Summary

September 20, 2021

Contents
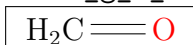
0.1 Loaded Graphs

0.1.1 Formaldehyde

H
|
C
O   H
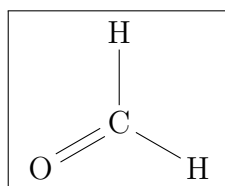
File: out/000_g_0_10300000

$H_2C = O$

File: out/000_g_0_11310100

0.1.2 Glycolaldehyde
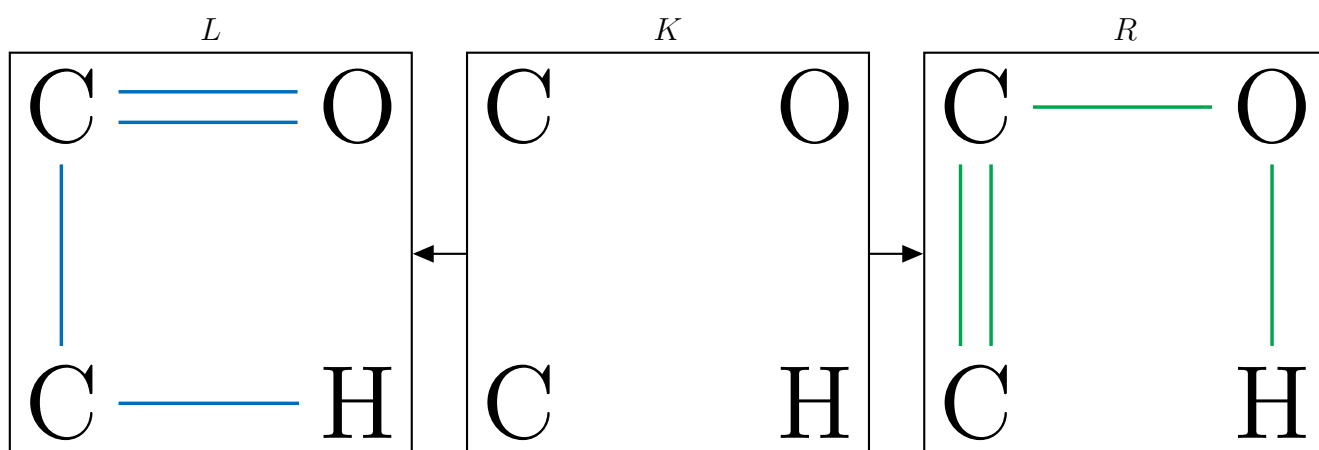
H
H
O — C
H   C — H
O
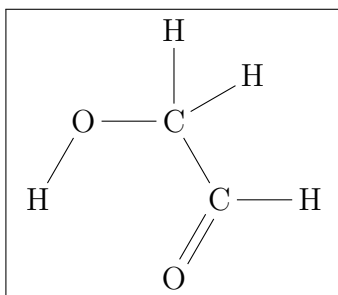
File: out/001_g_1_10300000
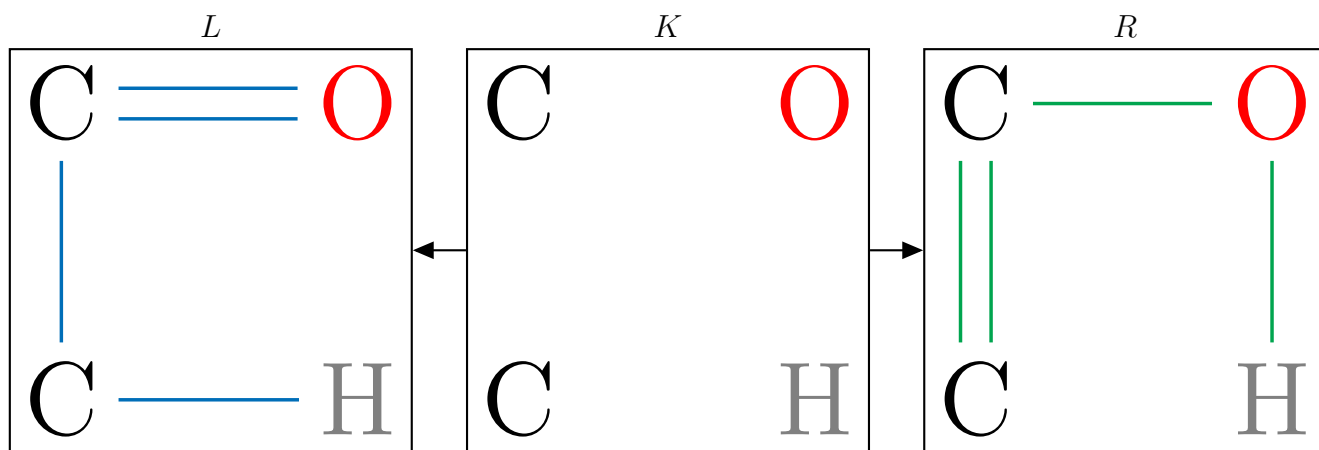
HO   O
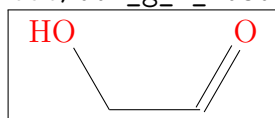
File: out/001_g_1_11310100

