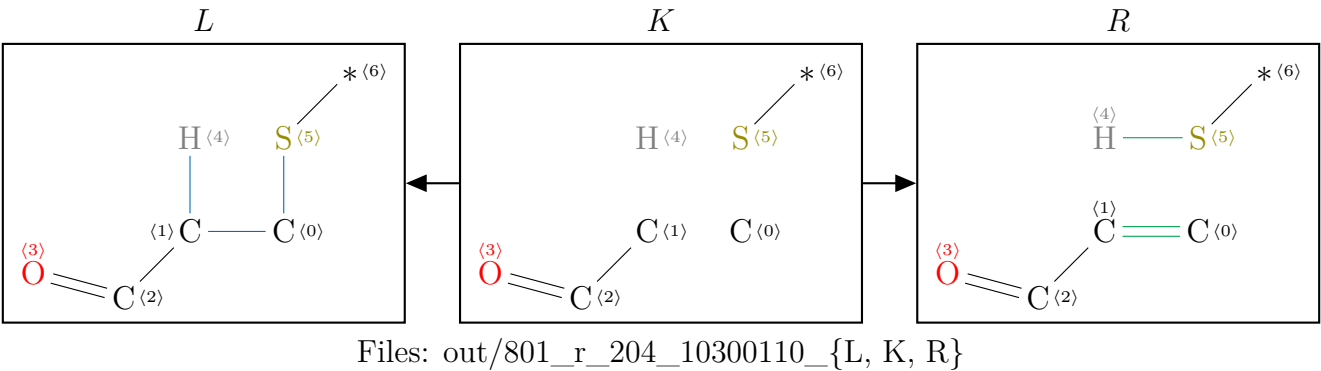
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\} = 0
\end{aligned}$$

