# Summary

December 7, 2024

# Contents

## 0.1 Loaded Graphs

### 0.1.1 g_{0}

$$N \equiv C \longrightarrow H$$

File: out/001_g_0_10300000

$$N \equiv CH$$

File: out/003_g_0_11310100

### 0.1.2 g_{1}

$$
\begin{array}{ccc}
H & & H \\
 & N & \\
 & H &
\end{array}
$$

File: out/005_g_1_10300000

$$NH_3$$

File: out/007_g_1_11310100

### 0.1.3 g_{2}

$$
\begin{array}{ccc}
H & & H \\
 & O &
\end{array}
$$

File: out/009_g_2_10300000

$$H_2O$$
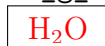
File: out/011_g_2_11310100

## 0.2 Product Graphs

### 0.2.1 p_{0,56}

File: out/013_g_1088_10300000
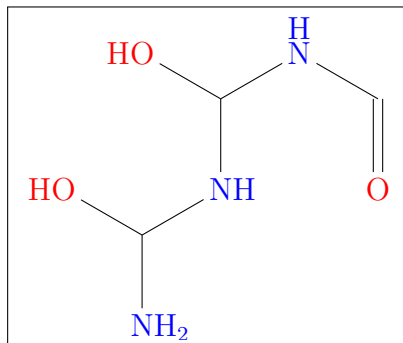
File: `out/015_g_1088_11310100`

# 0.3 Enumerated Flows

## 0.3.1 Solution 0

**Overall Data**

```
Objective value (non-integral): -0.131064
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  1.000000  0
g_{2}        3  0   -5.068043  1.000000  0
p_{0,13}     0  0   -21.240678 -9.000000 65
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
p_{0,5}      0  0   -16.158998 1.000000  64
```

# Filtered Graph
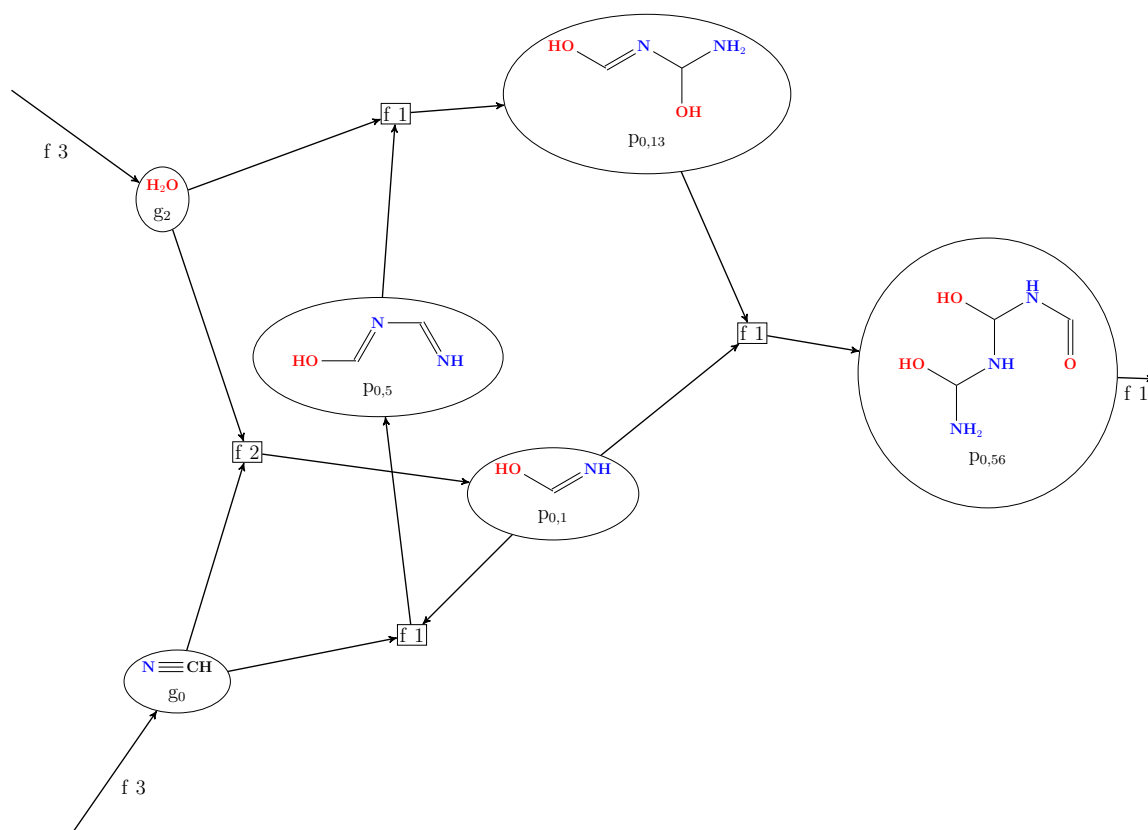


File: `out/029_dg_0_11100_f_0_0_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,5}$ | 0 | 0 | $-42425.44262$ | $1.0$ | $-42422.116835$ | 64 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | 65 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 2 | $-95.803747$ | $-95.803747$ |
| 14 | $g_0, p_{0,1},$ | $p_{0,5},$ | 1 | $-113.75722$ | $-113.75722$ |
| 123 | $g_2, p_{0,5},$ | $p_{0,13},$ | 1 | $-81.533092$ | $-81.533092$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $-52.84784$ | $-52.84784$ |
| Sum | | | | | $-344.1086723480411$ |

$\Delta G$ = -43.97456408759082

$\Delta E$ = -0.13106407145277477

|E| = 5

|U| = 4

## 0.3.2 Solution 1

**Overall Data**

```
Objective value (non-integral): -0.131064
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  0
p_{0,13}     0  0   -21.240678 0.613824   63
p_{0,15}     0  0   -10.625174 -7.010180  2
p_{0,17}     0  0   -21.248887 1.000000   64
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
p_{0,5}      0  0   -16.158998 1.000000   62
```

**Filtered Graph**
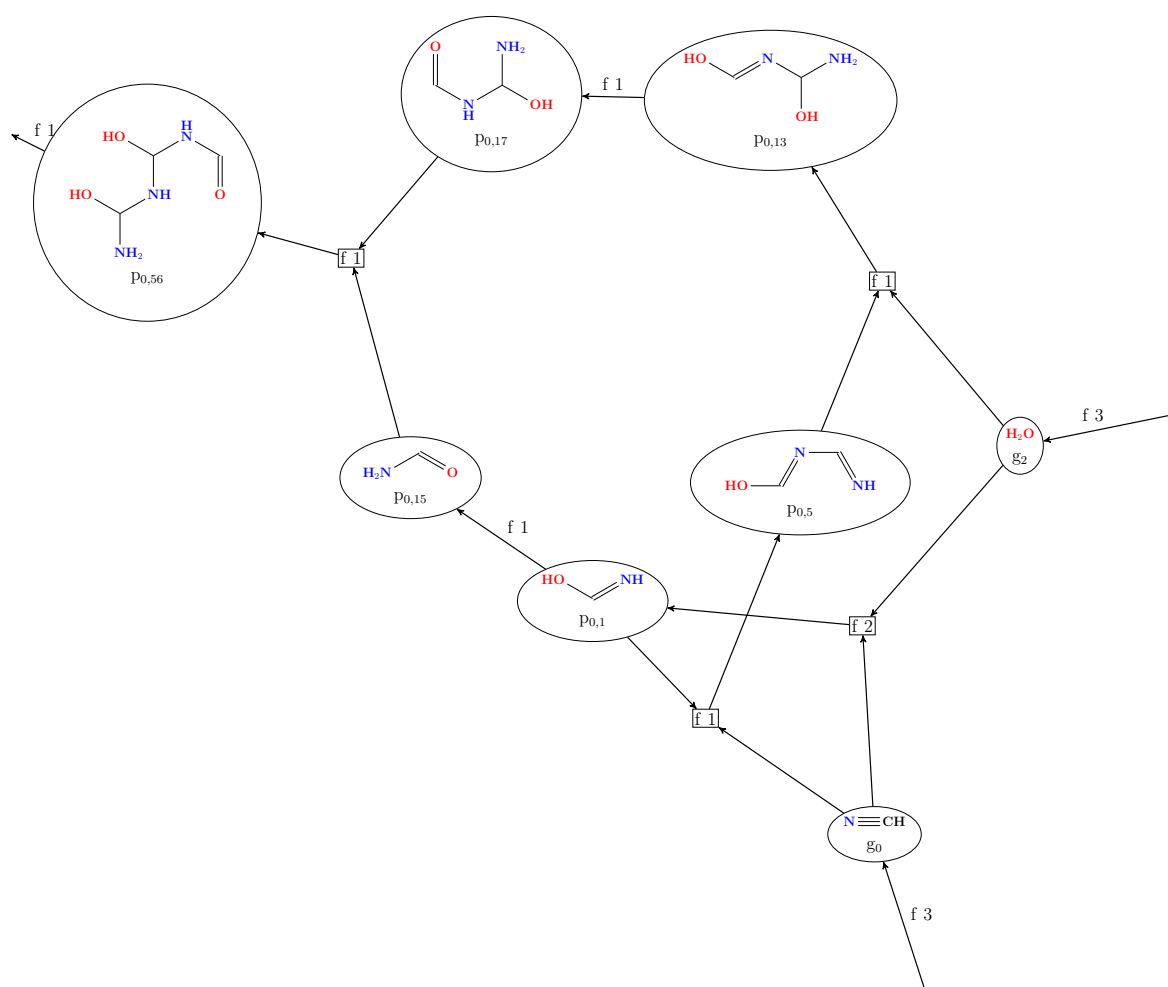


File: `out/042_dg_0_11100_f_0_1_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|-------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,5}$ | 0 | 0 | $-42425.44262$ | $1.0$ | $-42422.116835$ | 62 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $0.613824$ | $-55765.349681$ | 63 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $-7.01018$ | $-27919.704315$ | 2 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $1.0$ | $-55785.61853$ | 64 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 2 | $-54.231434$ | $-54.231434$ |
| 14 | $g_0, p_{0,1},$ | $p_{0,5},$ | 1 | $-113.75722$ | $-113.75722$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-72.87308$ | $-72.87308$ |
| 123 | $g_2, p_{0,5},$ | $p_{0,13},$ | 1 | $0.006113$ | $0.006113$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $0.006113$ | $0.006113$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-19.947765$ | $-19.947765$ |
| Sum | | | | | $-344.1086723480394$ |

$\Delta G = $ -31.502870278989164

$\Delta E = $ -0.13106407145277413

$|\text{E}| = 7$

$|\text{U}| = 6$

### 0.3.3 Solution 2

**Overall Data**

```
Objective value (non-integral): -0.131064
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  1.000000  0
g_{2}        3  0   -5.068043  1.000000  0
p_{0,13}     0  0   -21.240678 1.000000  33
p_{0,17}     0  0   -21.248887 -9.000000 65
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
p_{0,5}      0  0   -16.158998 -8.613824 31
```