0.2 Loaded Rules

0.2.1 Keto-enol isomerization ->

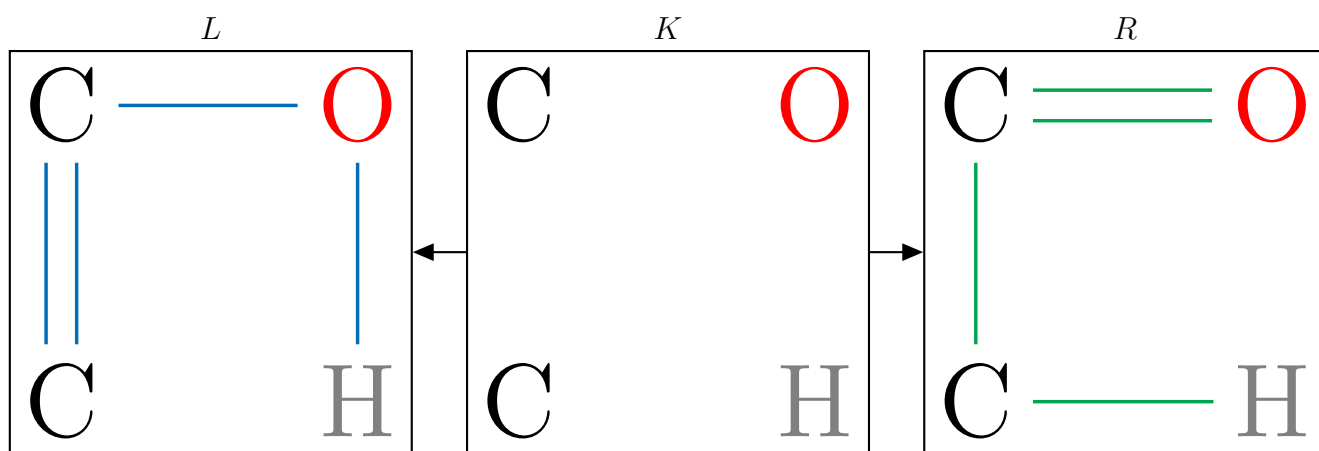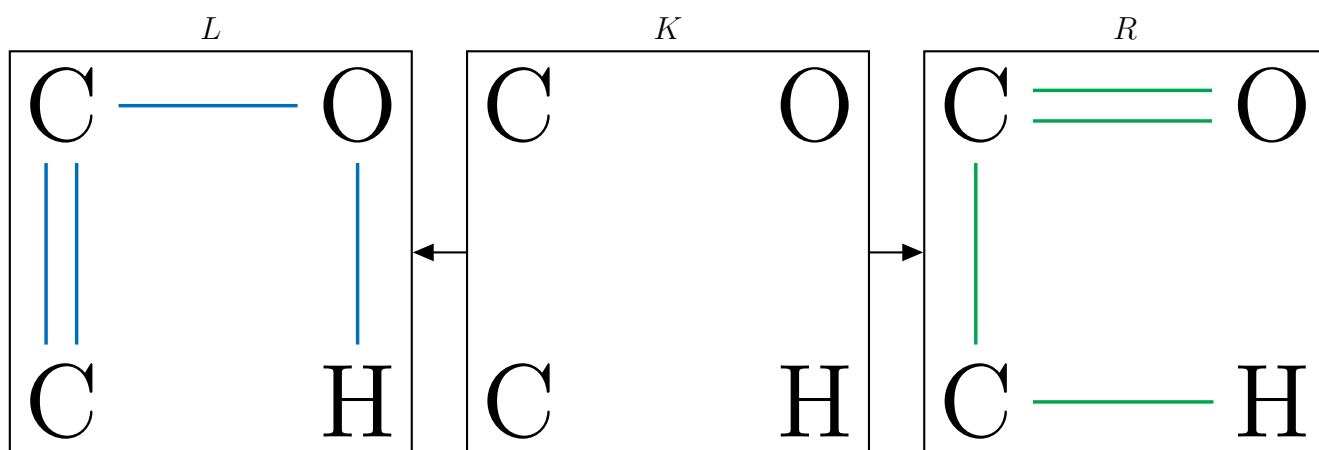L   K   R

C === O   C   O   C — O

C — H   C   H   C   H

Files: out/003_r_0_10300000_{L, K, R}

Files: out/004_r_0_11300100_{L, K, R}

$$|\{e \in \text{outEdges}(1) \mid$$
$$\text{label}(\text{target}(e)) \in \{\text{`O'}\}$$
$$\}| = 1$$
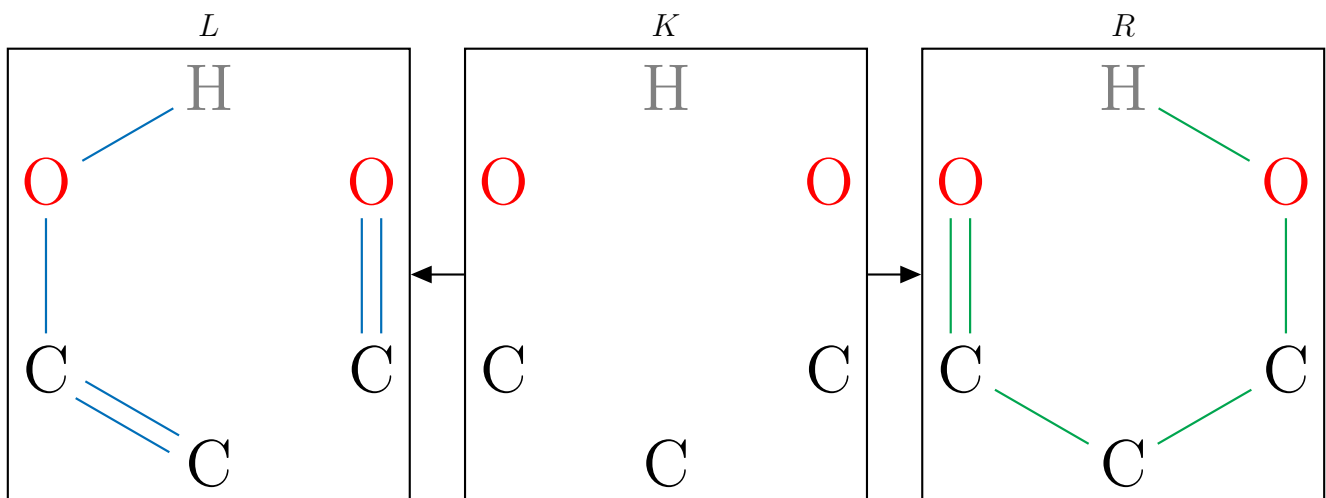
0.2.2 Keto-enol isomerization <-