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

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

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

1.0.201 Michael Addition 0,1, (reverse)



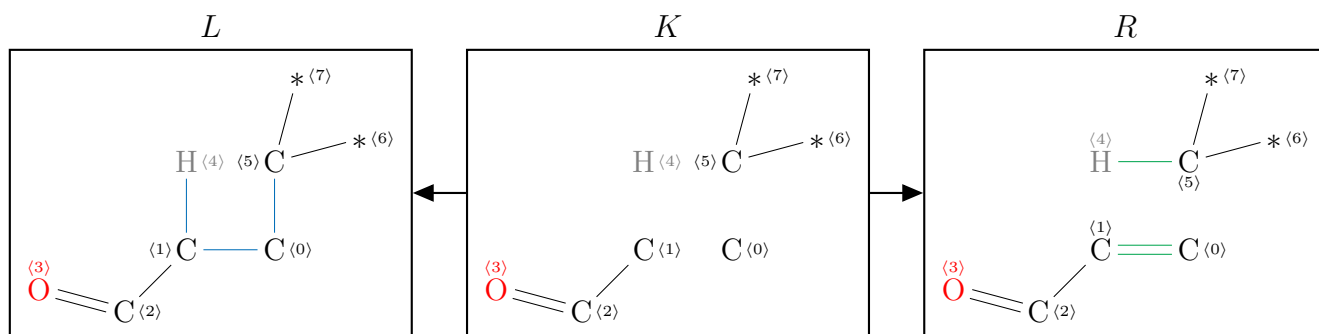
File: out/802_r_204_combined

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

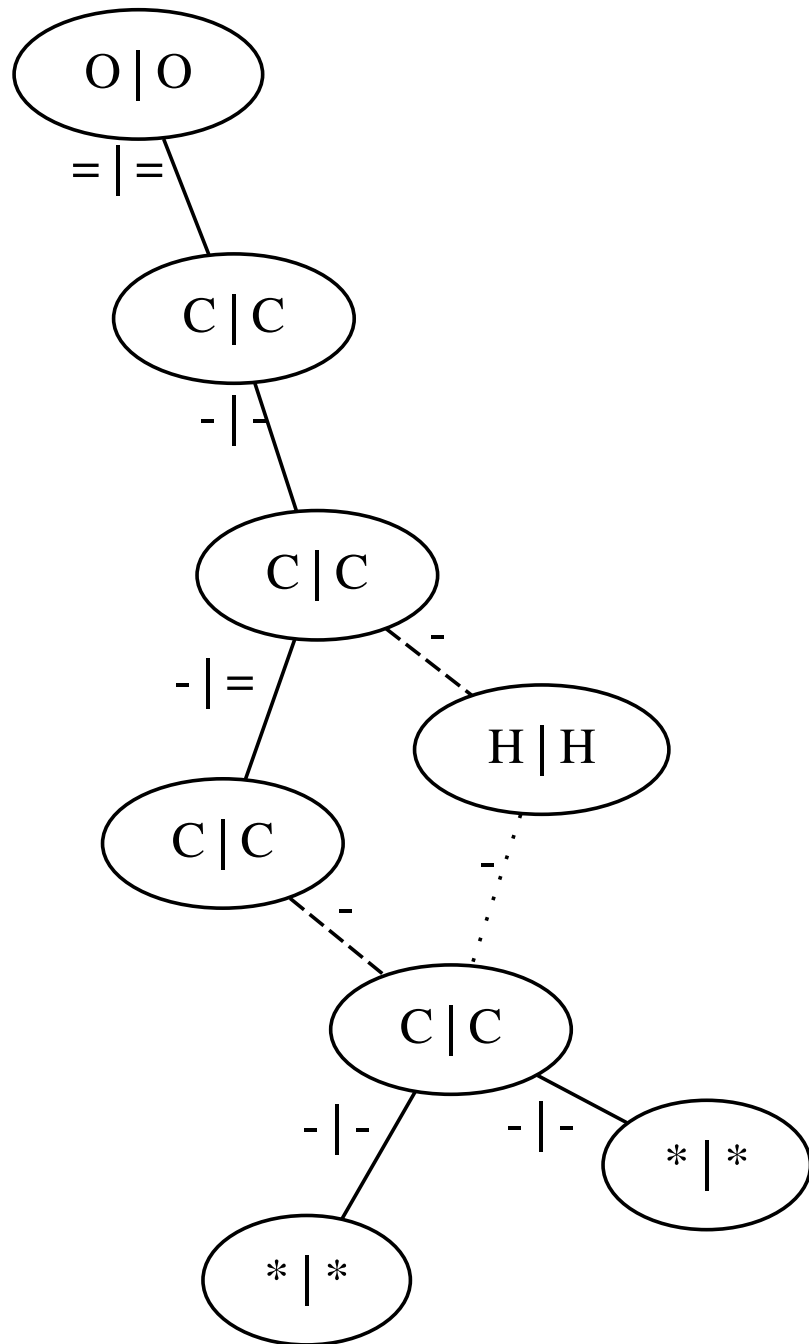
$$\begin{aligned} &|\{e \in \text{outEdges}(1) \mid \\ &\quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ &\quad \wedge \\ &\quad \text{label}(e) \in \{\text{'-'}\} \\ &\quad \}\mid = 0 \end{aligned}$$

