Summary

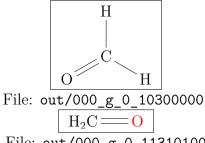
October 16, 2019

Contents

0.1	Loade	d Graphs	2
	0.1.1	Formaldehyde	2
	0.1.2	Glycolaldehyde	2
0.2	Loade	d Rules	2
	0.2.1	Keto-enol isomerization ->	2
	0.2.2	Keto-enol isomerization <	3
	0.2.3	Aldol Addition ->	4
	0.2.4	Aldol Addition <	5
	0.2.5	DG Hyper, dg_0	6
0.3	Flow S	Solutions, id 0	6
	0.3.1	Solution 0	6
0.4	Flow S	Solutions, id 1	7
	0.4.1	Solution 0	7

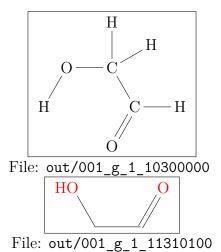
0.1 Loaded Graphs

0.1.1Formaldehyde



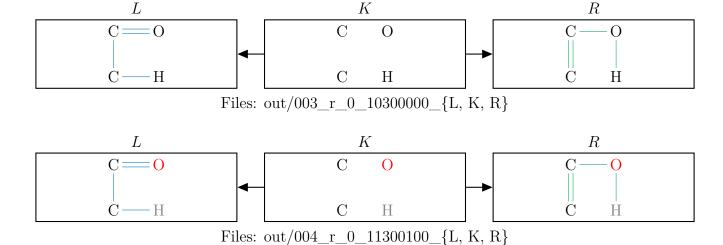
File: out/000_g_0_11310100

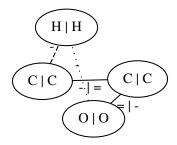
Glycolaldehyde 0.1.2



Loaded Rules 0.2

Keto-enol isomerization \rightarrow 0.2.1





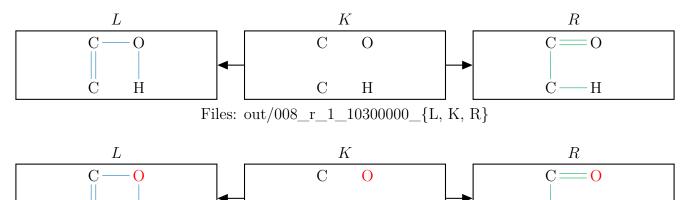
File: $out/005_r_0_combined$

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

0.2.2 Keto-enol isomerization <-

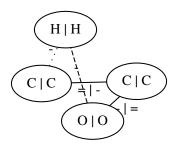
 \mathbf{C}

Н



Files: out/009_r_1_11300100_{L, K, R}

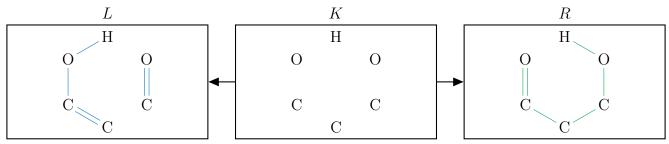
Н



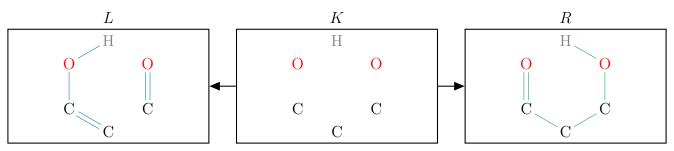
File: out/010_r_1_combined

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

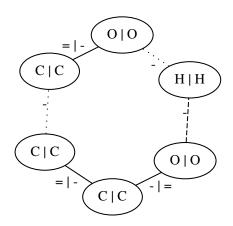
0.2.3 Aldol Addition ->



Files: $out/013_r_2_10300000_{L, K, R}$



Files: out/014_r_2_11300100_{L, K, R}

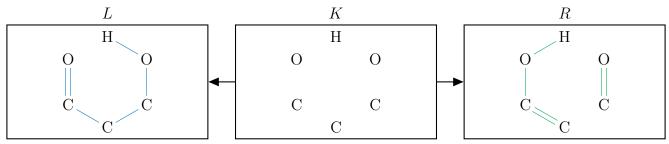


File: out/015_r_2_combined

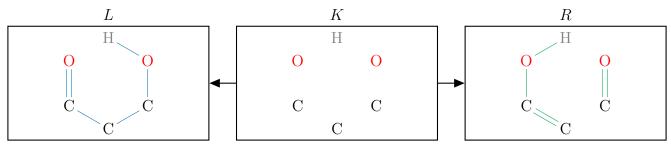