Files: out/007_r_1_10300000_{L, K, R}

Files: out/008_r_1_11300100_{L, K, R}

0.2.3 Aldol Addition ->

L	K	R
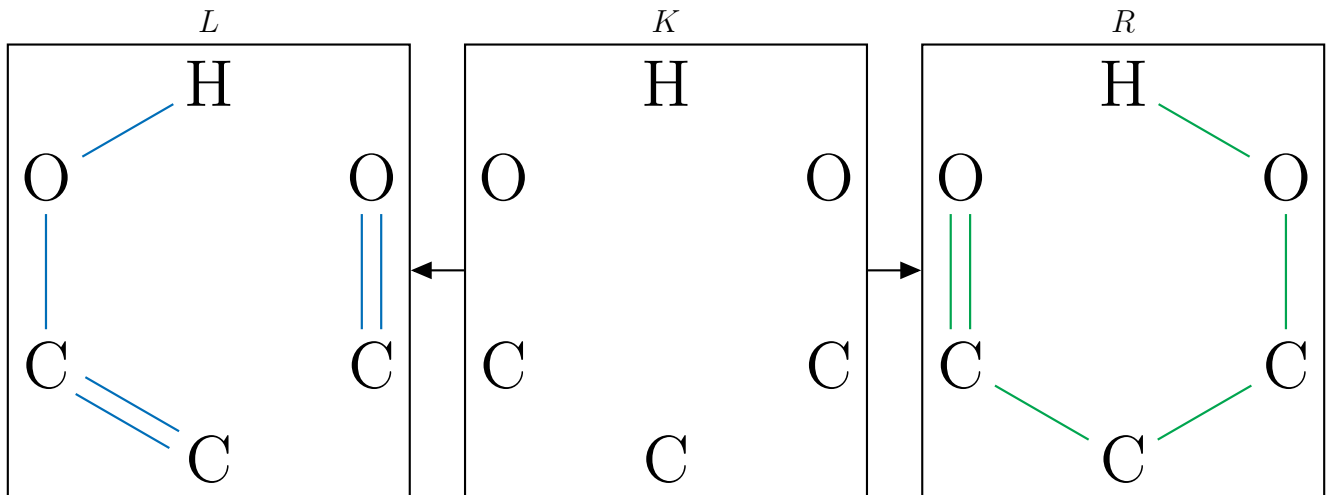
Files: out/011_r_2_10300000_{L, K, R}

L	K	R

Files: out/012_r_2_11300100_{L, K, R}

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

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

0.2.4 Aldol Addition <-
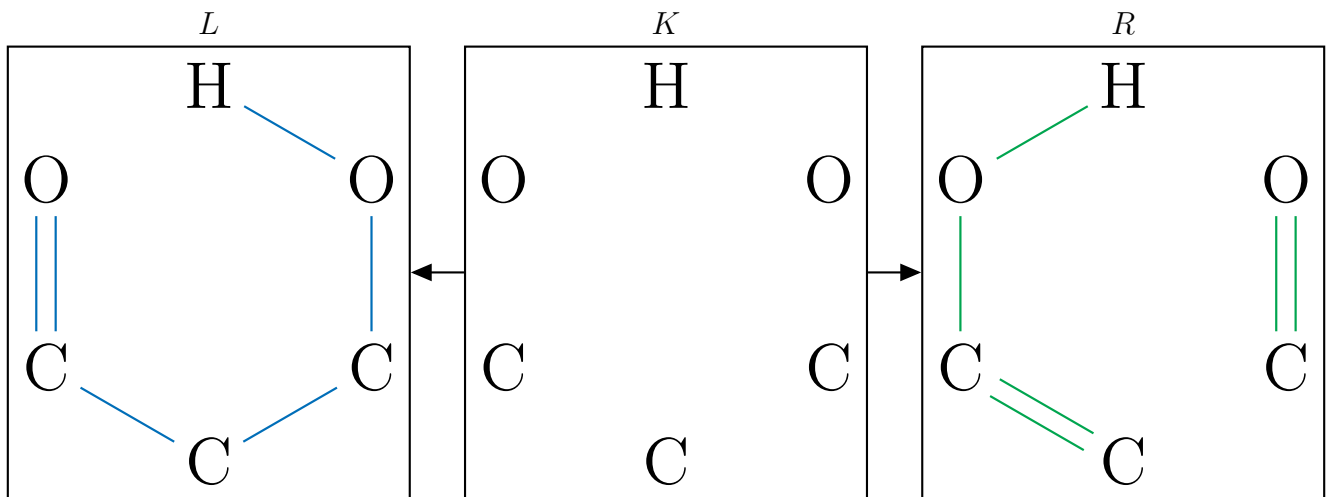
Files: out/015__r_3_10300000__{L, K, R}
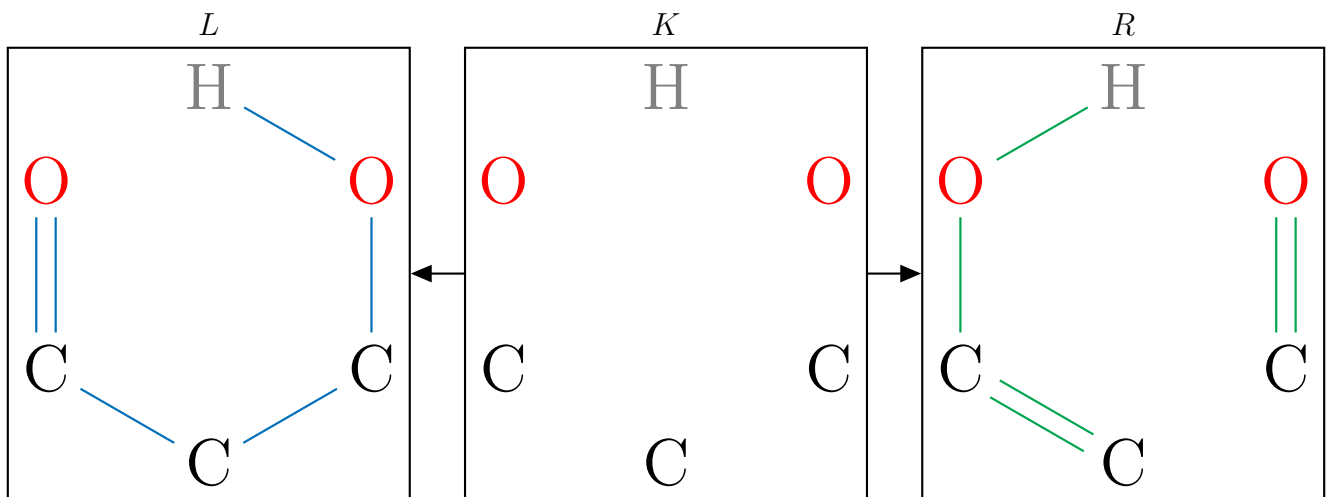
Files: out/016__r_3_11300100__{L, K, R}