**Filtered Graph**
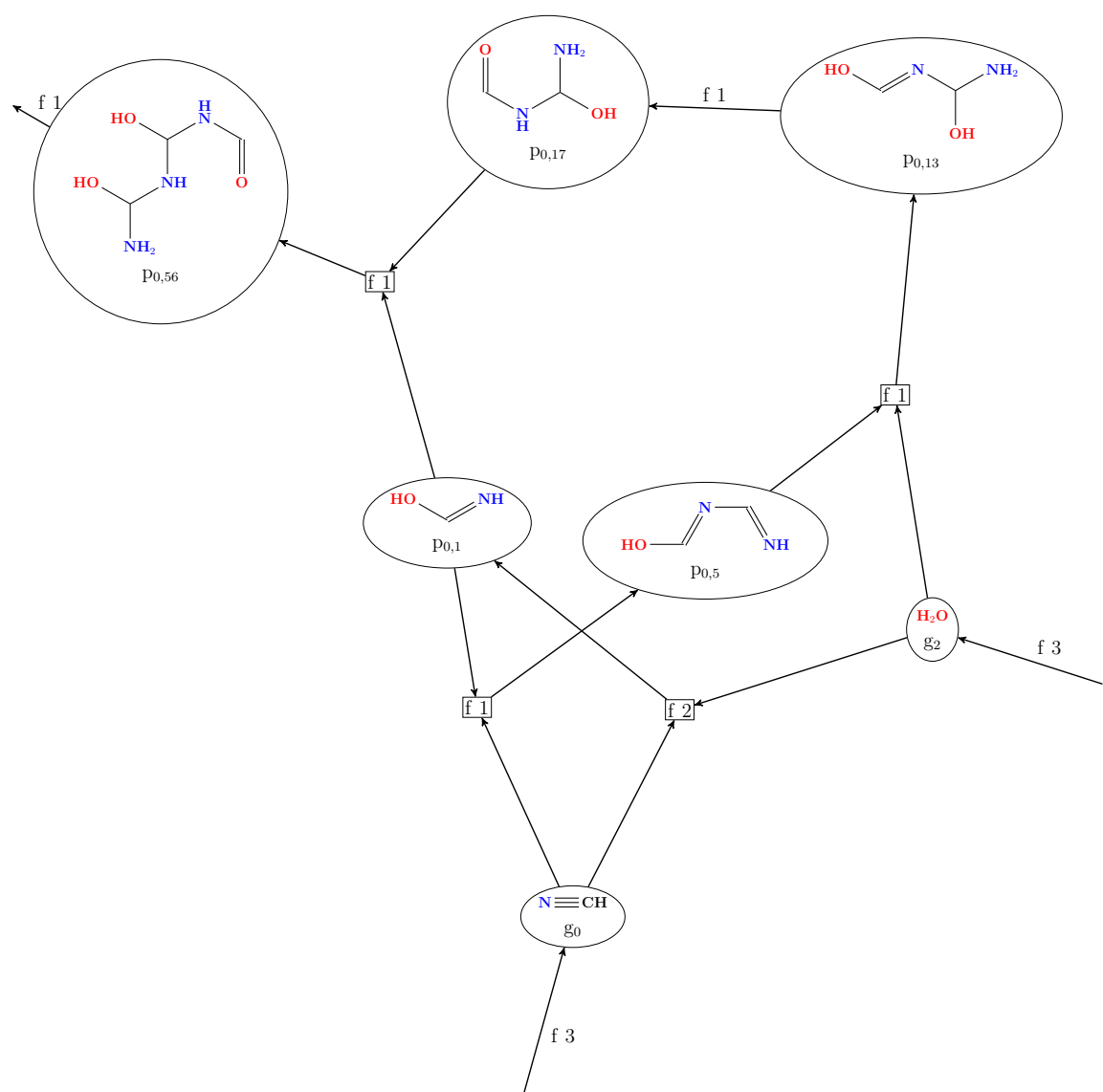


File: `out/051_dg_0_11100_f_0_2_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | $0$ |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | $0$ |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | $1$ |
| $p_{0,5}$ | 0 | 0 | $-42425.44262$ | $-8.613824$ | $-42454.090349$ | $31$ |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $1.0$ | $-55764.065344$ | $33$ |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $-9.0$ | $-55818.87638$ | $65$ |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | $67$ |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 2 | $-95.803747$ | $-95.803747$ |
| 14 | $g_0, p_{0,1},$ | $p_{0,5},$ | 1 | $-153.724111$ | $-153.724111$ |
| 123 | $g_2, p_{0,5},$ | $p_{0,13},$ | 1 | $0.006113$ | $0.006113$ |
| 196 | $p_{0,1}, p_{0,17},$ | $p_{0,56},$ | 1 | $-31.294654$ | $-31.294654$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-63.125499$ | $-63.125499$ |
| Sum | | | | | $-344.108672348038$ |

$\Delta G$ = -43.97456408759082
$\Delta E$ = -0.13106407145277357
|E| = 6
|U| = 5

### 0.3.4 Solution 3

**Overall Data**

```
Objective value (non-integral): -0.131064
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  1.000000   0
p_{0,13}     0  0   -21.240678 1.000000   64
p_{0,15}     0  0   -10.625195 -9.000000  2
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
p_{0,5}      0  0   -16.158998 -8.613824  63
```
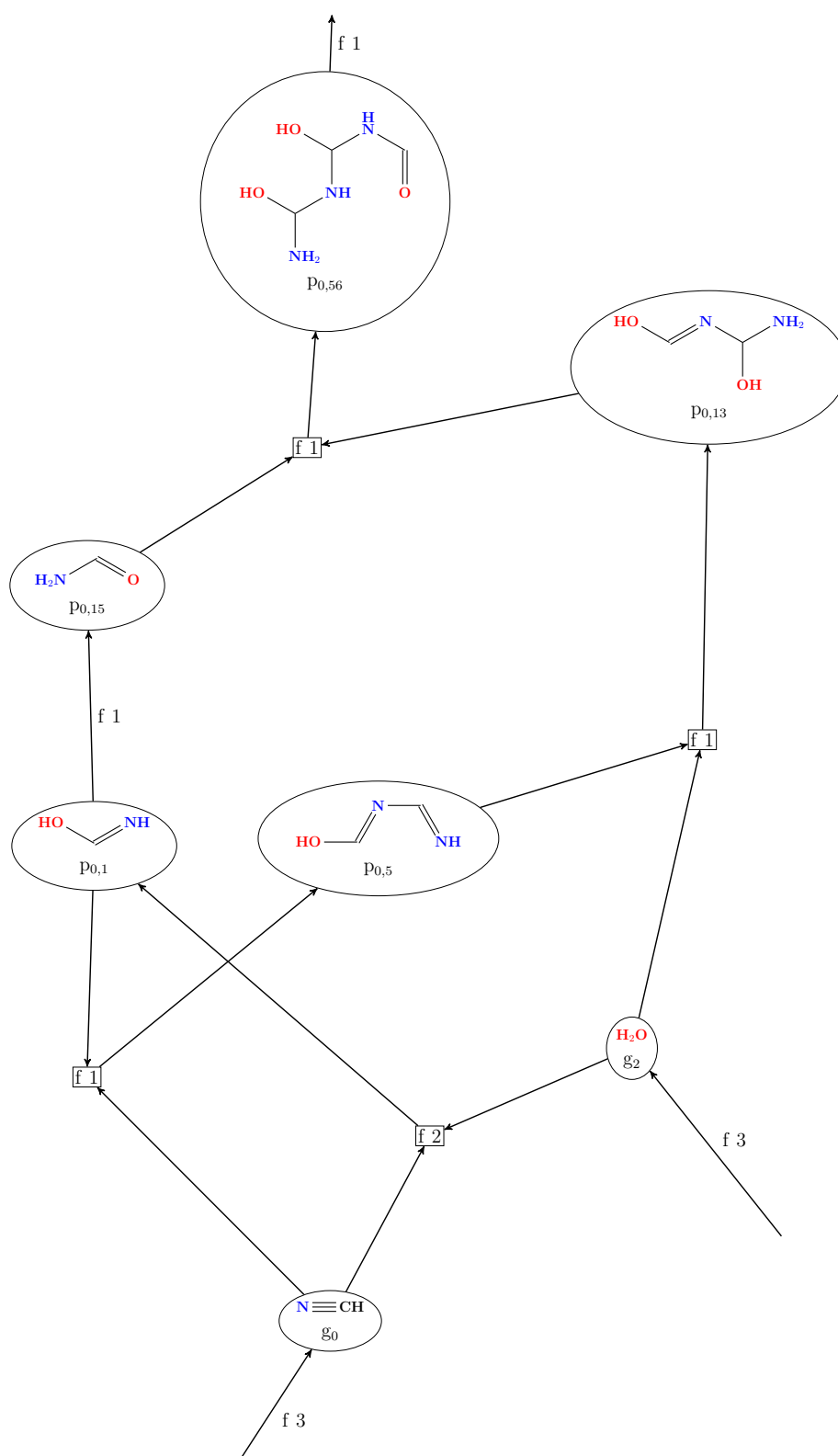
File: `out/060_dg_0_11100_f_0_3_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,5}$ | 0 | 0 | $-42425.44262$ | $-8.613824$ | $-42454.090349$ | 63 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $1.0$ | $-55764.065344$ | 64 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-9.0$ | $-27926.377821$ | 2 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 2 | $-95.803747$ | $-95.803747$ |
| 14 | $g_0, p_{0,1},$ | $p_{0,5},$ | 1 | $-153.724111$ | $-153.724111$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-81.201014$ | $-81.201014$ |
| 123 | $g_2, p_{0,5},$ | $p_{0,13},$ | 1 | $0.006113$ | $0.006113$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $-13.219139$ | $-13.219139$ |
| Sum | | | | | $-344.1086723480332$ |

$\Delta G$ = -43.97456408759082

$\Delta E$ = -0.13106407145277177

|E| = 6

|U| = 5

## 0.3.5   Solution 4

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  0
p_{0,15}     0  0   -10.625195 -6.996759  2
p_{0,17}     0  0   -21.248887 1.000000   64
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

# Filtered Graph
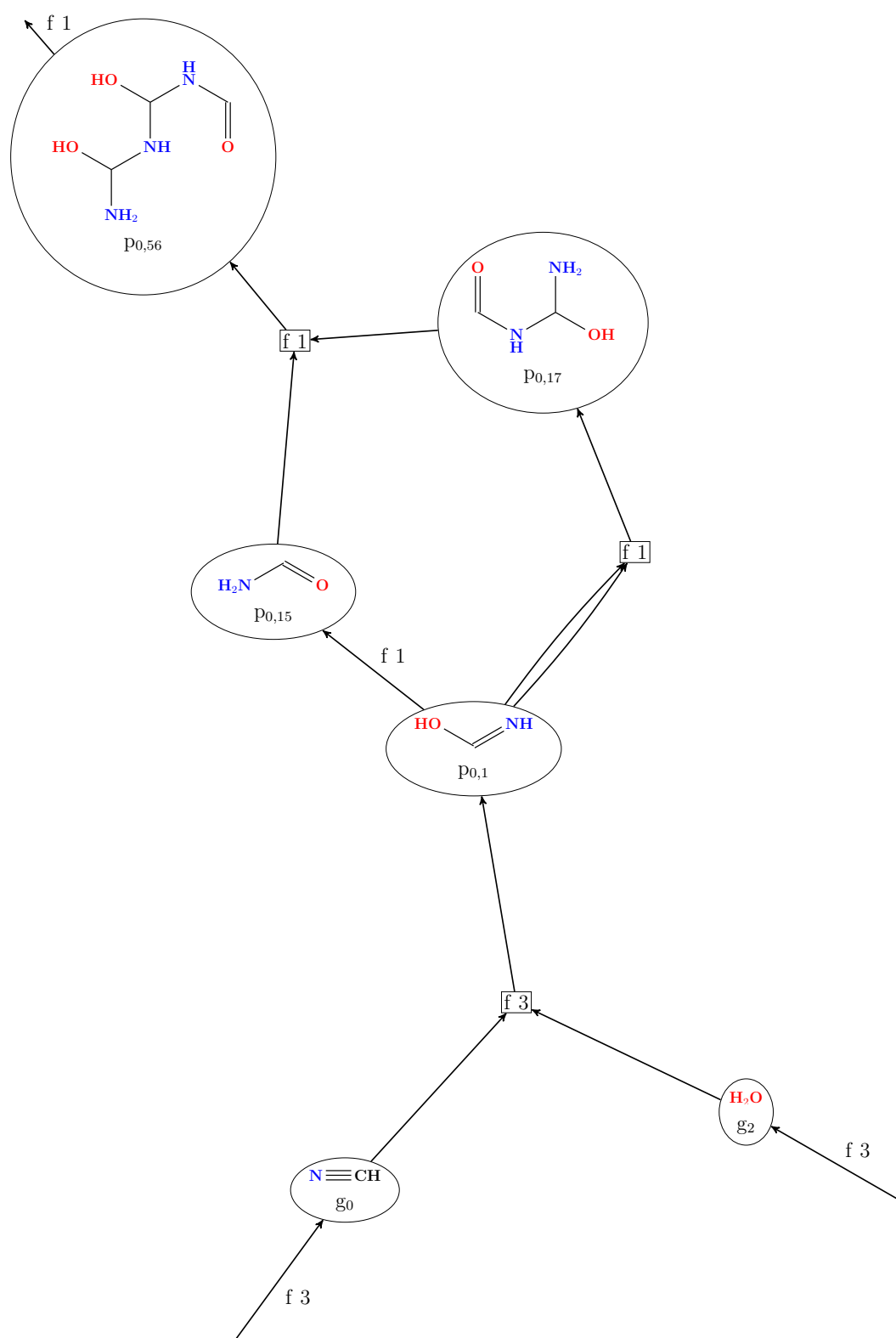
| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-6.996759$ | $-27919.715474$ | 2 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $1.0$ | $-55785.61853$ | 64 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-72.87308$ | $-72.87308$ |
| 40 | $p_{0,1}, p_{0,1},$ | $p_{0,17},$ | 1 | $-79.467437$ | $-79.467437$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $0.006113$ | $0.006113$ |
| Sum | | | | | $-248.3051087917569$ |

