Summary

June 10, 2020

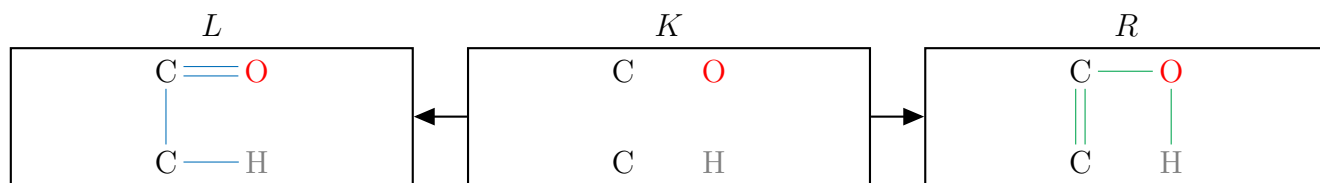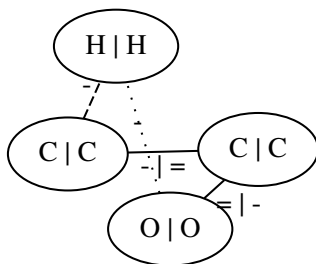# Contents

0.1 Input Rules

0.1.1 Keto-enol isomerization
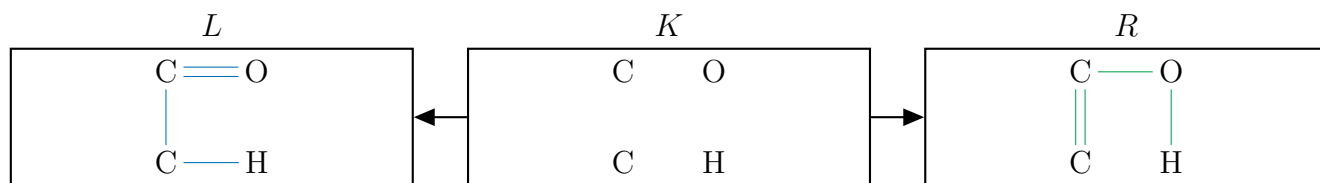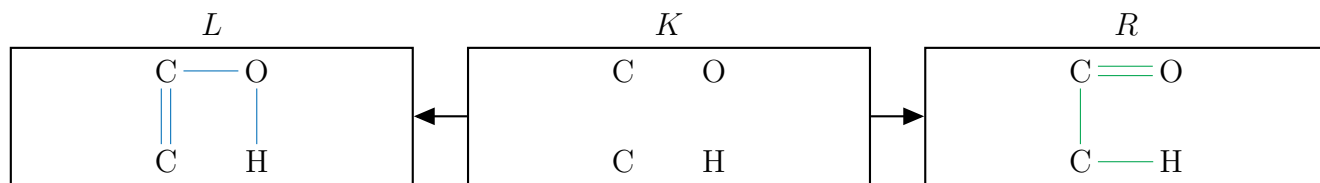

Files: out/001_r_0_10300000_{L, K, R}

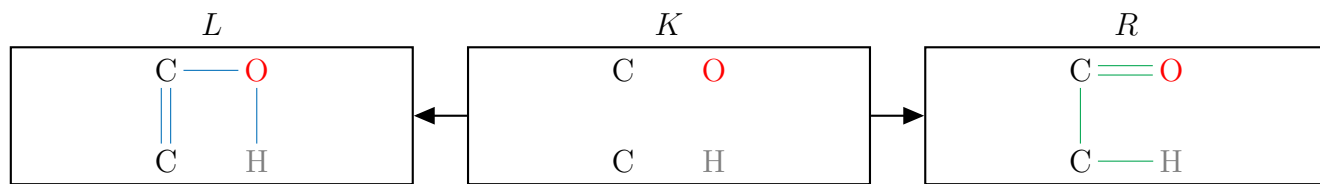Files: out/002_r_0_11300100_{L, K, R}

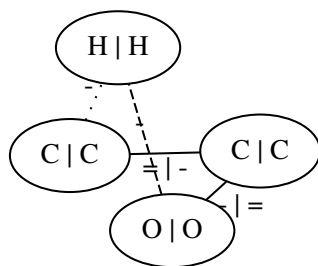File: out/003_r_0_combined