$$|\{e \in \text{outEdges}(1) \mid$$
$$\quad \text{label}(\text{target}(e)) \in \{\text{‘O’}\}$$
$$\}| = 1$$

$$|\{e \in \text{outEdges}(5) \mid$$
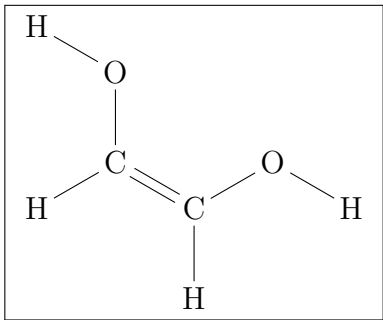$$\quad \text{label}(\text{target}(e)) \in \{\text{‘O’}\}$$
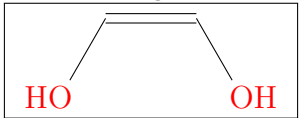$$\}| = 1$$

0.2.5 DG Hyper, `dg_0`
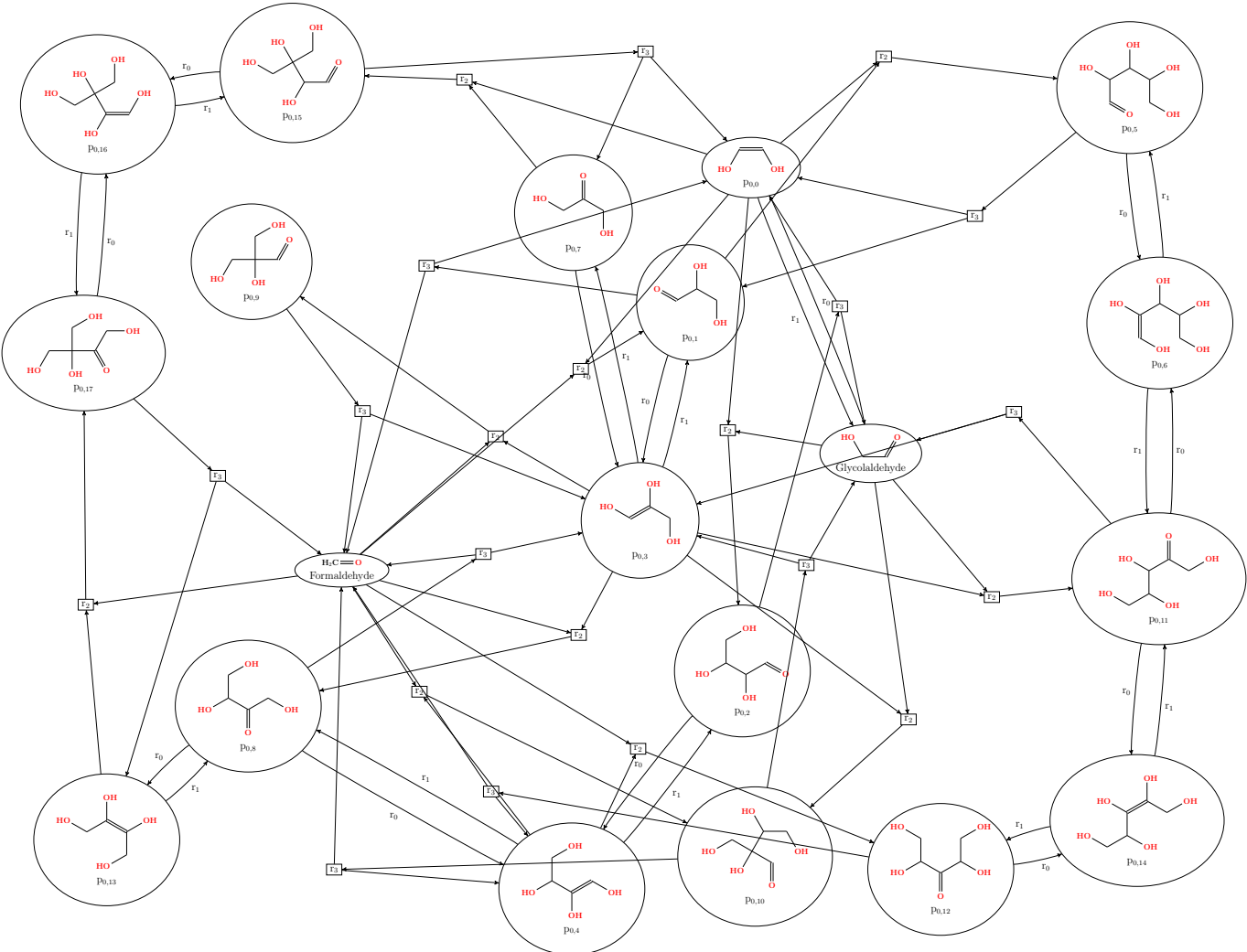
File: `out/037_dg_0_11100`
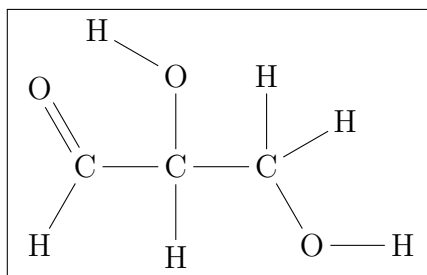
0.3 Product Graphs
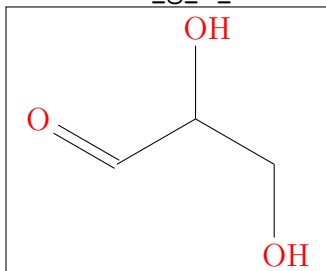
0.3.1 `p_{0,0}`