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

1.0.202 Michael Addition 0,2, (reverse)



Files: out/805_r_205_10300110_{L, K, R}



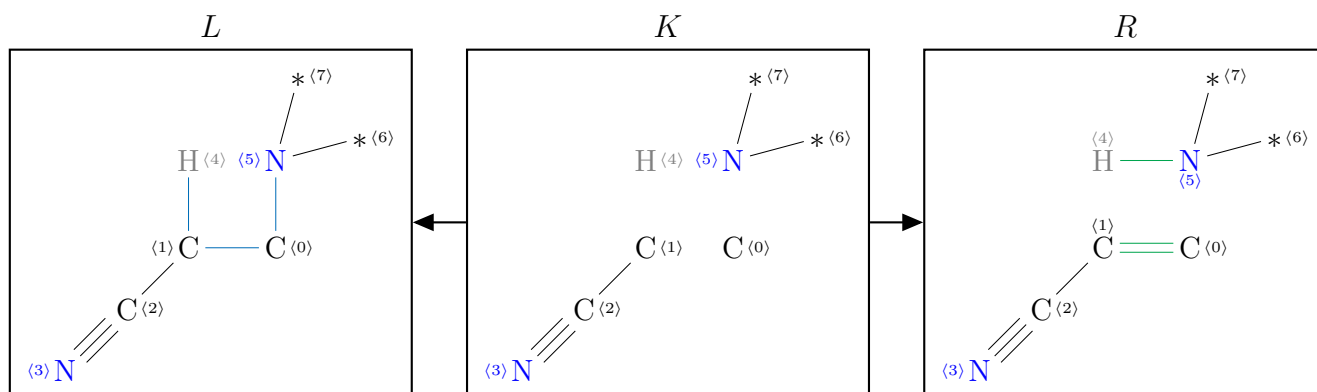
File: out/806_r_205_combined

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

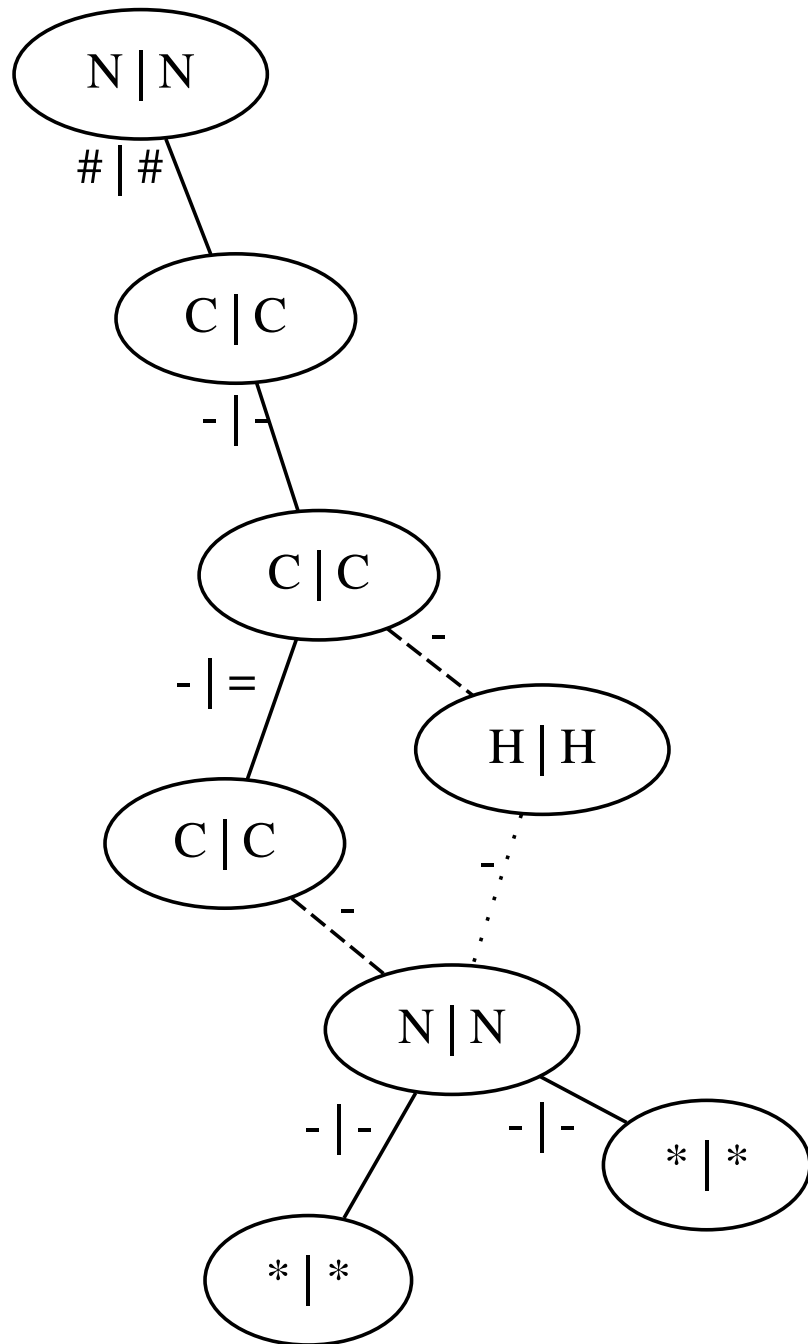
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \quad \}| = 0
\end{aligned}$$