0.1.2 Keto-enol isomerization, inverse
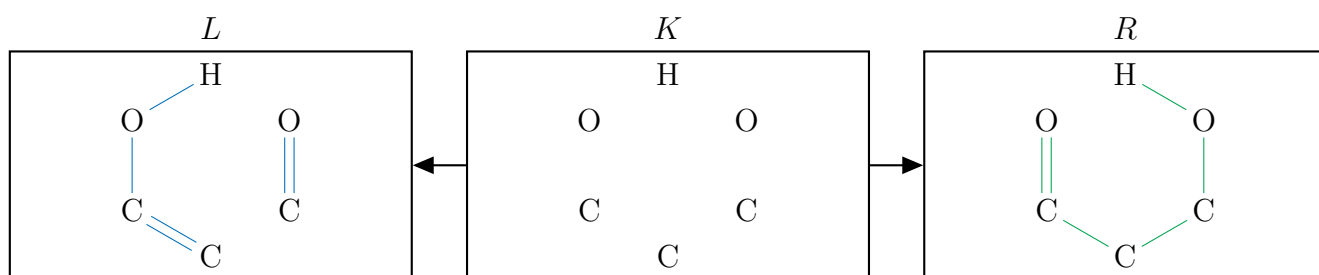

Files: out/006_r_1_10300000_{L, K, R}
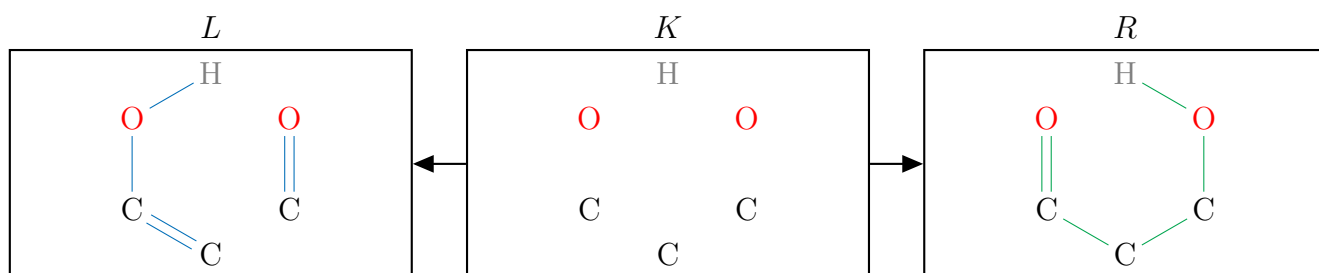

Files: out/007_r_1_11300100_{L, K, R}

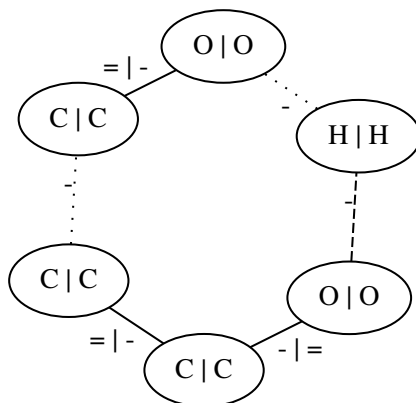File: out/008_r_1_combined

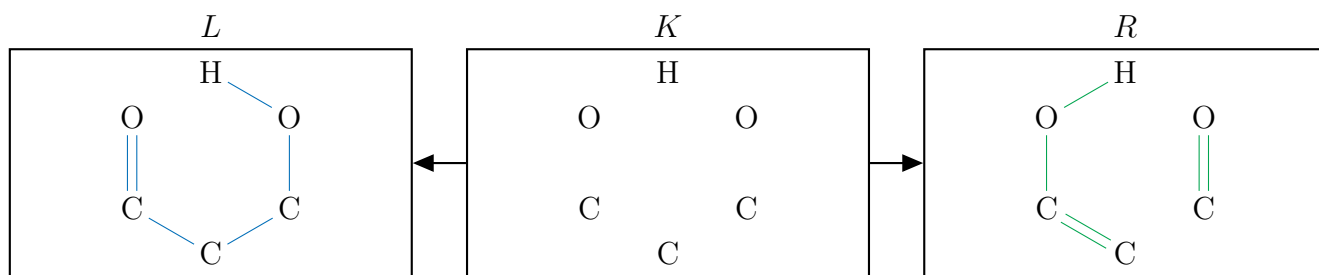## 0.1.3 Aldol Addition

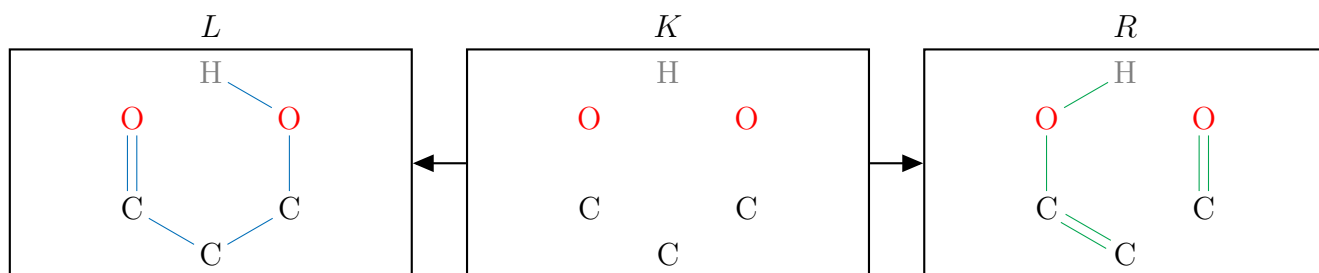Files: out/011_r_2_10300000_{L, K, R}

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