$\Delta G$ = -31.502870278989164
$\Delta E$ = -0.09457442121033222
|E| = 6
|U| = 4

### 0.3.6  Solution 5

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK      t_order
g_{0}         3   0  -5.507152  1.000000  0
g_{2}         3   0  -5.068043  1.000000  20
p_{0,17}      0   0  -21.248844 1.000000  43
p_{0,1}       0   0  -10.610080 1.000000  21
p_{0,56}      0   1  -31.869324 -9.000000 67
```

**Filtered Graph**
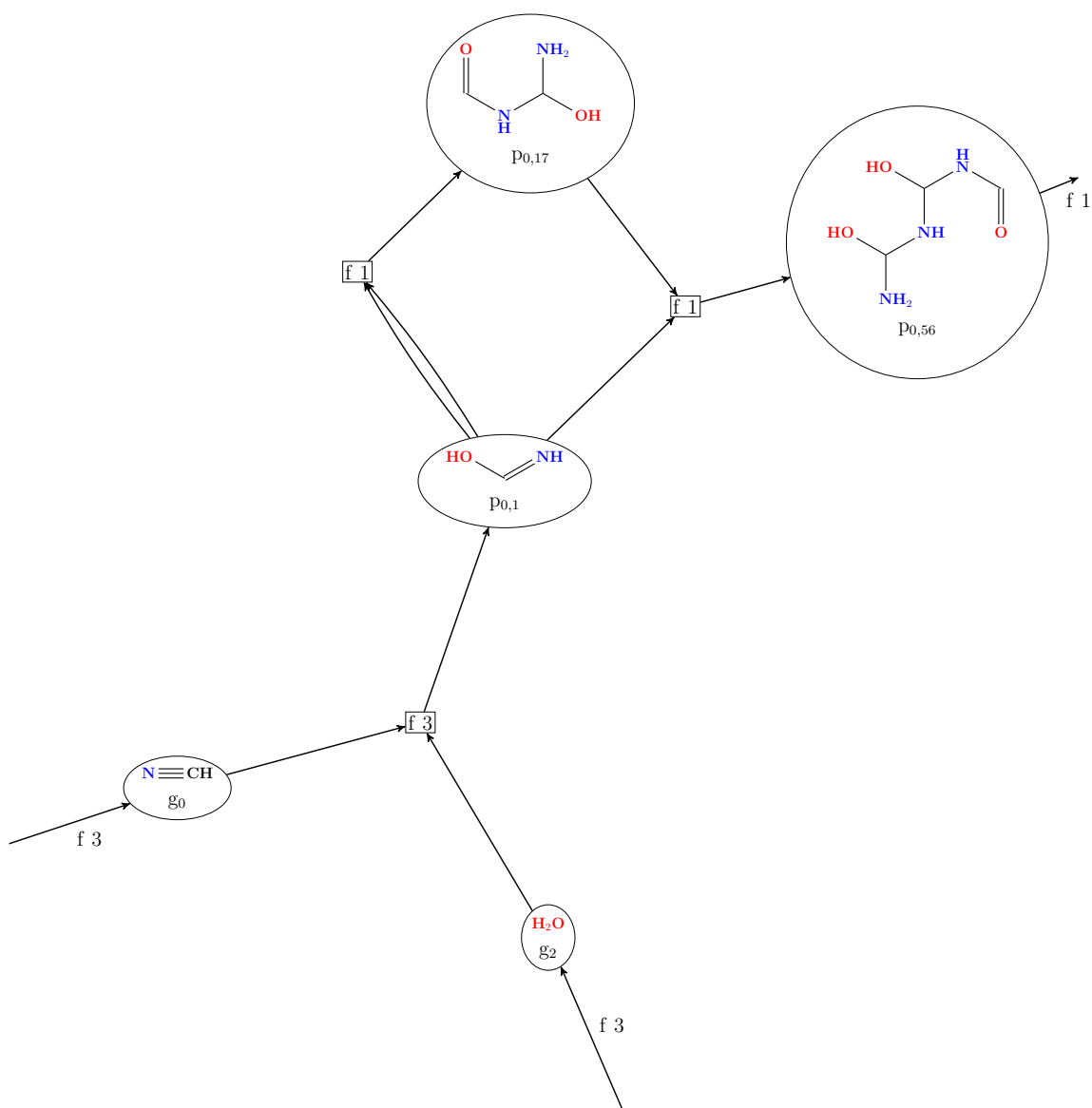


File: `out/078_dg_0_11100_f_0_5_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 20 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 21 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 43 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 40 | $p_{0,1}, p_{0,1},$ | $p_{0,17},$ | 1 | $-79.467287$ | $-79.467287$ |
| 196 | $p_{0,1}, p_{0,17},$ | $p_{0,56},$ | 1 | $-73.034258$ | $-73.034258$ |
| Sum | | | | | $-248.3051087917554$ |

$\Delta G = $ -43.97456356249089

$\Delta E = $ -0.09457442121033165

$|E| = 5$
$|U| = 3$

### 0.3.7 Solution 6

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}        3   0   -5.507152  1.000000   0
g_{2}        3   0   -5.068043  1.000000   20
p_{0,13}     0   0   -21.240635 1.000000   45
p_{0,1}      0   0   -10.610080 1.000000   21
p_{0,56}     0   1   -31.869324 -9.000000  67
```

**Filtered Graph**
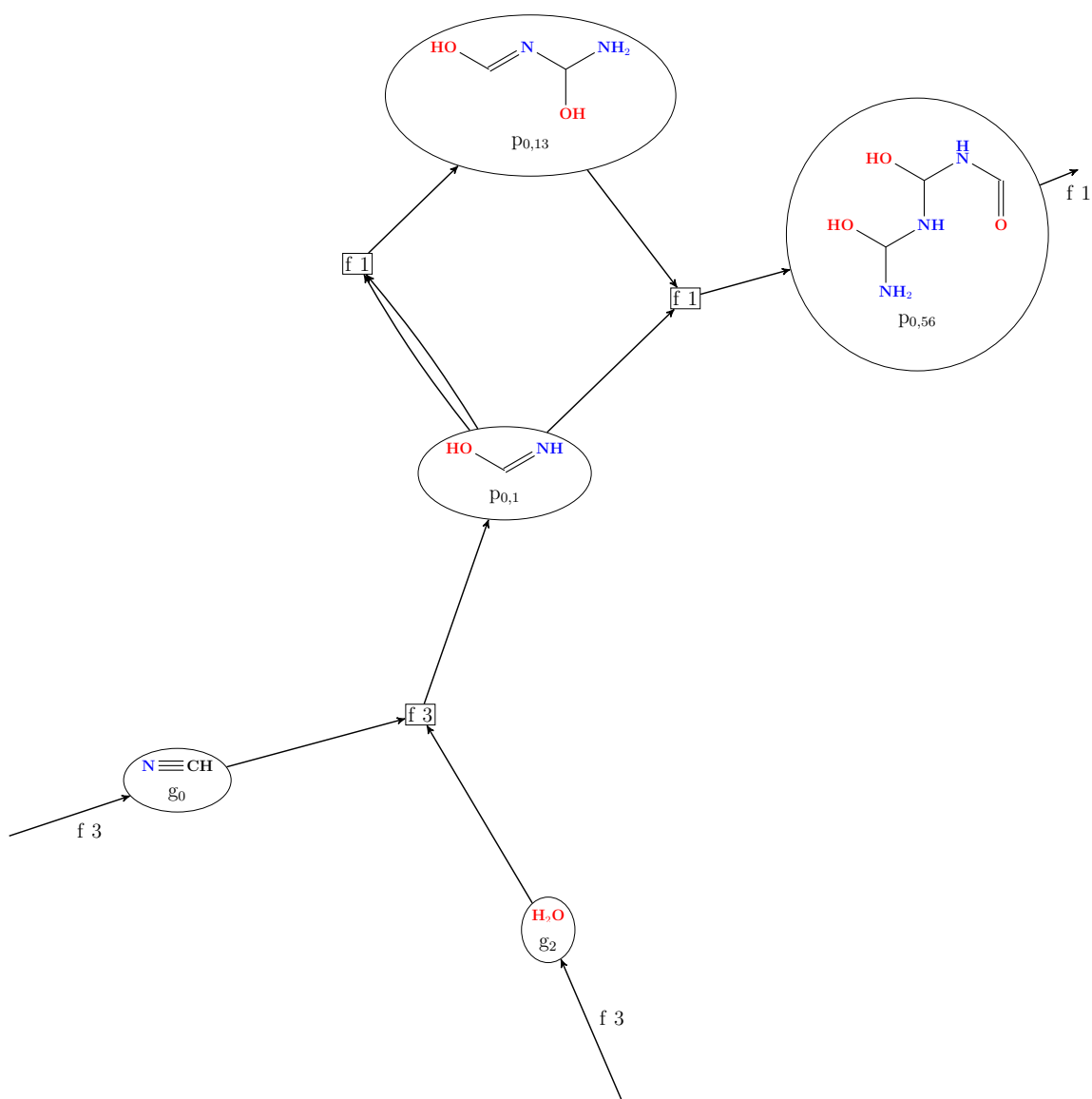


File: `out/087_dg_0_11100_f_0_6_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 20 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 21 |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | $1.0$ | $-55763.953809$ | 45 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 30 | $p_{0,1}, p_{0,1},$ | $p_{0,13},$ | 1 | $-57.914144$ | $-57.914144$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $-94.587401$ | $-94.587401$ |
| Sum | | | | | $-248.3051087917554$ |