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

1.0.203 Michael Addition 2,0, (reverse)



Files: out/809_r_206_10300110_{L, K, R}



File: out/810_r_206_combined

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

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

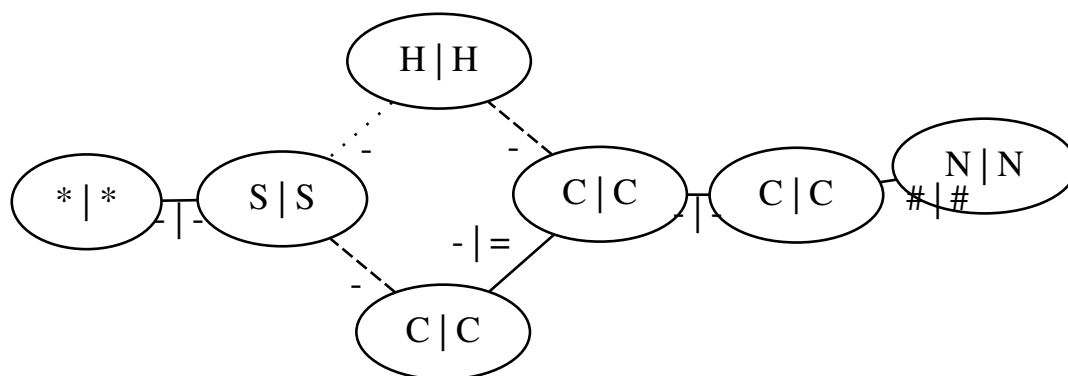
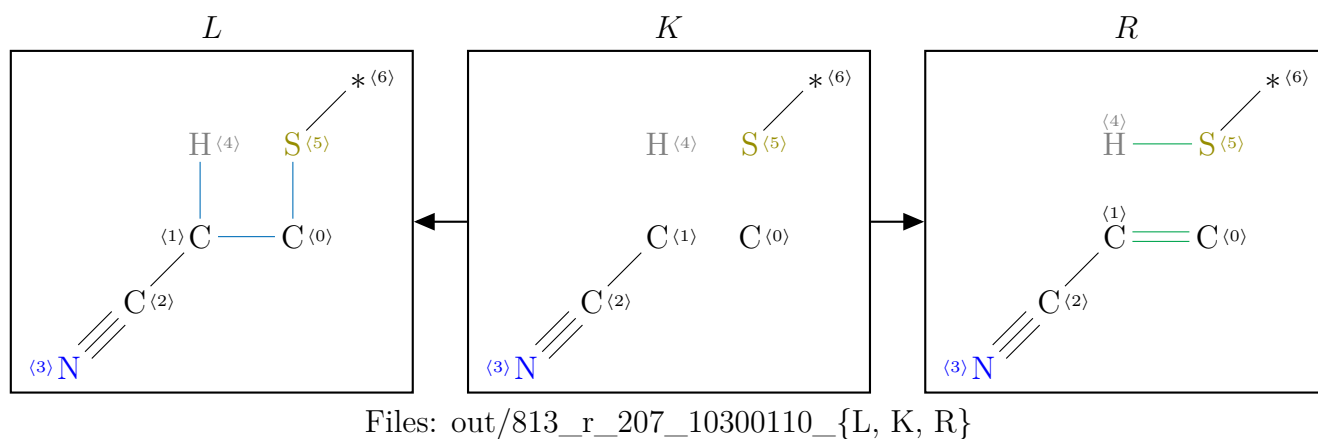
$$\begin{aligned}
& |\{e \in \text{outEdges}(0) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{\text{'N'}, \text{'0'}\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{\text{'-'}\} \\
& \}\} = 0
\end{aligned}$$