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\begin{aligned} |\{e \in \text{outEdges}(1) \mid \\ \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\ \}| = 1 \end{aligned}
```

$$\begin{aligned} |\{e \in \text{outEdges}(5) \mid \\ \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\ \}| = 1 \end{aligned}$$

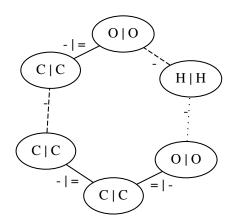
0.2.4 Aldol Addition <-



Files: $out/018_r_3_10300000_{L, K, R}$



Files: out/019_r_3_11300100_{L, K, R}

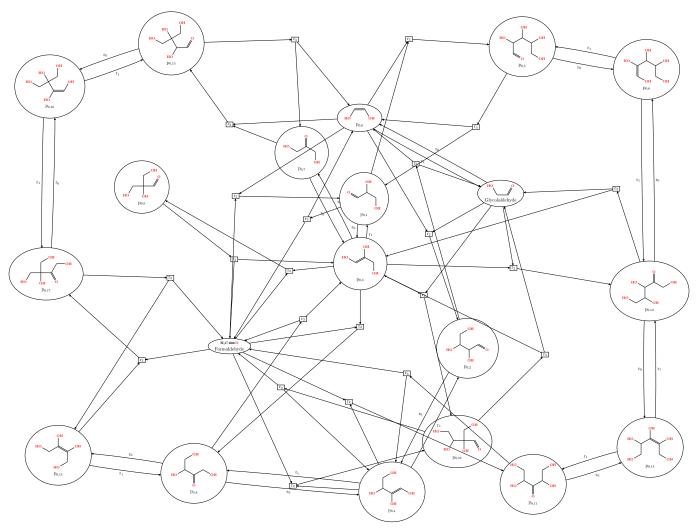


File: out/020_r_3_combined

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

$$\begin{aligned} |\{e \in \text{outEdges}(5) \mid \\ \text{label}(\text{target}(e)) \in \{\text{`0'}\} \\ \}| = 1 \end{aligned}$$

0.2.5 DG Hyper, dg_0



File: out/041_dg_0_11100

0.3 Flow Solutions, id 0

0.3.1 Solution 0

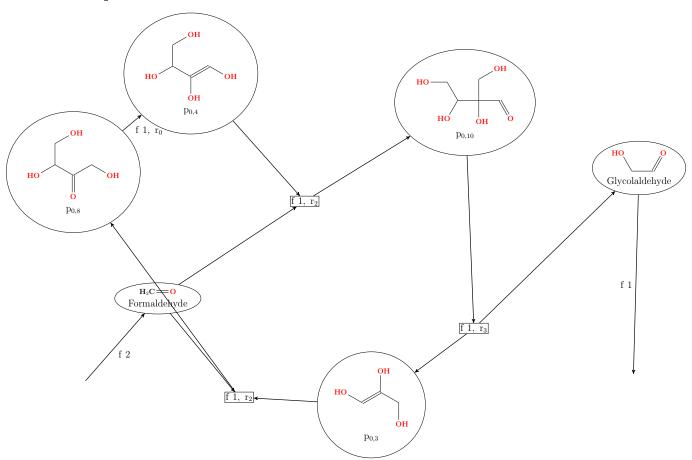
Overall Data

Solution 0 from flow model 0

Objective value: 6

Formaldehyde: inFlow = 2 outFlow = 0 isInCycle = false Glycolaldehyde: inFlow = 0 outFlow = 1 isInCycle = false

Filtered Graph



File: out/045_dg_0_11100_f_0_0_filt

0.4 Flow Solutions, id 1

0.4.1 Solution 0

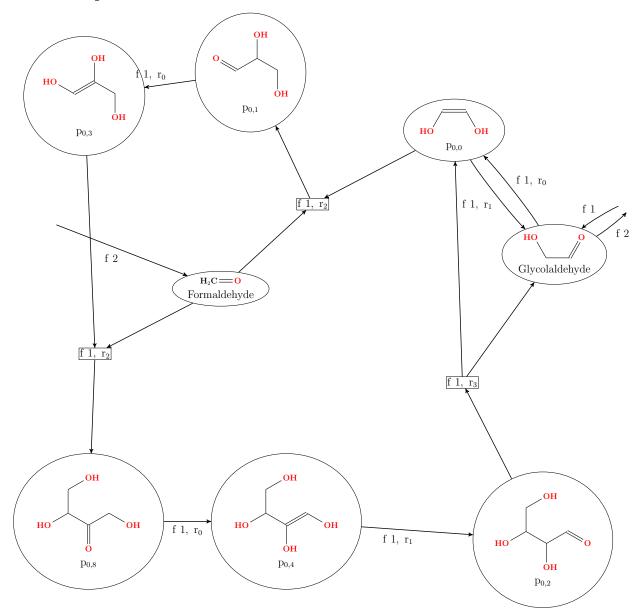
Overall Data

Solution 0 from flow model 1

Objective value: 12

Formaldehyde: inFlow = 2 outFlow = 0 isOverallAutocata = 0 isInCycle = false Glycolaldehyde: inFlow = 1 outFlow = 2 isOverallAutocata = 1 isInCycle = true

Filtered Graph



 $File: \ \mathtt{out/049_dg_0_11100_f_1_0_filt}$