$\Delta G$ = -43.97456356249089

$\Delta E$ = -0.0945744212103165

$|E| = 5$

$|U| = 3$

## 0.3.8   Solution 7

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152  1.000000   0
g_{2}         3  0   -5.068043  1.000000   0
p_{0,13}      0  0   -21.240635 -3.410779  39
p_{0,15}      0  0   -10.625195 -7.795844  27
p_{0,17}      0  0   -21.248887 -9.000000  26
p_{0,1}       0  0   -10.610080 1.000000   11
p_{0,56}      0  1   -31.869324 -9.000000  67
```

# Filtered Graph
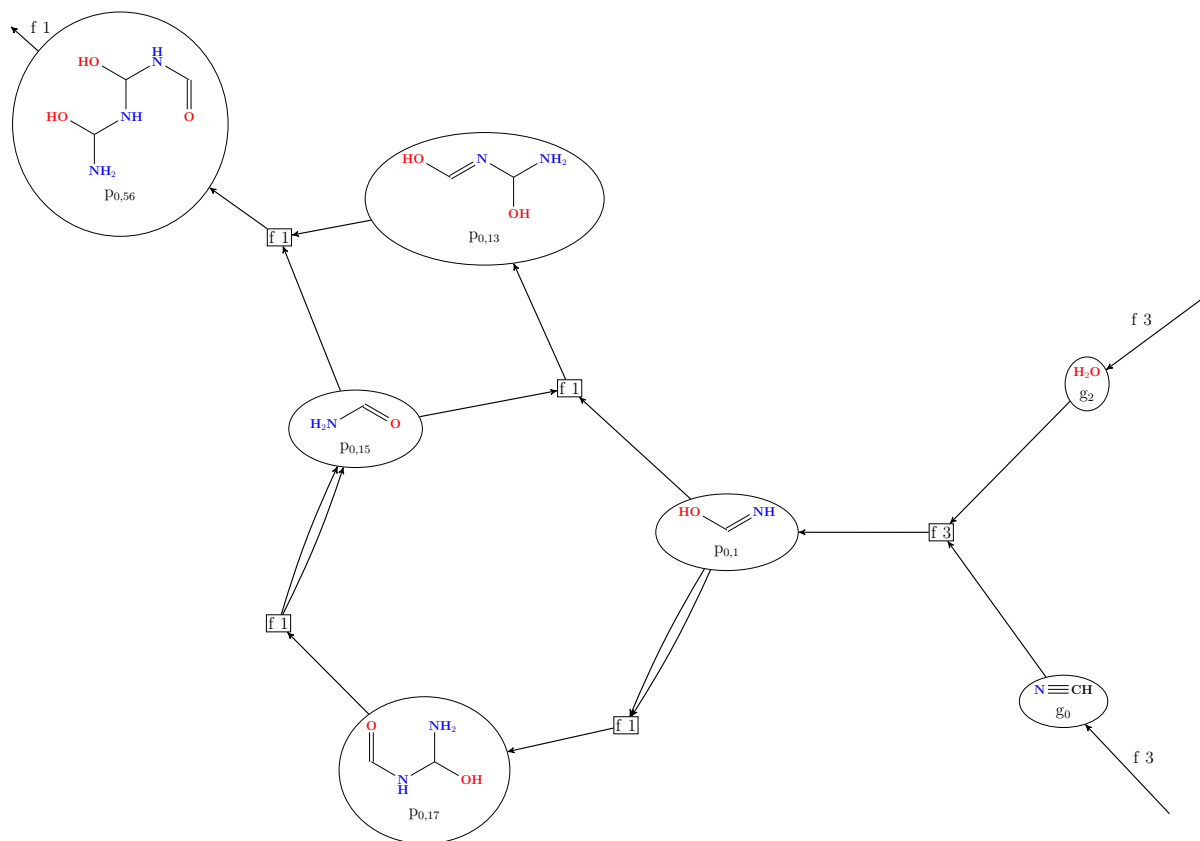


File: `out/096_dg_0_11100_f_0_7_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 11 |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | $-3.410779$ | $-55778.623112$ | 39 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-7.795844$ | $-27922.373057$ | 27 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $-9.0$ | $-55818.87638$ | 26 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 40 | $p_{0,1}, p_{0,1},$ | $p_{0,17},$ | 1 | $-121.151178$ | $-121.151178$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $0.0$ | $0.0$ |
| 192 | $p_{0,1}, p_{0,15},$ | $p_{0,13},$ | 1 | $0.0$ | $0.0$ |
| 237 | $p_{0,17},$ | $p_{0,15}, p_{0,15},$ | 1 | $-31.350368$ | $-31.350368$ |
| Sum | | | | | $-248.30510879175392$ |

$\Delta G$ = -43.97456356249089

$\Delta E$ = -0.09457442121033108

|E| = 7

|U| = 5

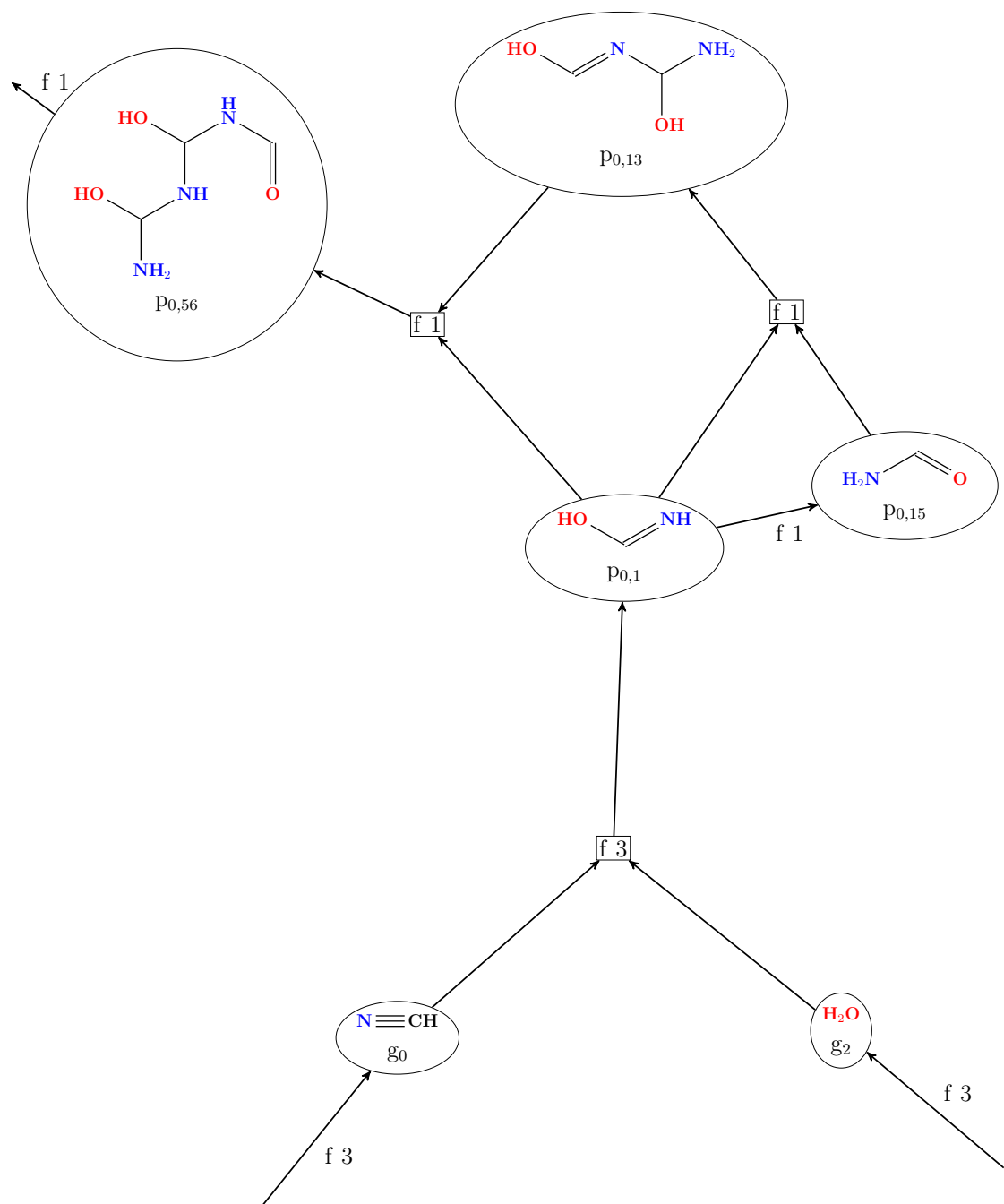### 0.3.9 Solution 8

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK      t_order
g_{0}       3  0   -5.507152  1.000000  0
g_{2}       3  0   -5.068043  1.000000  0
p_{0,13}    0  0   -21.240678 -3.136761 44
p_{0,15}    0  0   -10.625195 1.000000  23
p_{0,1}     0  0   -10.610101 -7.536724 1
p_{0,56}    0  1   -31.869260 1.000000  67
```

**Filtered Graph**

f 1

HO N H

HO NH

NH₂

O

$p_{0,56}$

HO N NH₂

OH

$p_{0,13}$

f 1

f 1

HO NH

$p_{0,1}$

f 1

H₂N O

$p_{0,15}$

f 3

N≡CH

$g_0$

H₂O

$g_2$

f 3

f 3

File: out/105_dg_0_11100_f_0_8_filt

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | $0$ |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | $0$ |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $-7.536724$ | $-27881.882578$ | $1$ |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-3.136761$ | $-55777.823322$ | $44$ |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $1.0$ | $-27893.119971$ | $23$ |
| $p_{0,56}$ | 0 | 1 | $-83672.731446$ | $1.0$ | $-83669.405661$ | $67$ |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-131.292882$ | $-131.292882$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-4.139566$ | $-4.139566$ |
| 192 | $p_{0,1}, p_{0,15},$ | $p_{0,13},$ | 1 | $0.006113$ | $0.006113$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $0.006113$ | $0.006113$ |
| Sum | | | | | $-248.30510879175392$ |

$\Delta G$ = -39.800598058388196
$\Delta E$ = -0.09457442121033108
|E| = 6
|U| = 4

## 0.3.10 Solution 9

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  0
p_{0,13}     0  0   -21.240635 1.000000   3
p_{0,15}     0  0   -10.625174 1.000000   2
p_{0,17}     0  0   -21.248844 1.000000   64
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

**Filtered Graph**
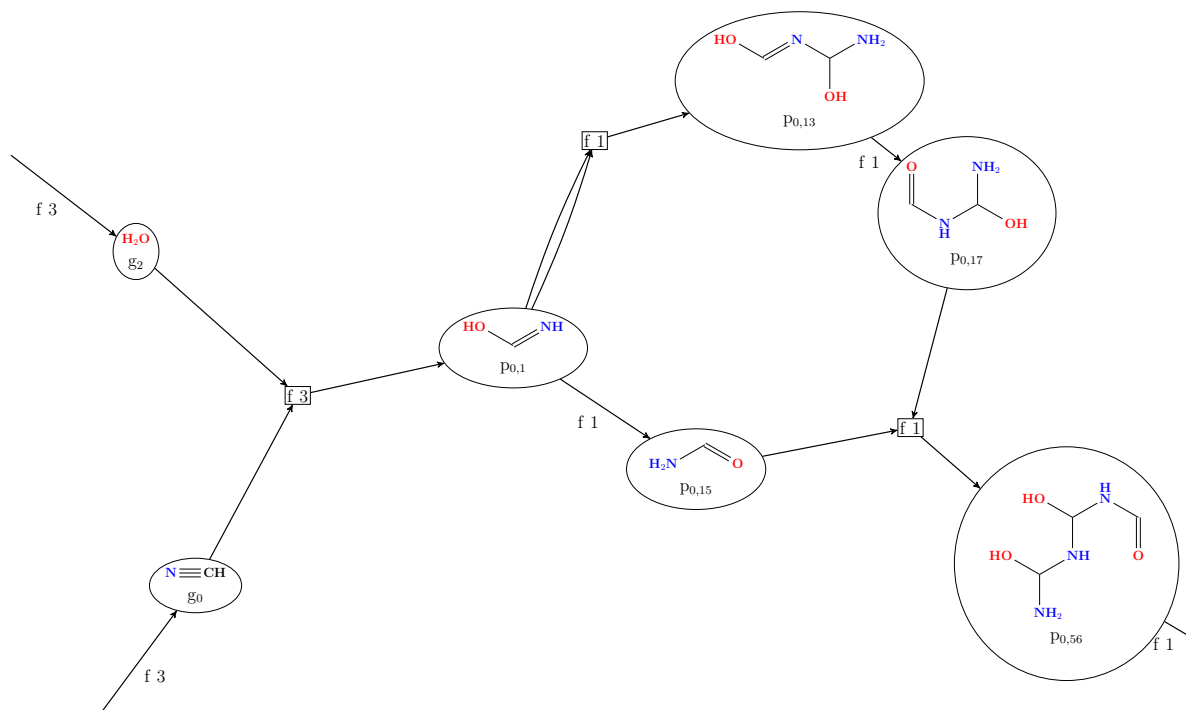


File: `out/114_dg_0_11100_f_0_9_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | 1.0 | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | 1.0 | $-27853.491269$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | 1.0 | $-55763.953809$ | 3 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | 1.0 | $-27893.064178$ | 2 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | 1.0 | $-55785.506952$ | 64 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 30 | $p_{0,1}, p_{0,1},$ | $p_{0,13},$ | 1 | $-57.802717$ | $-57.802717$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-39.572909$ | $-39.572909$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $-33.405636$ | $-33.405636$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-21.553143$ | $-21.553143$ |
| Sum | | | | | $-248.30510879175372$ |