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

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

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

1.0.204 Michael Addition 2,1, (reverse)

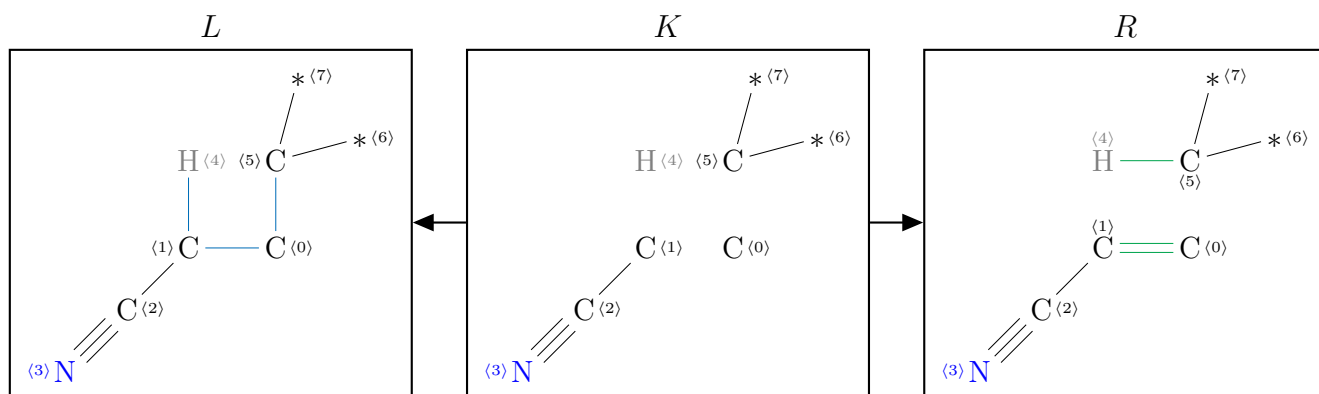


File: out/814_r_207_combined

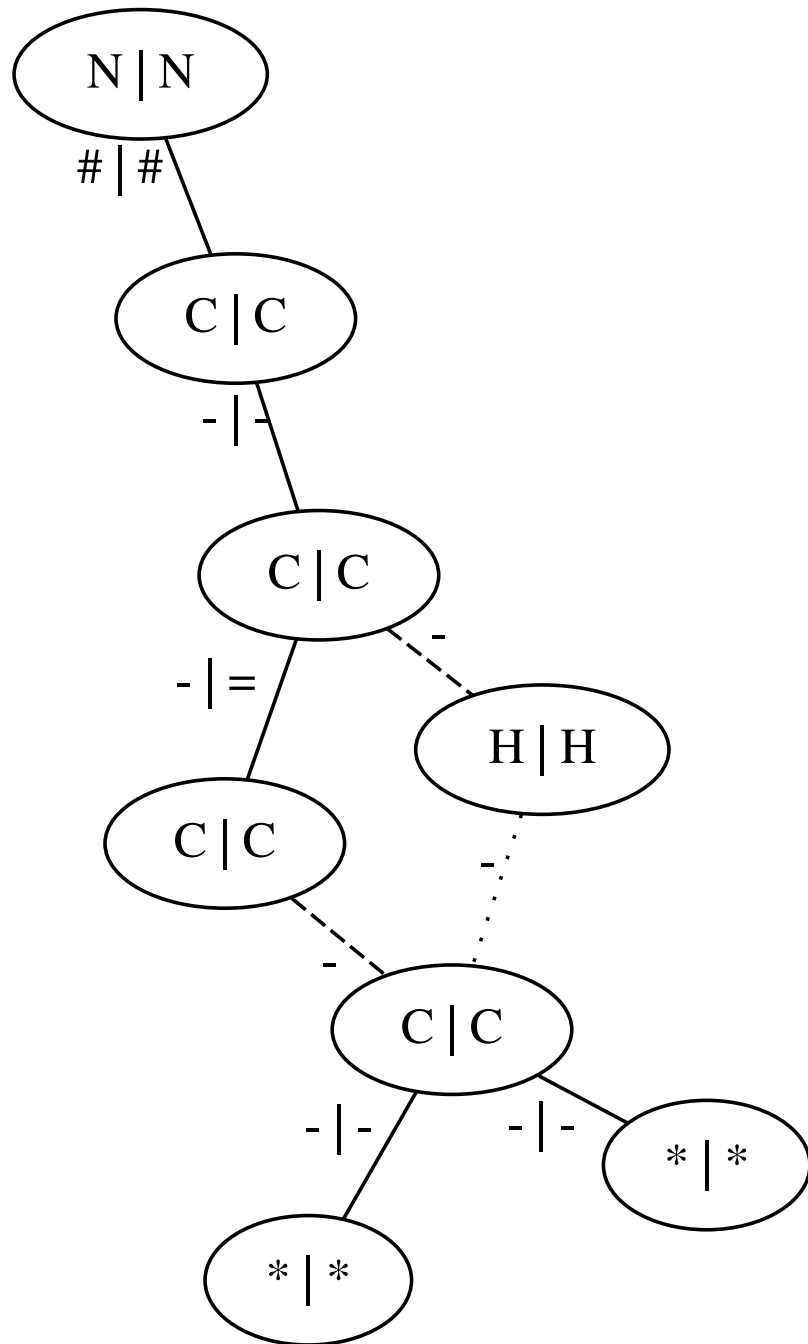
$$\begin{aligned} & |\{e \in \text{outEdges}(0) \mid \\ & \quad \text{label}(\text{target}(e)) \in \{\text{'0'}\} \\ & \quad \wedge \\ & \quad \text{label}(e) \in \{\text{'-'}\} \\ & \quad \} | = 0 \end{aligned}$$
$$\begin{aligned} & |\{e \in \text{outEdges}(1) \mid \\ & \quad \text{label}(\text{target}(e))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