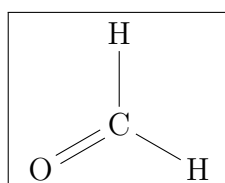### 0.1.4 Aldol Addition, inverse

Files: out/016_r_3_10300000_{L, K, R}

Files: out/017_r_3_11300100_{L, K, R}
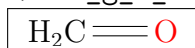

File: out/018_r_3_combined
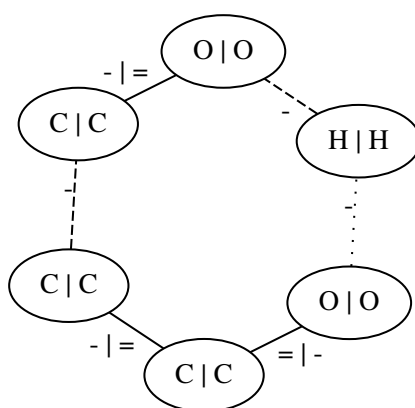
0.2 Input Graphs (Molecules)

0.2.1 Formaldehyde

$$H_2C = O$$

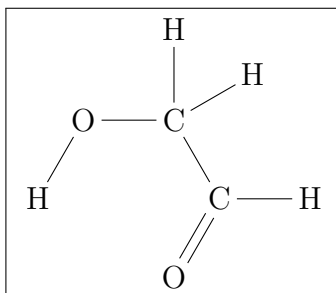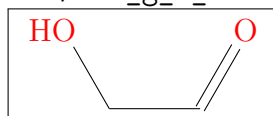## 0.2.2 Glycolaldehyde