$\Delta G$ = -31.502869753889232

$\Delta E$ = -0.09457442121033101

|E| = 7

|U| = 5

## 0.3.11  Solution 10
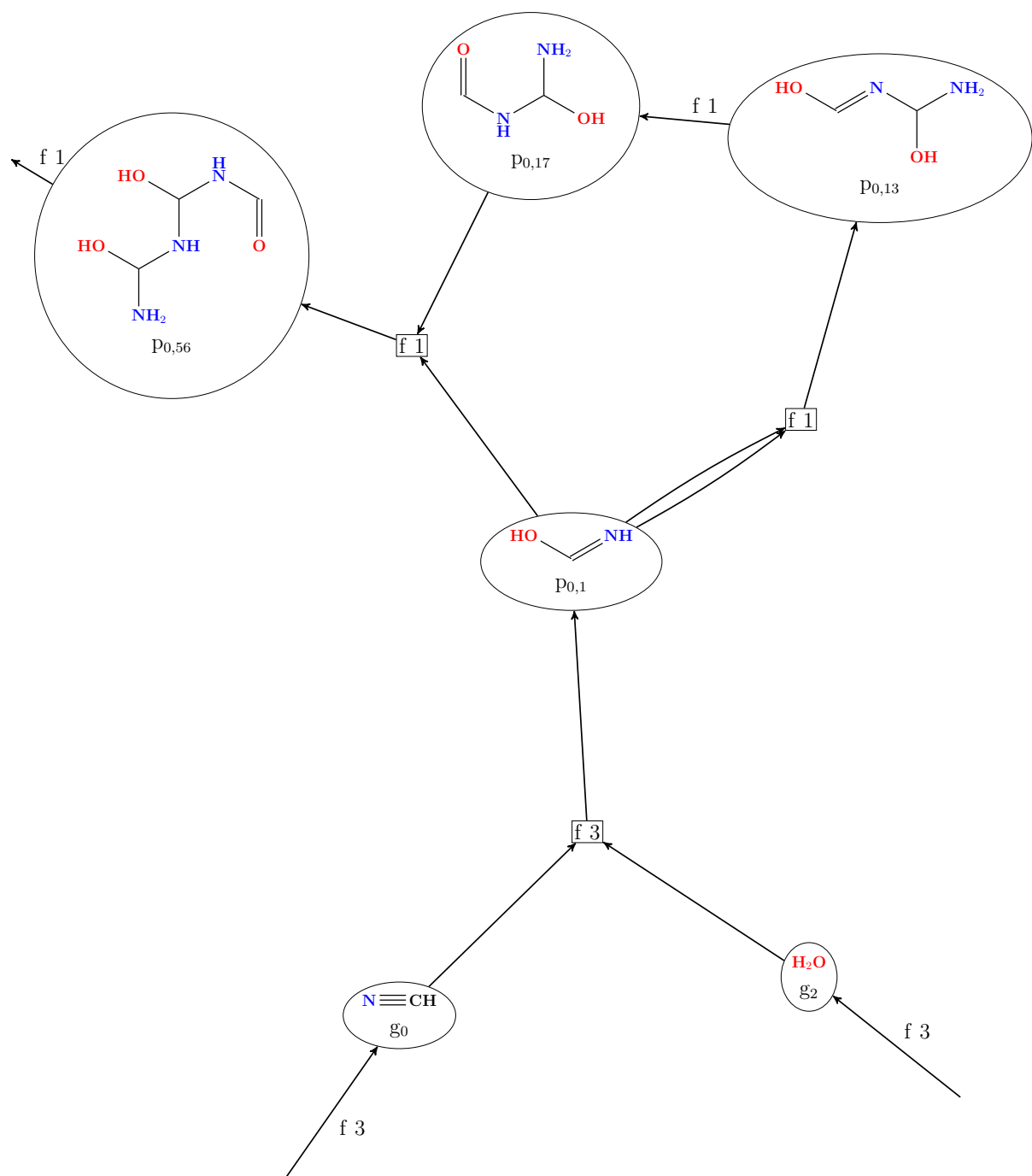
**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G         logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  20
p_{0,13}     0  0   -21.240635 1.000000   43
p_{0,17}     0  0   -21.248844 1.000000   45
p_{0,1}      0  0   -10.610080 1.000000   21
p_{0,56}     0  1   -31.869324 -9.000000  67
```

**Filtered Graph**



File: `out/123_dg_0_11100_f_0_10_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | $0$ |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | $20$ |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | $21$ |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | $1.0$ | $-55763.953809$ | $43$ |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | $45$ |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | $67$ |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.17572$ | $-54.17572$ |
| 30 | $p_{0,1}, p_{0,1},$ | $p_{0,13},$ | 1 | $-57.914144$ | $-57.914144$ |
| 196 | $p_{0,1}, p_{0,17},$ | $p_{0,56},$ | 1 | $-73.034258$ | $-73.034258$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-21.553143$ | $-21.553143$ |
| Sum | | | | | $-248.30510879175225$ |

$\Delta G$ = -31.5028700164392

$\Delta E$ = -0.09457442121033044

|E| = 6

|U| = 4

## 0.3.12   Solution 11

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK      t_order
g_{0}       3  0   -5.507152  -9.000000 0
g_{2}       3  0   -5.068043  -9.000000 0
p_{0,13}    0  0   -21.240635 1.000000  64
p_{0,15}    0  0   -10.625195 -3.386535 62
p_{0,17}    0  0   -21.248844 1.000000  65
p_{0,1}     0  0   -10.610080 1.000000  1
p_{0,56}    0  1   -31.869324 -9.000000 67
```

**Filtered Graph**
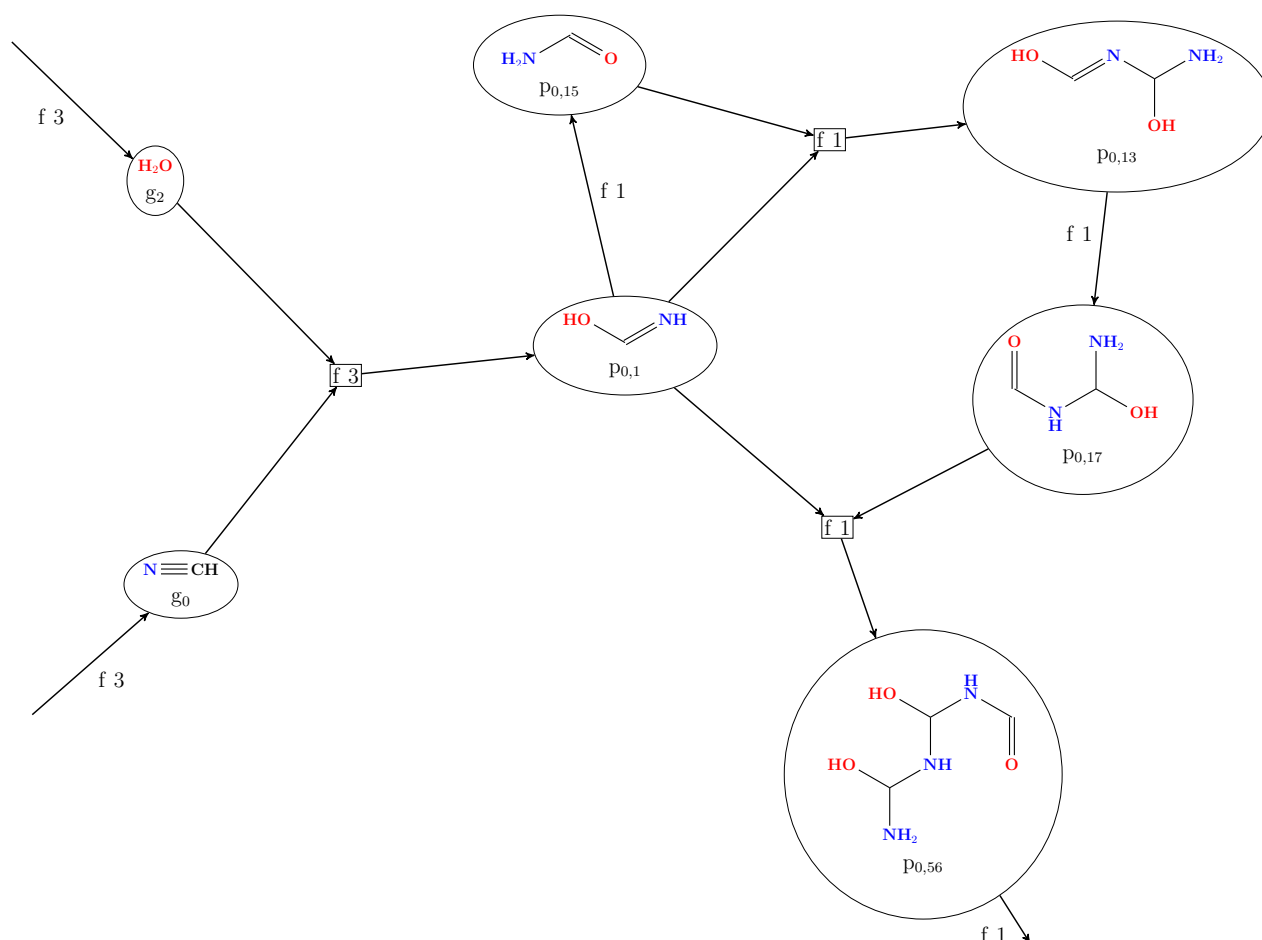


File: `out/132_dg_0_11100_f_0_11_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $-9.0$ | $-14488.957643$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | $1.0$ | $-55763.953809$ | 64 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-3.386535$ | $-27907.708644$ | 62 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 65 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-12.603407$ | $-12.603407$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-57.920257$ | $-57.920257$ |
| 192 | $p_{0,1}, p_{0,15},$ | $p_{0,13},$ | 1 | $0.006113$ | $0.006113$ |
| 196 | $p_{0,1}, p_{0,17},$ | $p_{0,56},$ | 1 | $-73.034258$ | $-73.034258$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-21.553143$ | $-21.553143$ |
| Sum | | | | | $-248.30510879175074$ |

$\Delta G$ = -19.03117594528758

$\Delta E$ = -0.0945744212103298

|E| = 7
|U| = 5

## 0.3.13  Solution 12

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  1.000000  0
g_{2}        3  0   -5.068043  -9.000000 0
p_{0,13}     0  0   -21.240678 -4.157665 44
p_{0,15}     0  0   -10.625174 1.000000  22
p_{0,17}     0  0   -21.248844 1.000000  3
p_{0,1}      0  0   -10.610101 -8.520524 1
p_{0,56}     0  1   -31.869324 -9.000000 67
```

**Filtered Graph**
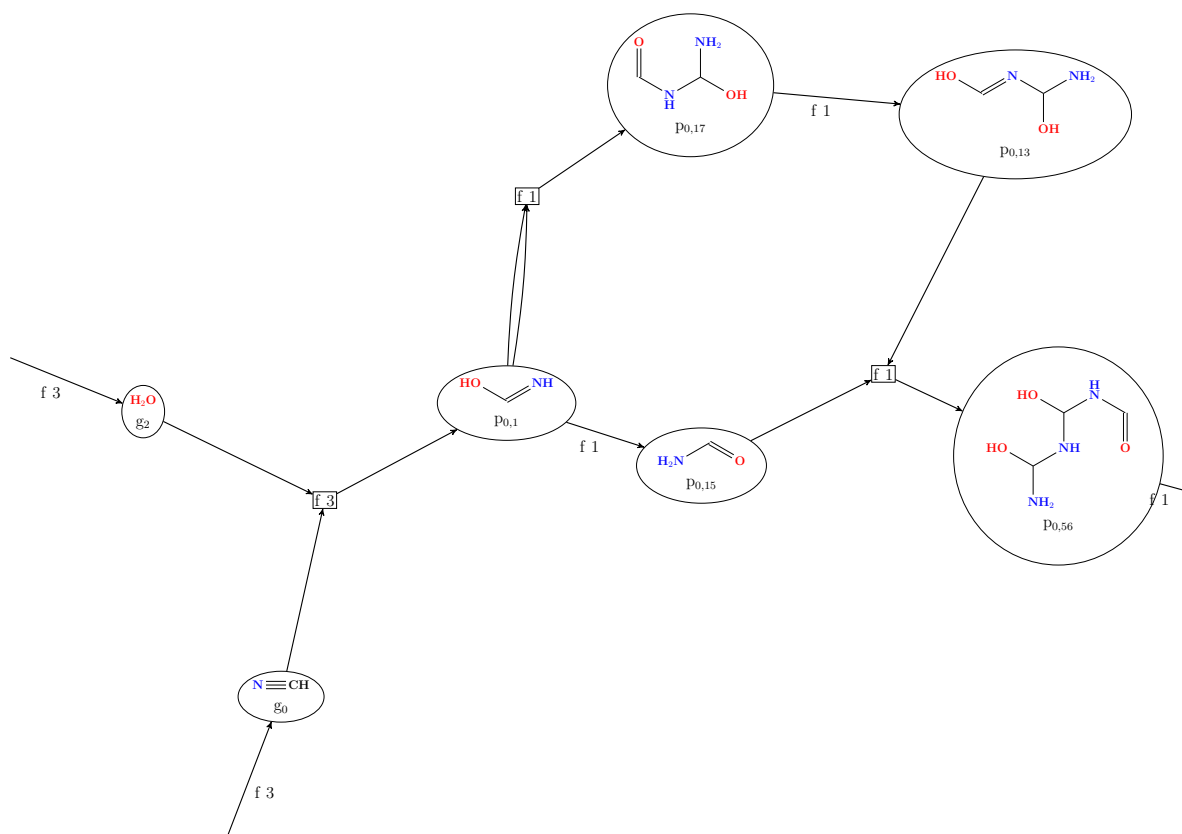


File: `out/141_dg_0_11100_f_0_12_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^{K}$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|-----------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $-8.520524$ | $-27885.154487$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-4.157665$ | $-55781.21863$ | 44 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | 22 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 3 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|-----------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-93.810455$ | $-93.810455$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $0.006113$ | $0.006113$ |
| 40 | $p_{0,1}, p_{0,1},$ | $p_{0,17},$ | 1 | $-0.197817$ | $-0.197817$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $-33.405636$ | $-33.405636$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $0.0$ | $0.0$ |
| Sum | | | | | $-248.30510879175074$ |

$\Delta G$ = -31.5028700164392

$\Delta E$ = -0.09457442121032987

|E| = 7

|U| = 5

## 0.3.14  Solution 13

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  1.000000  0
g_{2}        3  0   -5.068043  1.000000  0
p_{0,13}     0  0   -21.240678 -9.000000 65
p_{0,15}     0  0   -10.625195 1.000000  2
p_{0,17}     0  0   -21.248844 1.000000  4
p_{0,1}      0  0   -10.610080 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
```