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

1.0.205 Michael Addition 2,2, (reverse)



Files: out/817_r_208_10300110_{L, K, R}



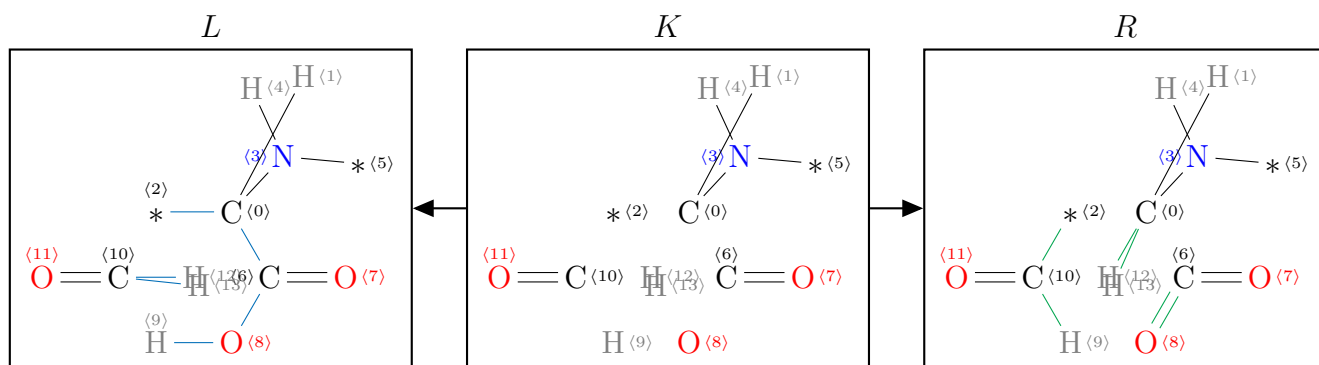
File: out/818_r_208_combined

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

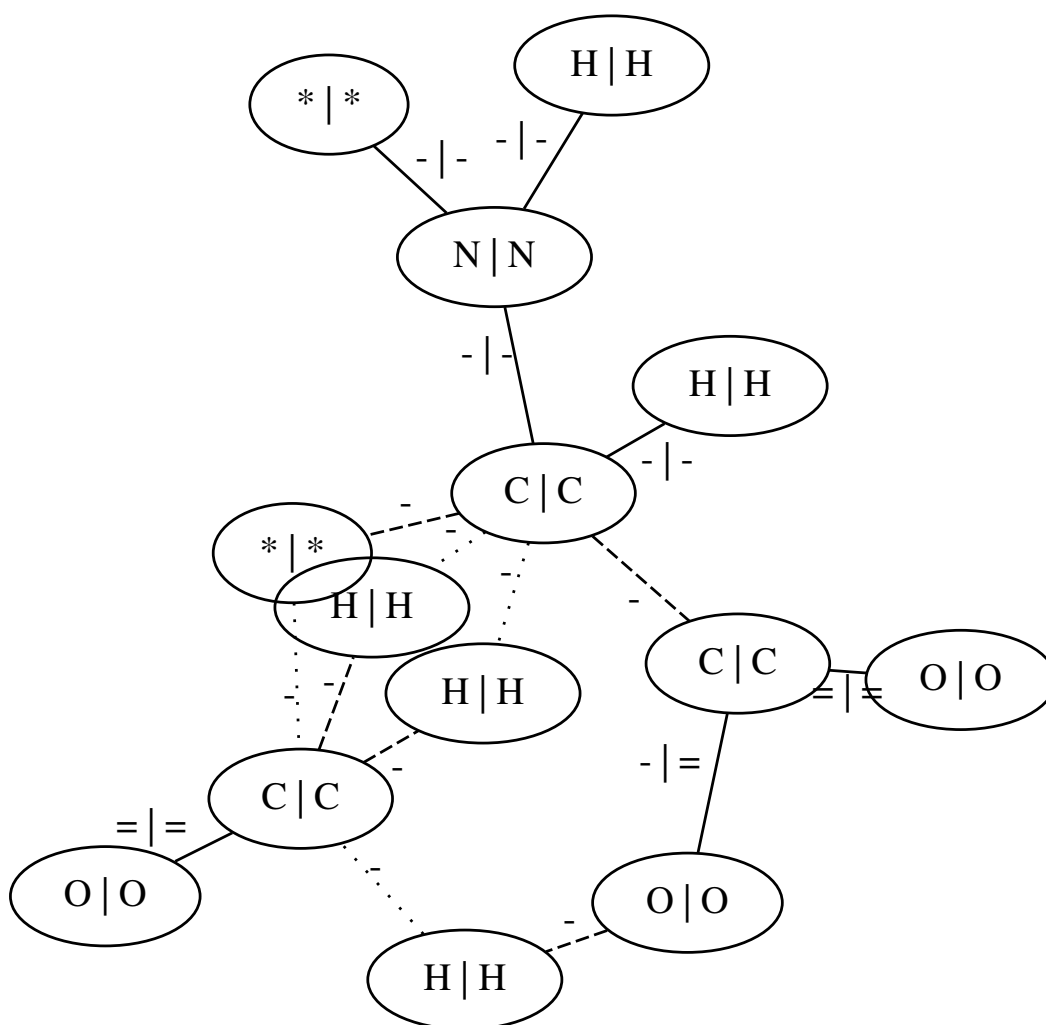
$$\begin{aligned}
& |\{e \in \text{outEdges}(1) \mid \\
& \quad \text{label}(\text{target}(e)) \in \{'0'\} \\
& \quad \wedge \\
& \quad \text{label}(e) \in \{'-\'} \\
& \quad \}\mid = 0
\end{aligned}$$