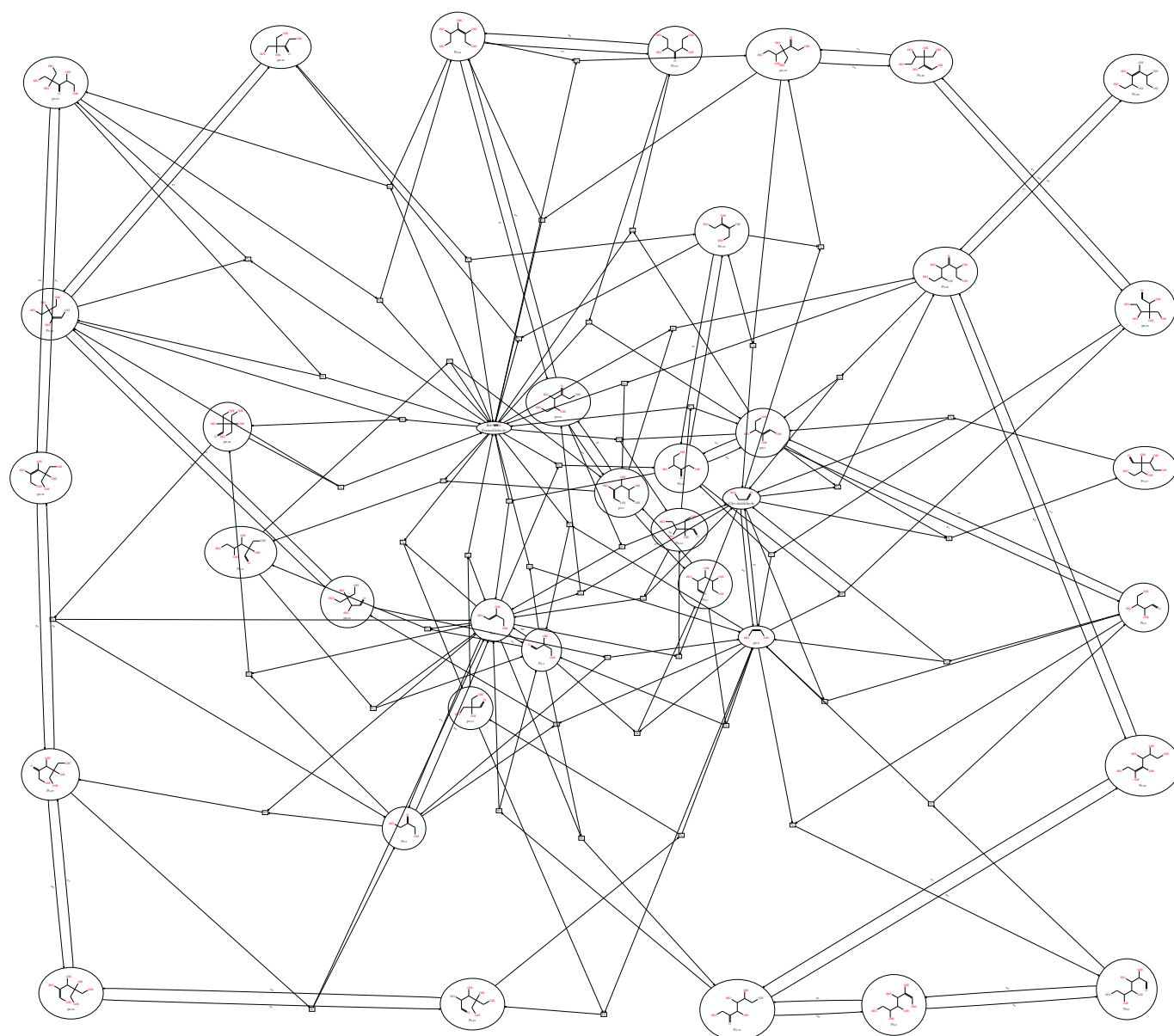File: out/021_g_1_10300000

File: out/021_g_1_11310100

0.2.3 DG Hyper, `dg_0`

File: `out/058_dg_0_11100`