# Filtered Graph
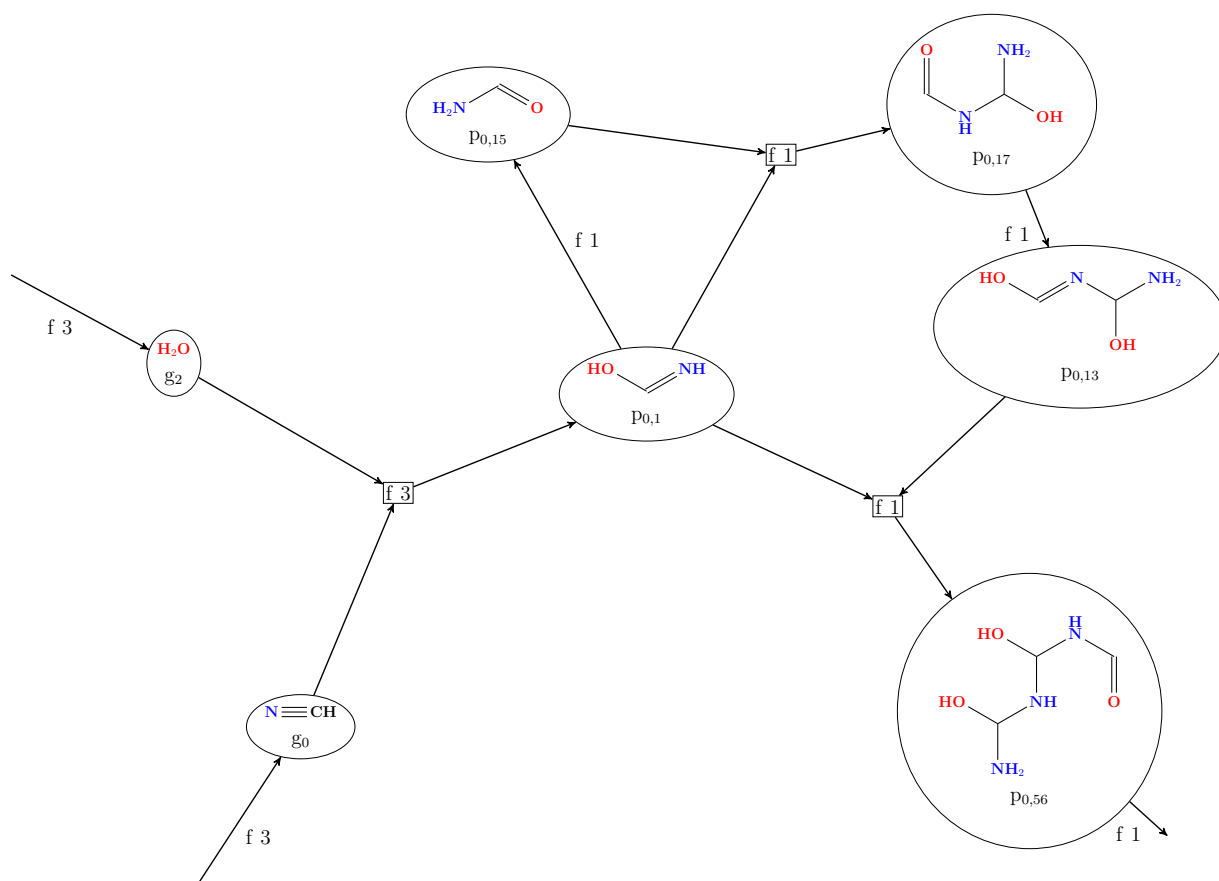


File: `out/150_dg_0_11100_f_0_13_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | 65 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $1.0$ | $-27893.119971$ | 2 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 4 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|-----------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-39.684415$ | $-39.684415$ |
| 183 | $p_{0,1}, p_{0,15},$ | $p_{0,17},$ | 1 | $-39.782872$ | $-39.782872$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $-20.130705$ | $-20.130705$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $-52.903554$ | $-52.903554$ |
| Sum | | | | | $-248.30510879176006$ |

$\Delta G$ = -43.97456329994093

$\Delta E$ = -0.0945744212103342

|E| = 7

|U| = 5

## 0.3.15   Solution 14
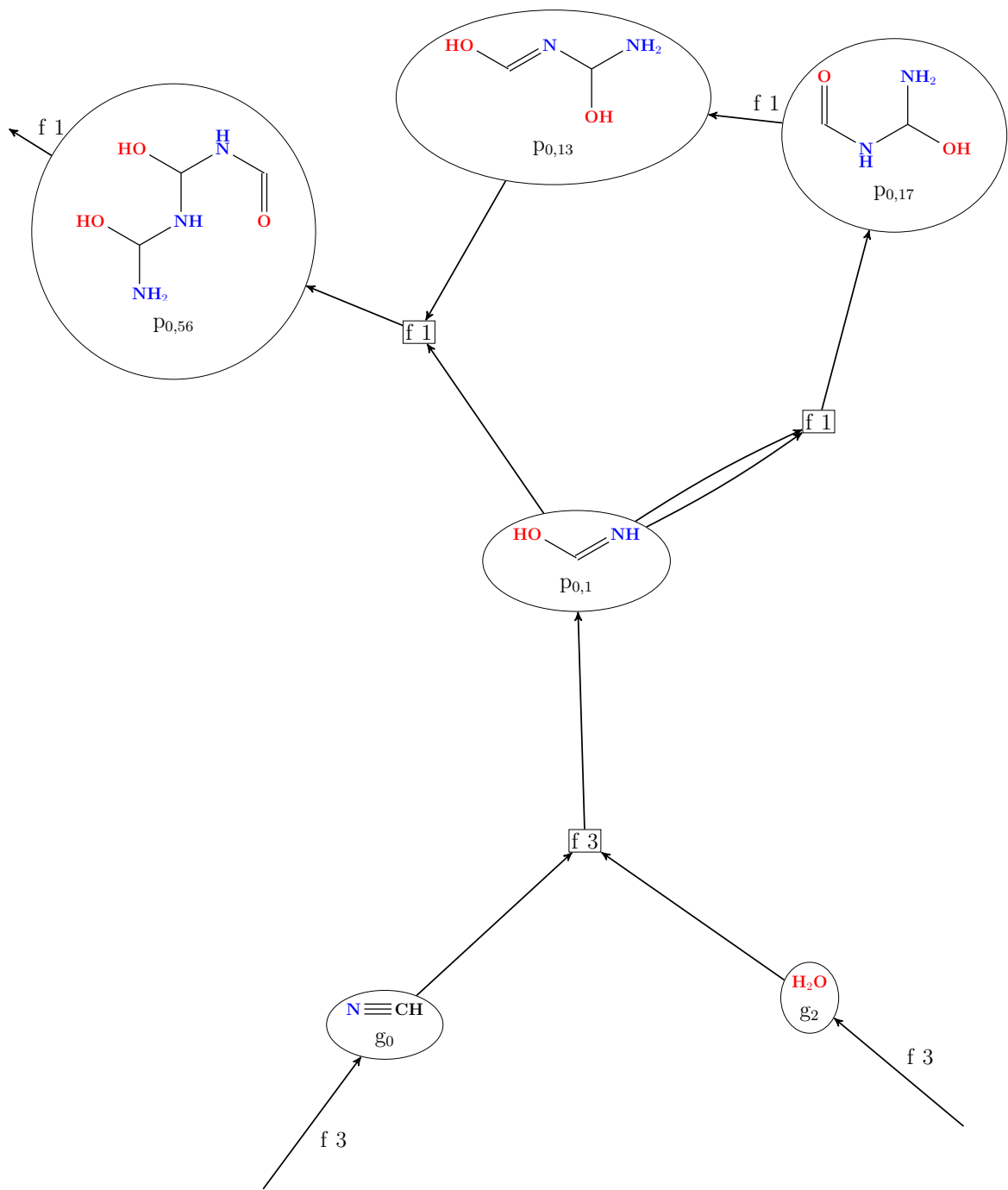
**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152 -9.000000 0
g_{2}         3  0   -5.068043 -9.000000 0
p_{0,13}      0  0   -21.240678 -9.000000 44
p_{0,17}      0  0   -21.248844 1.000000  43
p_{0,1}       0  0   -10.610080 1.000000  21
p_{0,56}      0  1   -31.869324 -9.000000 67
```

**Filtered Graph**

f 1

HO  N  NH₂
OH
p₀,₁₃

O  NH₂
N  OH
H
p₀,₁₇

f 1

HO  H
N
HO  NH  O
NH₂
p₀,₅₆

f 1

f 1

f 1

HO  NH
p₀,₁

f 3

N≡CH
g₀

H₂O
g₂

f 3

f 3

File: `out/159_dg_0_11100_f_0_14_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $-9.0$ | $-14488.957643$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 21 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | 44 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 43 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-12.603407$ | $-12.603407$ |
| 40 | $p_{0,1}, p_{0,1},$ | $p_{0,17},$ | 1 | $-79.467287$ | $-79.467287$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $-20.130705$ | $-20.130705$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $-52.903554$ | $-52.903554$ |
| Sum | | | | | $-248.30510879175858$ |

$\Delta G$ = -19.03117620783754
$\Delta E$ = -0.09457442121033285
|E| = 6
|U| = 4

## 0.3.16   Solution 15

**Overall Data**

```
Objective value (non-integral): -0.0945744
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  0
p_{0,13}     0  0   -21.240678 -2.181264  64
p_{0,15}     0  0   -10.625195 -9.000000  2
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

f 1

HO

H
N

HO

NH

O

NH₂

p₀,₅₆

f 1

HO

N

NH₂

OH

p₀,₁₃

f 1

H₂N

O

p₀,₁₅

f 1

f 1

HO

NH

p₀,₁

f 3

H₂O

g₂

f 3

N≡CH

g₀

f 3

File: `out/168_dg_0_11100_f_0_15_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-2.181264$ | $-55774.645545$ | 64 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-9.0$ | $-27926.377821$ | 2 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|-----------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 30 | $p_{0,1}, p_{0,1},$ | $p_{0,13},$ | 1 | $-71.139503$ | $-71.139503$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 1 | $-81.201014$ | $-81.201014$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $0.006113$ | $0.006113$ |
| Sum | | | | | $-248.30510879174759$ |

$\Delta G$ = -31.502870278989164
$\Delta E$ = -0.09457442121032866
|E| = 6
|U| = 4
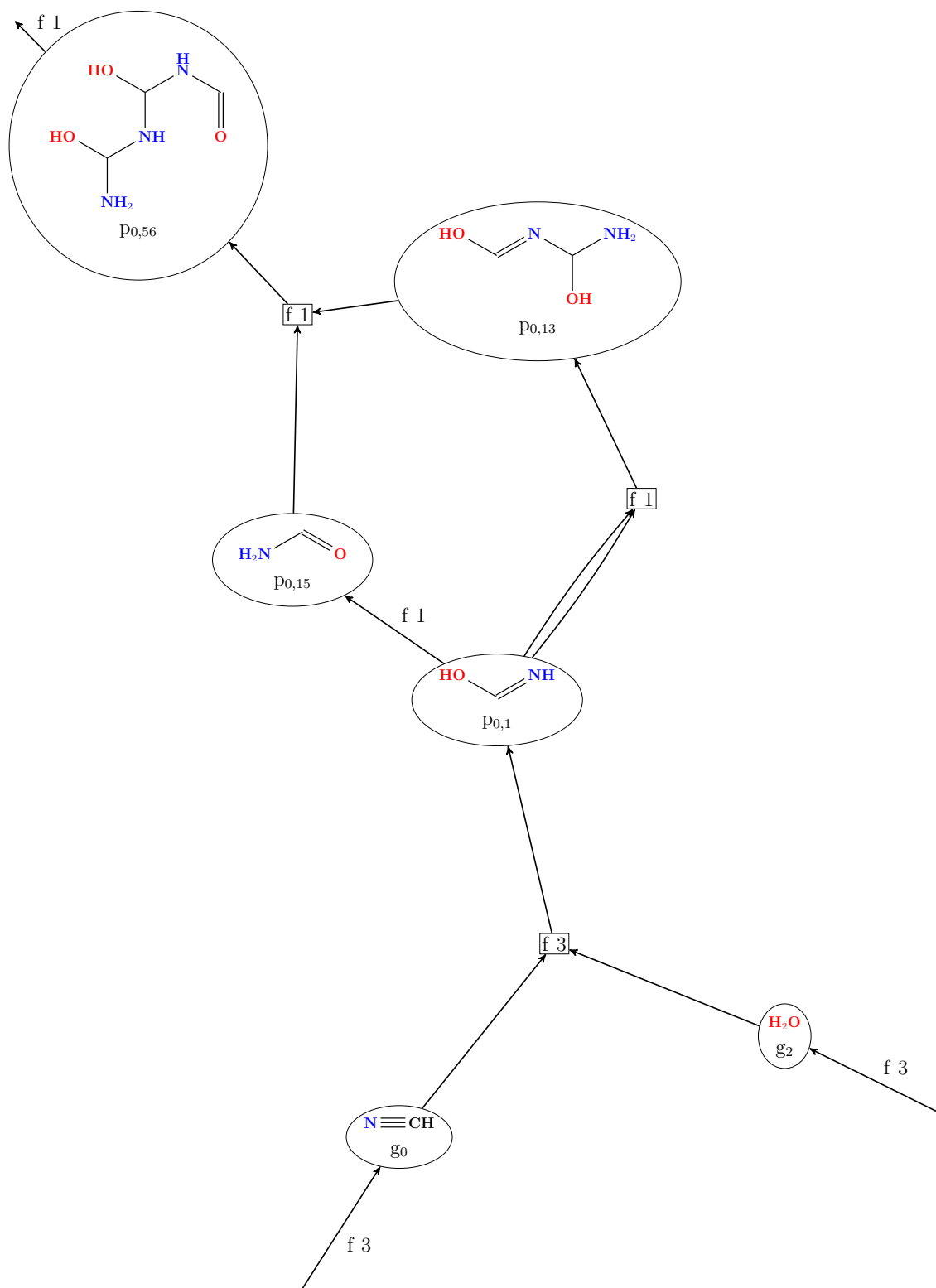
## 0.3.17   Solution 16