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

1.0.206 Strecker Degradation, HH

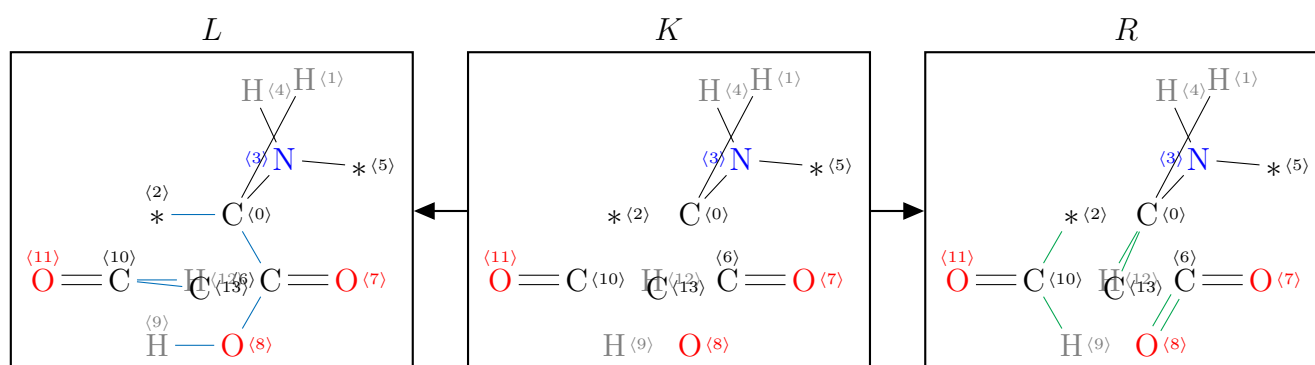


Files: out/821_r_209_10300110_{L, K, R}

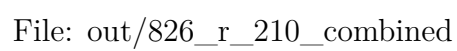


File: out/822_r_209_combined

1.0.207 Strecker Degradation, HC

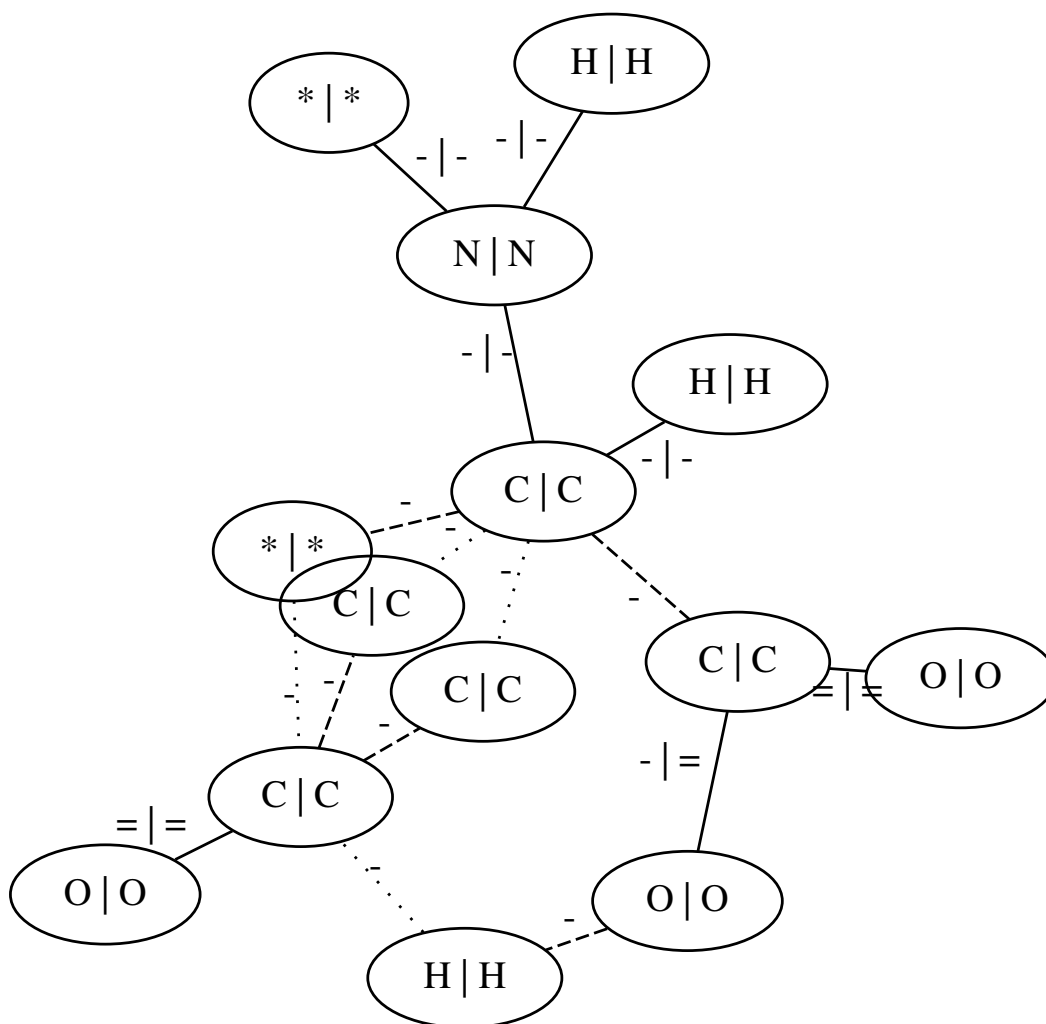