File: `out/019_g_2_10300000`
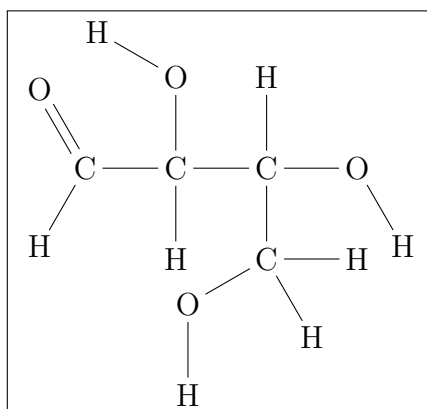

File: `out/019_g_2_11310100`
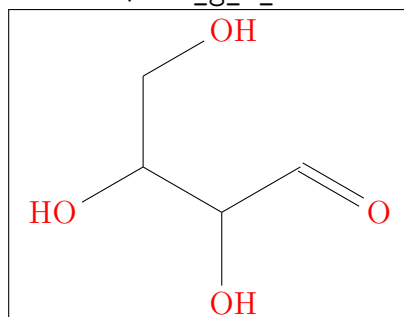
0.3.2 p_{0,1}

File: out/020_g_6_10300000

File: out/020_g_6_11310100

0.3.3 p_{0,2}
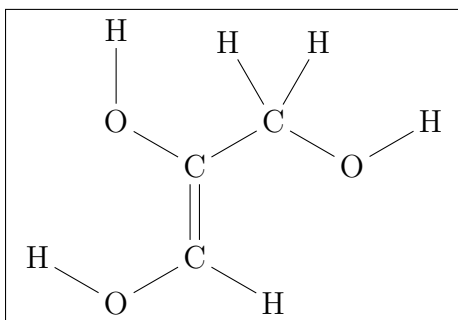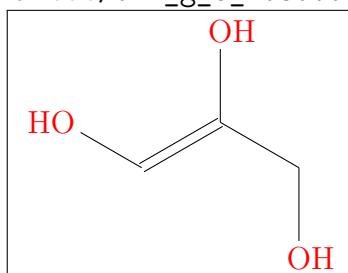

File: out/021_g_7_10300000
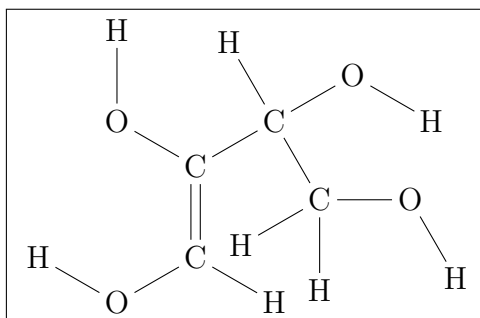

File: out/021_g_7_11310100
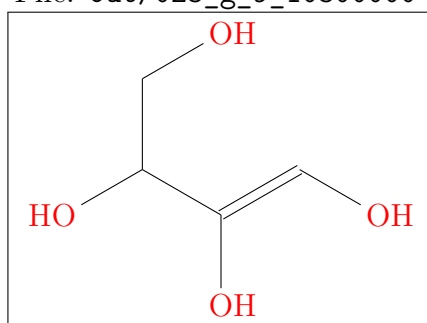
0.3.4 p_{0,3}

File: out/022_g_8_10300000
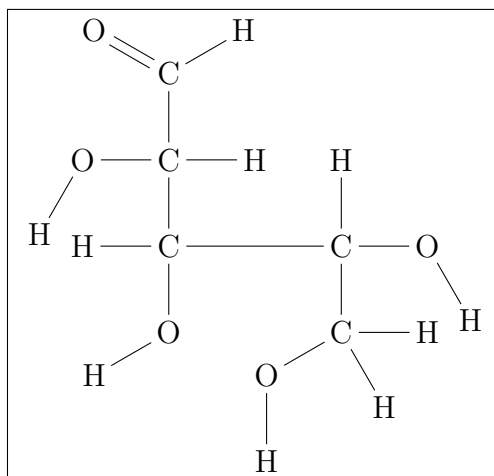

File: out/022_g_8_11310100
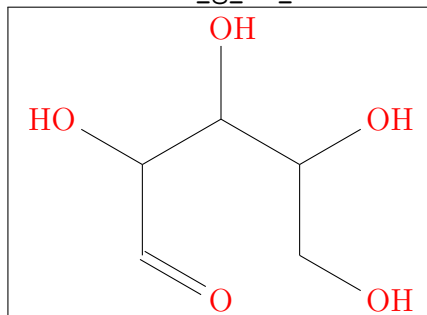
0.3.5 p_{0,4}

File: out/023_g_9_10300000
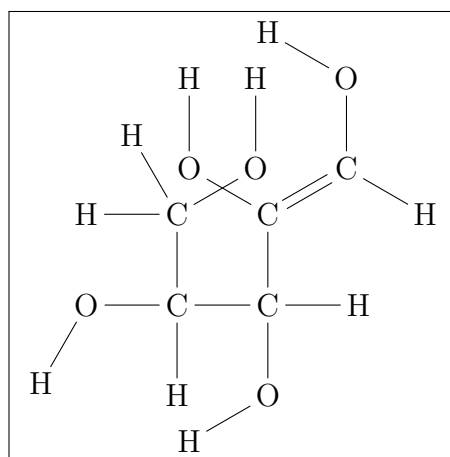

File: out/023_g_9_11310100

0.3.6 p_{0,5}

File: out/024_g_10_10300000
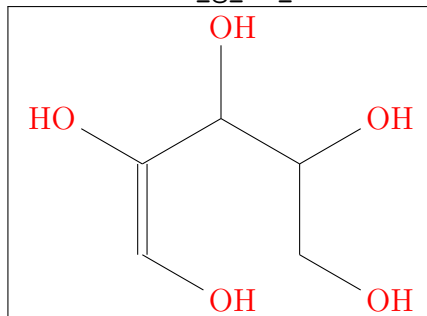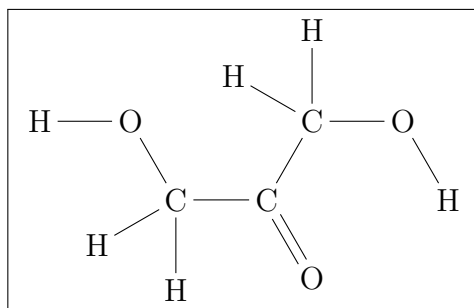