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G         logK       t_order
g_{0}        3  0   -5.507152  -9.000000 0
g_{2}        3  0   -5.068043  -9.000000 0
p_{0,13}     0  0   -21.240678 -9.000000 64
p_{0,15}     0  0   -10.625174 0.974002  31
p_{0,17}     0  0   -21.248844 1.000000  63
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
```

# Filtered Graph
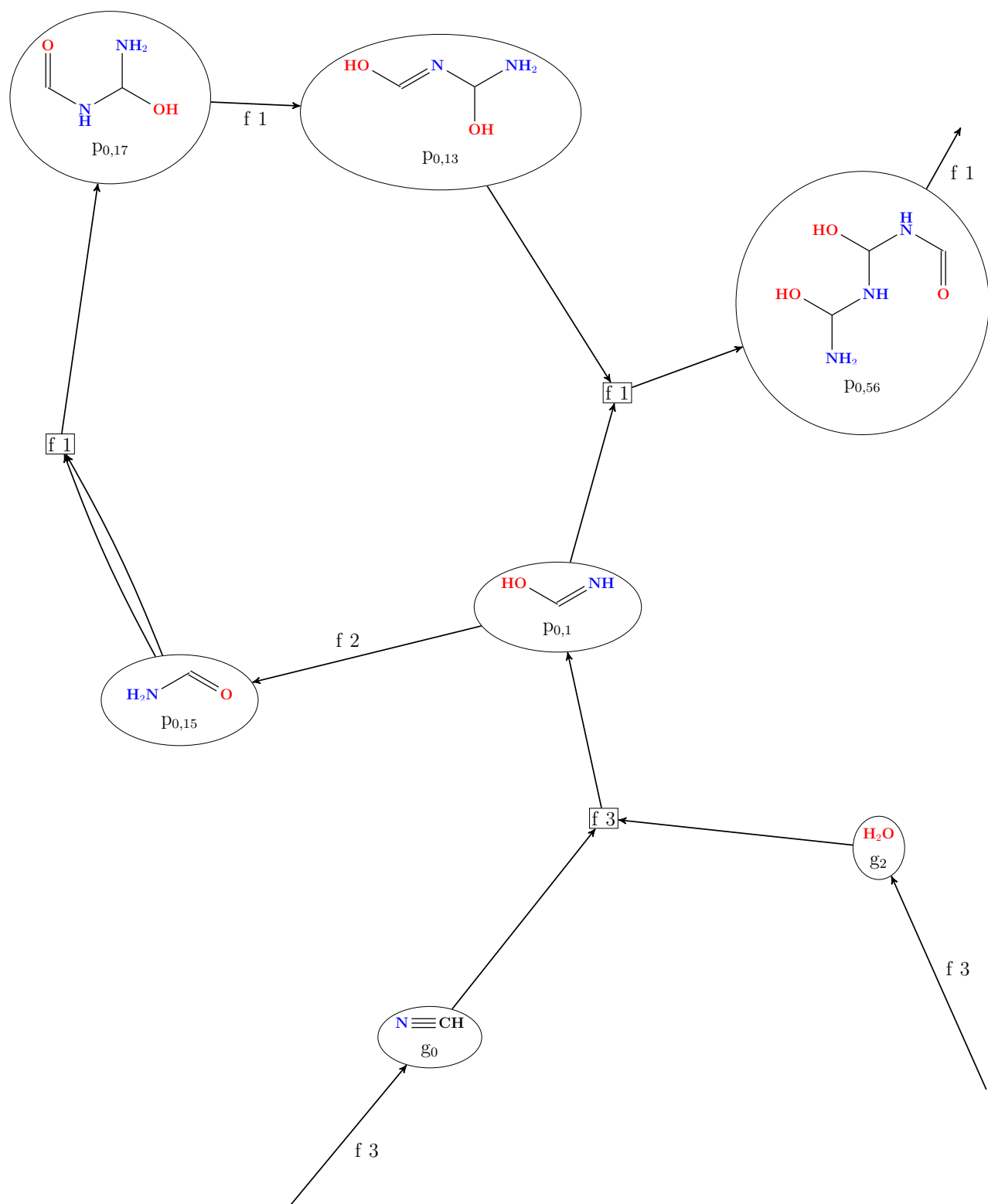


File: `out/177_dg_0_11100_f_0_16_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $-9.0$ | $-14488.957643$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | 64 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $0.974002$ | $-27893.15064$ | 31 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 63 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-12.659121$ | $-12.659121$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-39.680986$ | $-39.680986$ |
| 180 | $p_{0,15}, p_{0,15},$ | $p_{0,17},$ | 1 | $0.006113$ | $0.006113$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $-20.130705$ | $-20.130705$ |
| 263 | $p_{0,1}, p_{0,13},$ | $p_{0,56},$ | 1 | $-52.84784$ | $-52.84784$ |
| Sum | | | | | $-208.67648668796497$ |

$\Delta G = \text{-19.03117594528758}$

$\Delta E = \text{-0.0794806761920923}$

$|\text{E}| = 8$

$|\text{U}| = 5$

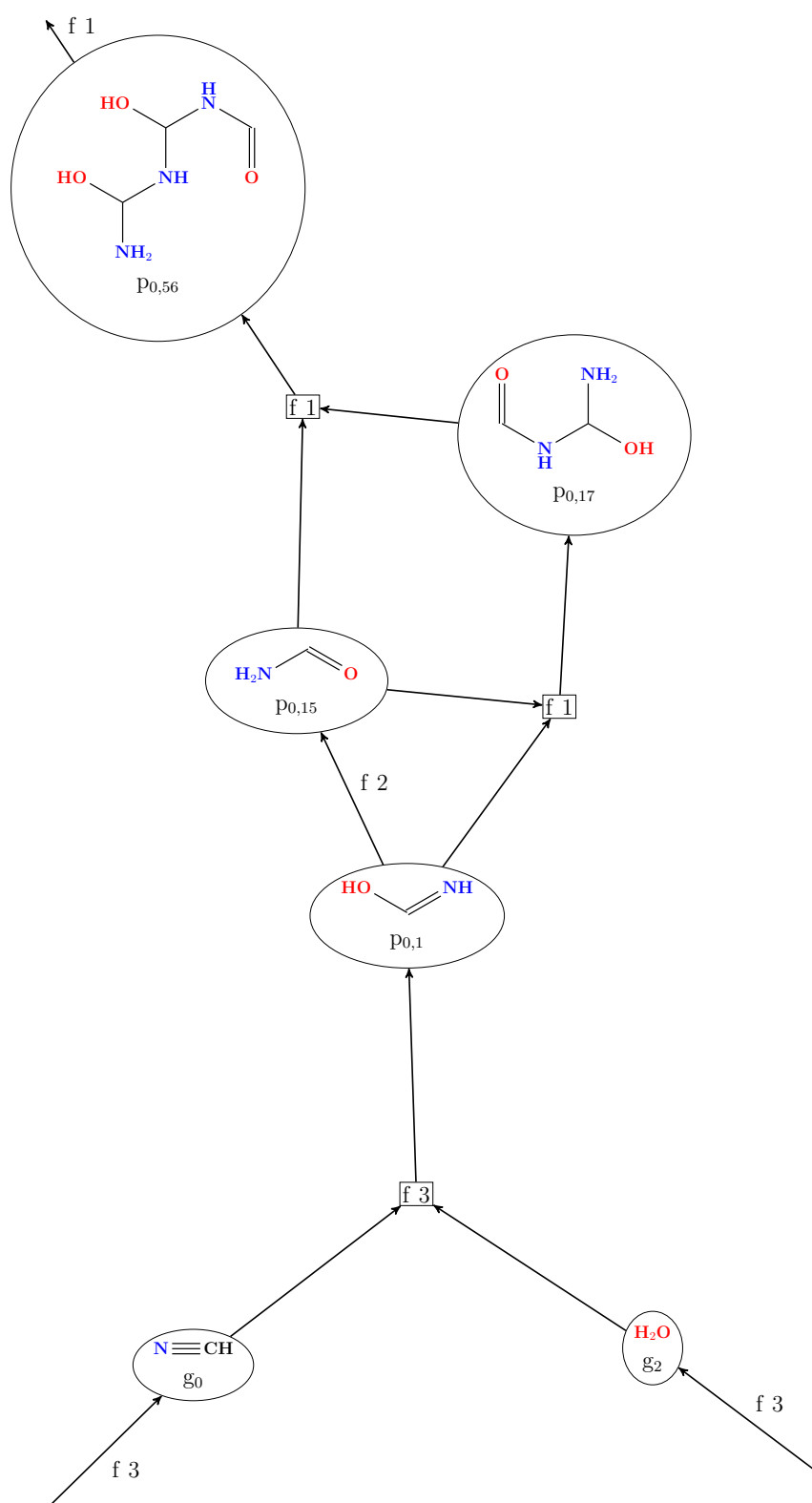## 0.3.18 Solution 17

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152  1.000000   0
g_{2}         3  0   -5.068043  -9.000000  20
p_{0,15}      0  0   -10.625195 -6.996759  22
p_{0,17}      0  0   -21.248887 1.000000   44
p_{0,1}       0  0   -10.610101 1.000000   21
p_{0,56}      0  1   -31.869324 -9.000000  67
```

**Filtered Graph**



File: `out/186_dg_0_11100_f_0_17_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 20 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 21 |
| $p_{0,15}$ | 0 | 0 | $-27896.445756$ | $-6.996759$ | $-27919.715474$ | 22 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $1.0$ | $-55785.61853$ | 44 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-72.87308$ | $-72.87308$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $0.006113$ | $0.006113$ |
| 183 | $p_{0,1}, p_{0,15},$ | $p_{0,17},$ | 1 | $-6.594357$ | $-6.594357$ |
| Sum | | | | | $-208.67648668796178$ |

$\Delta G$ = -31.502870278989164
$\Delta E$ = -0.0794806761920911
|E| = 7
|U| = 4