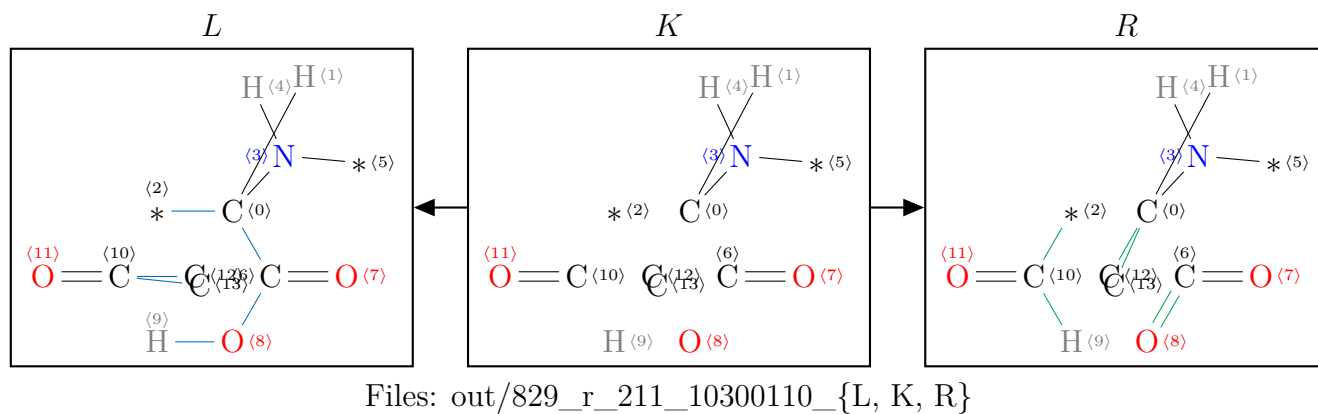


Files: out/825_r_210_10300110_{L, K, R}



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1.0.208 Strecker Degradation, CC



File: out/830_r_211_combined

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

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