File: out/024_g_10_11310100

0.3.7 p_{0,6}

File: out/025_g_18_10300000

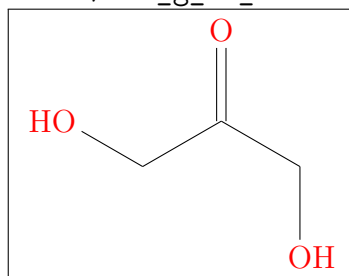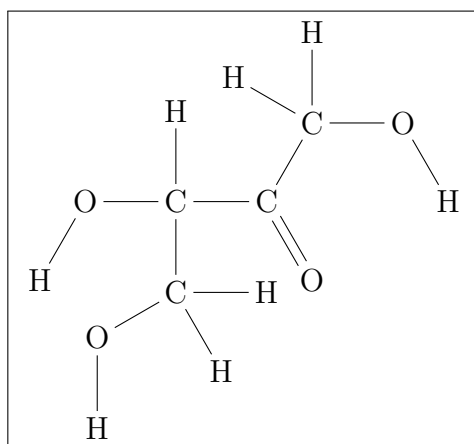

File: out/025_g_18_11310100
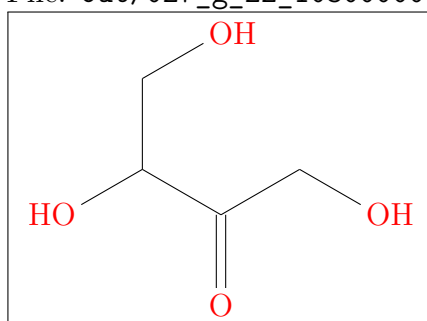
0.3.8 p_{0,7}

File: out/026_g_20_10300000

File: out/026_g_20_11310100

0.3.9 p_{0,8}
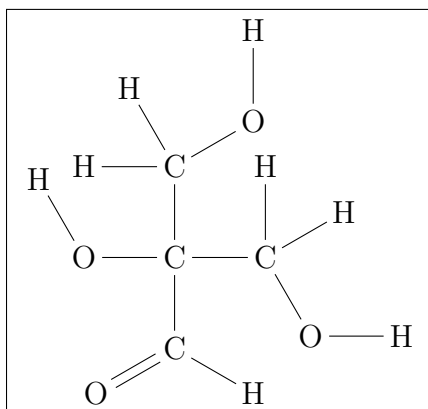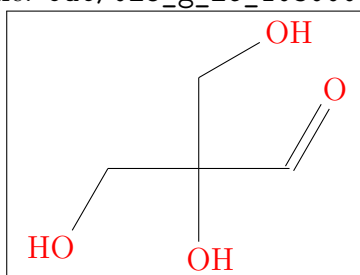

File: out/027_g_22_10300000
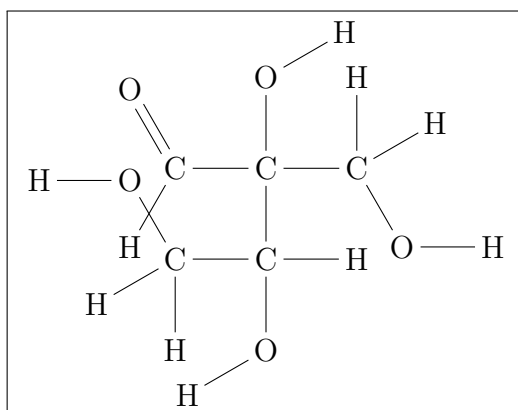

File: out/027_g_22_11310100
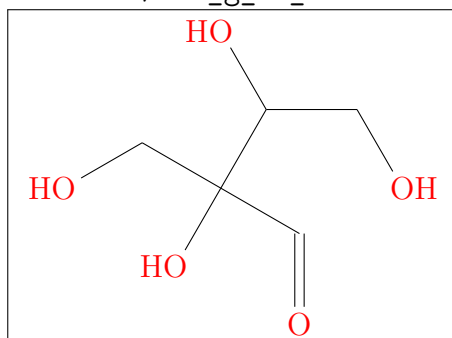
0.3.10 p_{0,9}

File: out/028_g_26_10300000
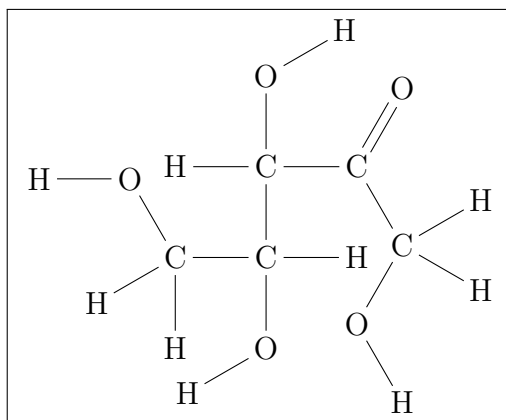

File: out/028_g_26_11310100
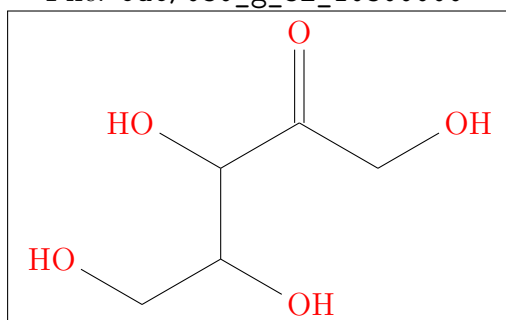
0.3.11 p_{0,10}

File: out/029_g_27_10300000
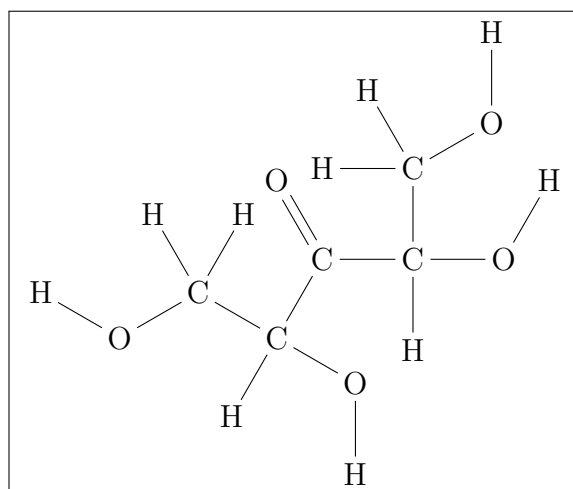

File: out/029_g_27_11310100

0.3.12 p_{0,11}

File: out/030_g_32_10300000
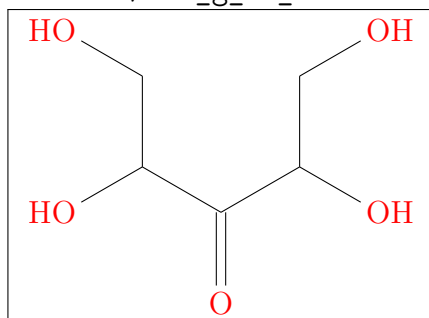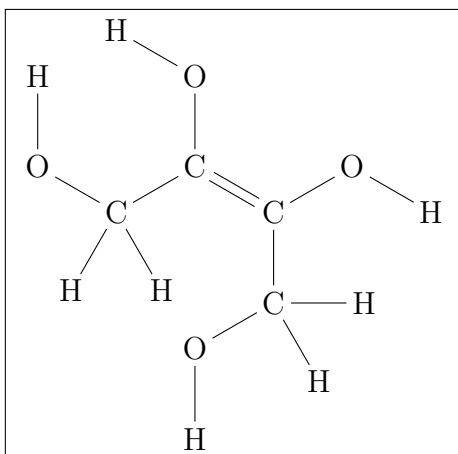

File: out/030_g_32_11310100

0.3.13 p_{0,12}

File: out/031_g_41_10300000
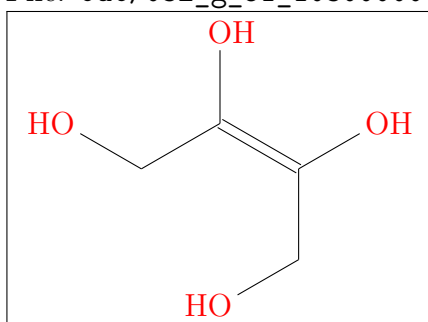

File: out/031_g_41_11310100

0.3.14 p_{0,13}
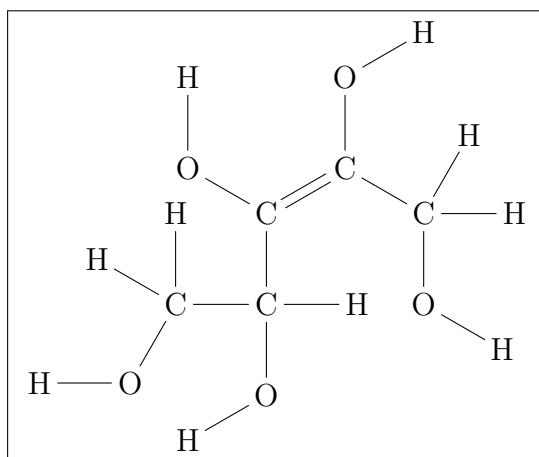

File: out/032_g_51_10300000
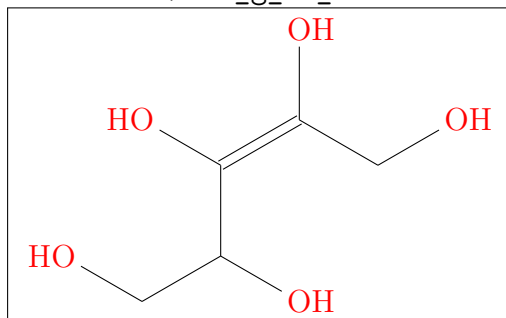

File: out/032_g_51_11310100

0.3.15 p_{0,14}
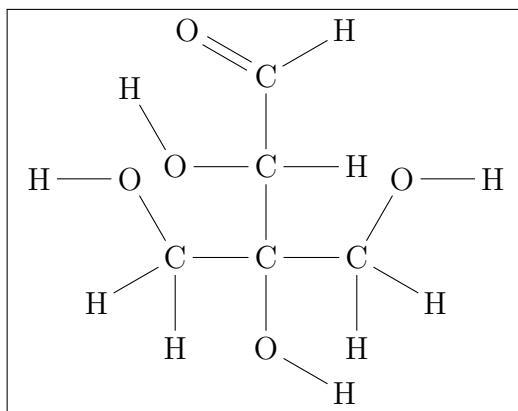

File: out/033_g_56_10300000
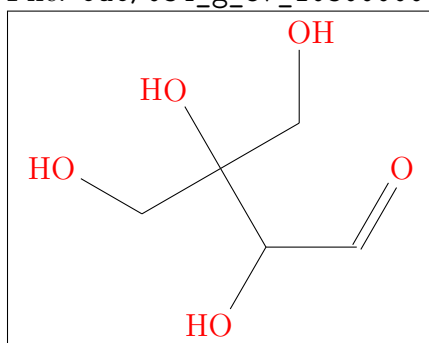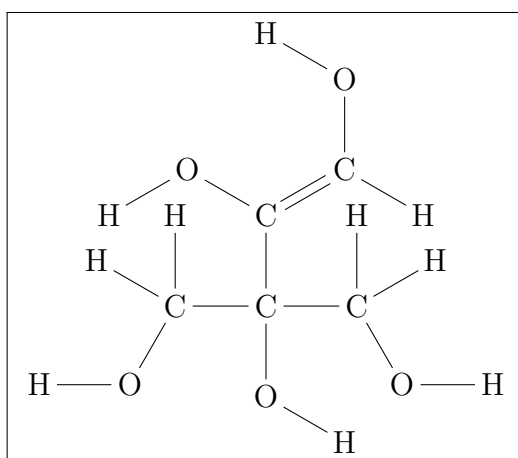

File: out/033_g_56_11310100
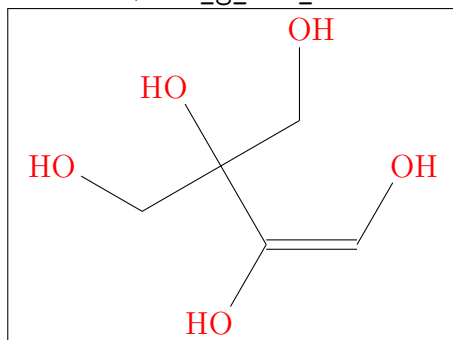
0.3.16 p_{0,15}

File: out/034_g_87_10300000

File: out/034_g_87_11310100

0.3.17 p_{0,16}
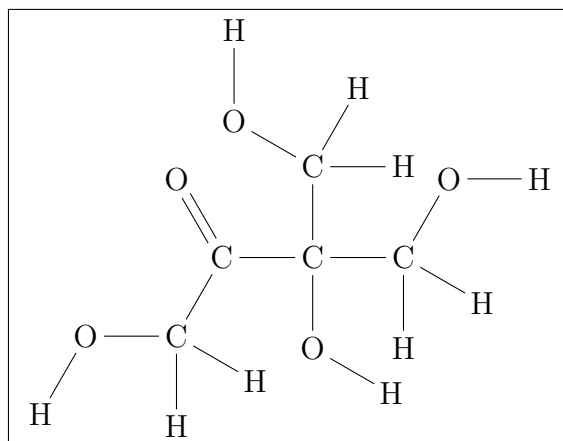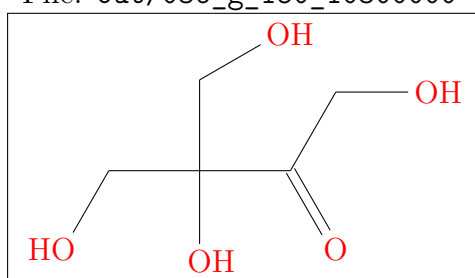

File: out/035_g_135_10300000

File: out/035_g_135_11310100

0.3.18 `p_{0,17}`

File: `out/036_g_150_10300000`

File: `out/036_g_150_11310100`

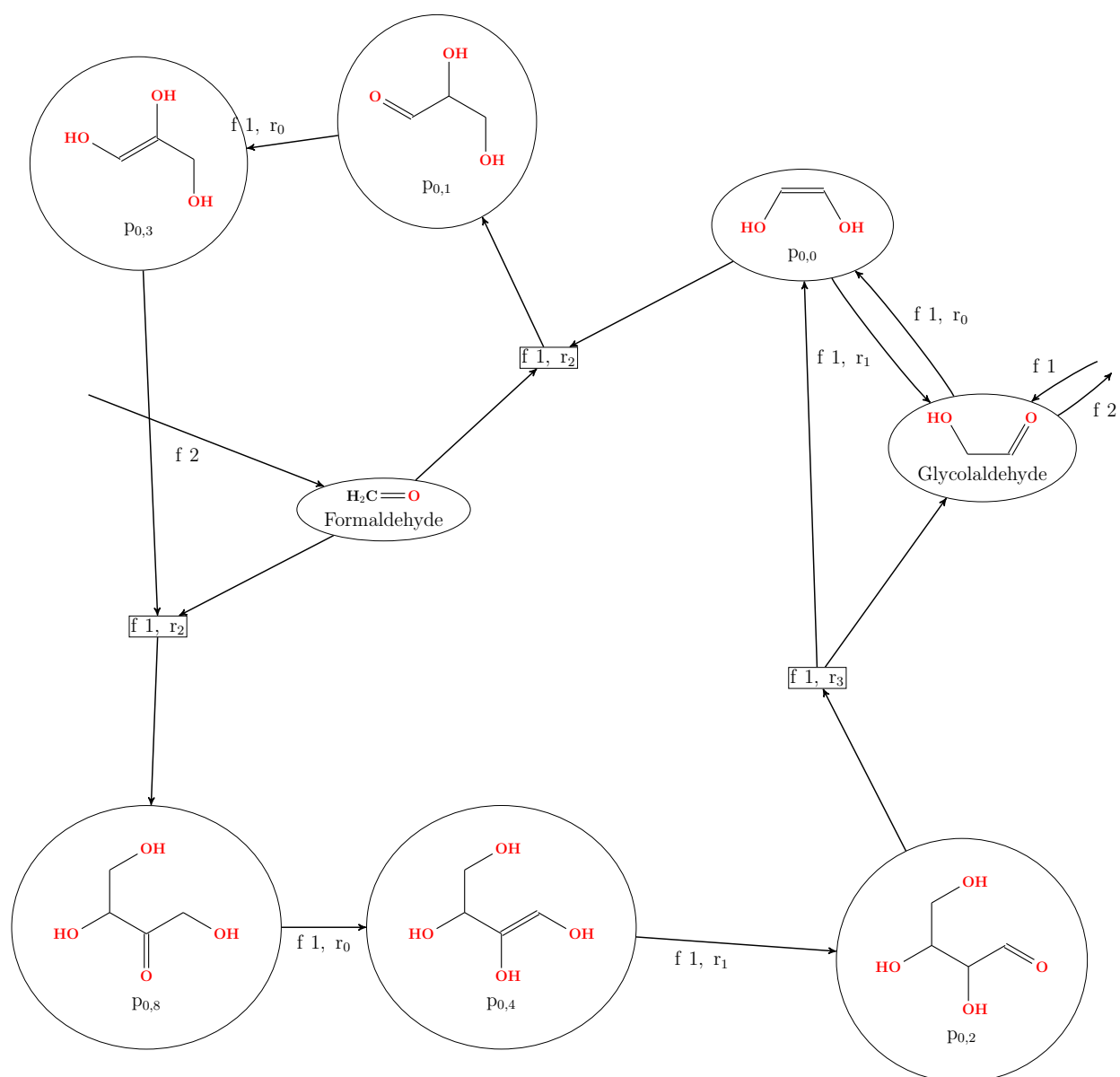# 0.4 Flow Solutions, id 0

0.4.1 Solution 0

Overall Data

```
Objective value (integral): 12
Vertex/Graph    In Out OA
Formaldehyde    2  0   0
Glycolaldehyde 1  2   1
```

Filtered Graph

File: out/041_dg_0_11100_f_0_0_filt