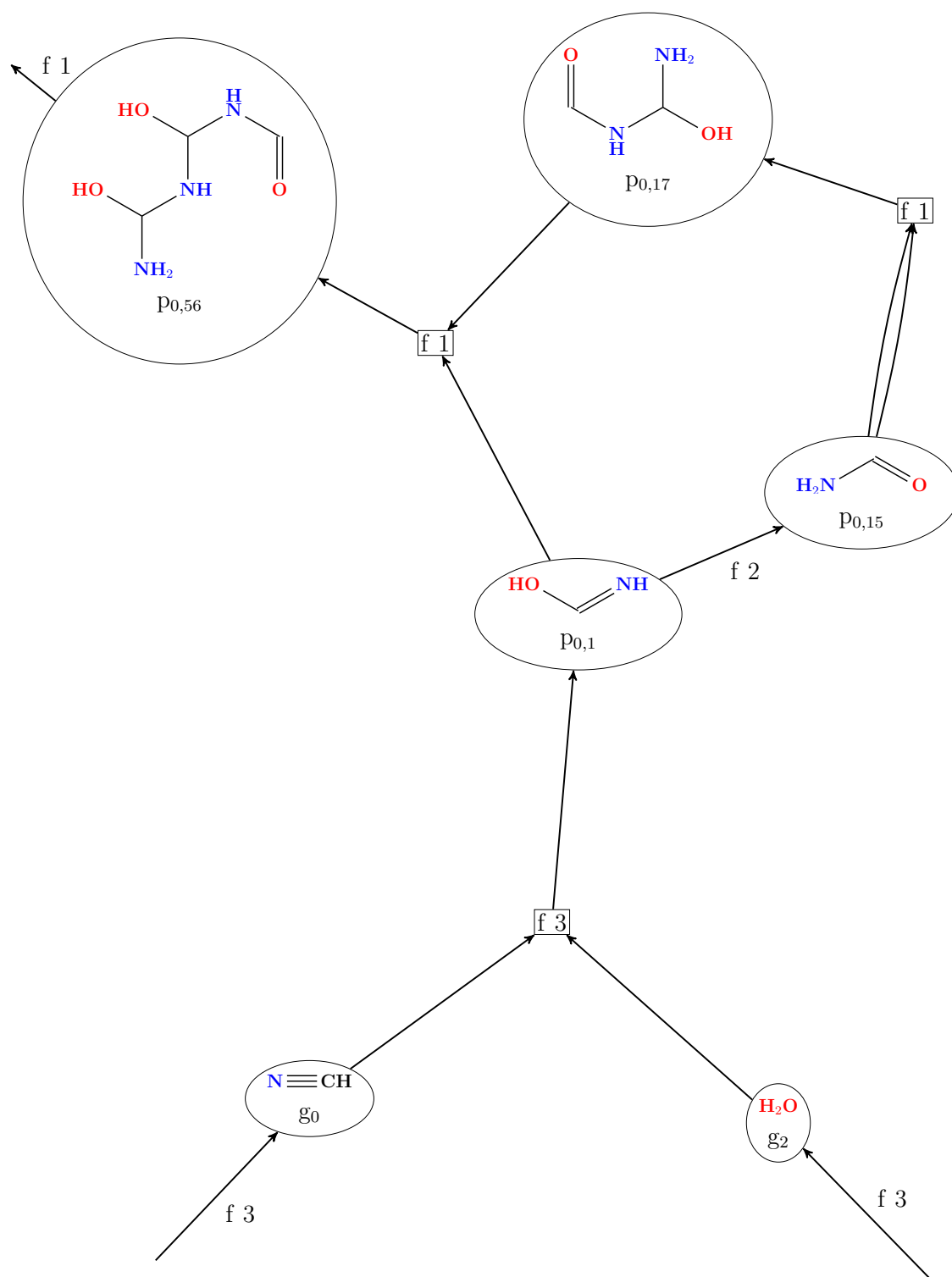## 0.3.19   Solution 18

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152  1.000000   0
g_{2}         3  0   -5.068043  1.000000   0
p_{0,15}      0  0   -10.625174 0.974002   22
p_{0,17}      0  0   -21.248844 1.000000   45
p_{0,1}       0  0   -10.610080 1.000000   21
p_{0,56}      0  1   -31.869324 -9.000000  67
```

# Filtered Graph



File: `out/195_dg_0_11100_f_0_18_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|---|---|---|---|---|---|---|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 21 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $0.974002$ | $-27893.15064$ | 22 |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | 45 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-39.7367$ | $-39.7367$ |
| 180 | $p_{0,15}, p_{0,15},$ | $p_{0,17},$ | 1 | $0.006113$ | $0.006113$ |
| 196 | $p_{0,1}, p_{0,17},$ | $p_{0,56},$ | 1 | $-73.034258$ | $-73.034258$ |
| Sum | | | | | $-208.67648668796178$ |

$\Delta G$ = -43.97456329994093
$\Delta E$ = -0.0794806761920911
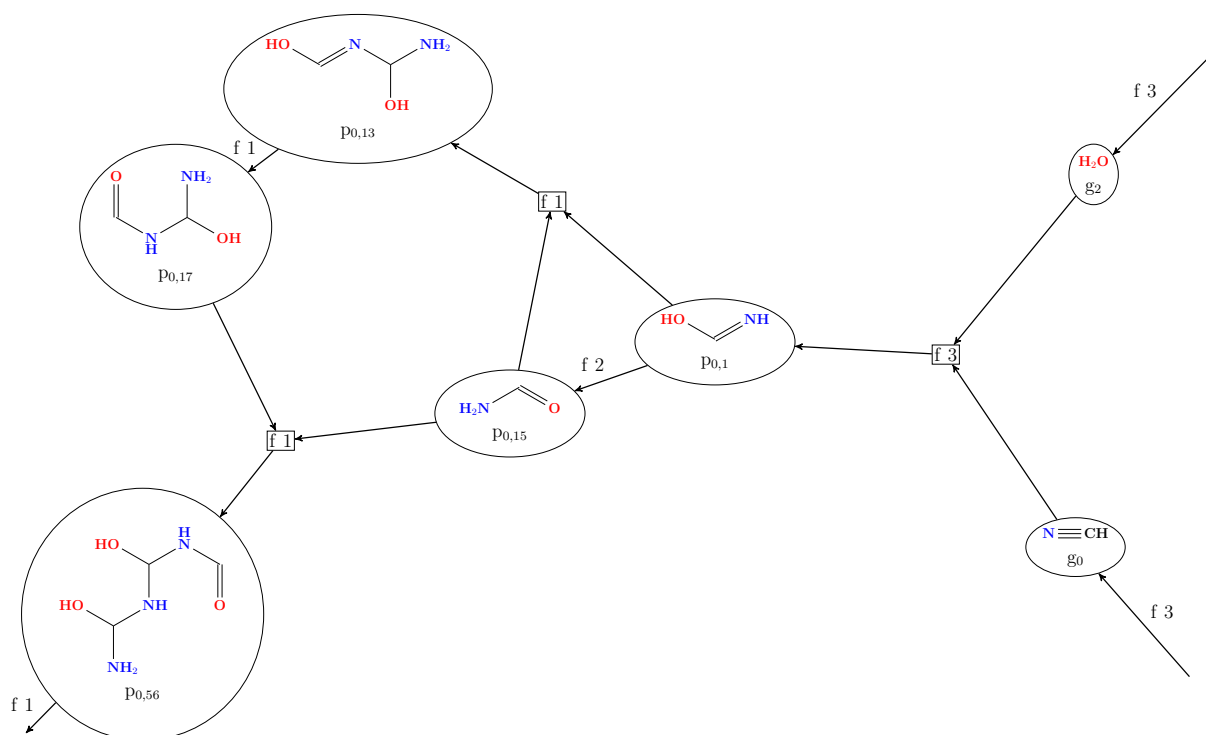|E| = 7
|U| = 4

## 0.3.20 Solution 19

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152  1.000000   0
g_{2}         3  0   -5.068043  -9.000000  0
p_{0,13}      0  0   -21.240635 1.000000   43
p_{0,15}      0  0   -10.625174 1.000000   22
p_{0,17}      0  0   -21.248887 -7.008710  44
p_{0,1}       0  0   -10.610101 1.000000   20
p_{0,56}      0  1   -31.869324 -9.000000  67
```

# Filtered Graph



File: `out/204_dg_0_11100_f_0_19_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 20 |
| $p_{0,13}$ | 0 | 0 | $-55767.279594$ | $1.0$ | $-55763.953809$ | 43 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | 22 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $-7.00871$ | $-55812.253777$ | 44 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-39.572909$ | $-39.572909$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $0.0$ | $0.0$ |
| 192 | $p_{0,1}, p_{0,15},$ | $p_{0,13},$ | 1 | $-18.229808$ | $-18.229808$ |
| 250 | $p_{0,13},$ | $p_{0,17},$ | 1 | $-54.958779$ | $-54.958779$ |
| Sum | | | | | $-208.67648668795562$ |

$\Delta G$ = -31.502869753889232
$\Delta E$ = -0.07948067619208875
|E| = 8
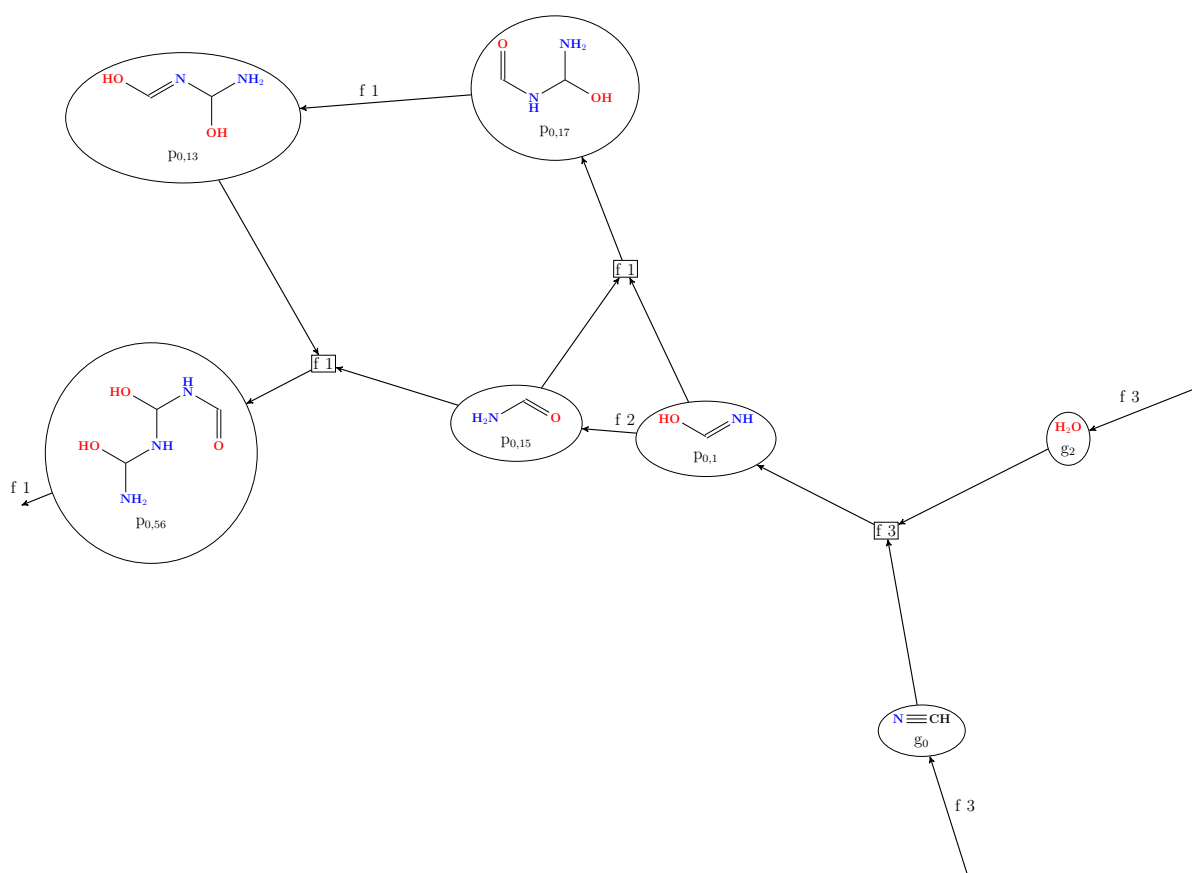|U| = 5

## 0.3.21 Solution 20

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  1.000000   0
p_{0,13}     0  0   -21.240678 -9.000000 64
p_{0,15}     0  0   -10.625174 1.000000  2
p_{0,17}     0  0   -21.248844 1.000000  4
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
```

**Filtered Graph**



File: `out/213_dg_0_11100_f_0_20_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | $0$ |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | $0$ |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | $1$ |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | $64$ |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | $2$ |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | $4$ |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | $67$ |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|------------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.803747$ | $-95.803747$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-39.572909$ | $-39.572909$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $-13.274931$ | $-13.274931$ |
| 183 | $p_{0,1}, p_{0,15},$ | $p_{0,17},$ | 1 | $-39.782951$ | $-39.782951$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $-20.130705$ | $-20.130705$ |
| Sum | | | | | $-208.67648668795562$ |

$\Delta G$ = -43.97456356249089

$\Delta E$ = -0.07948067619208875

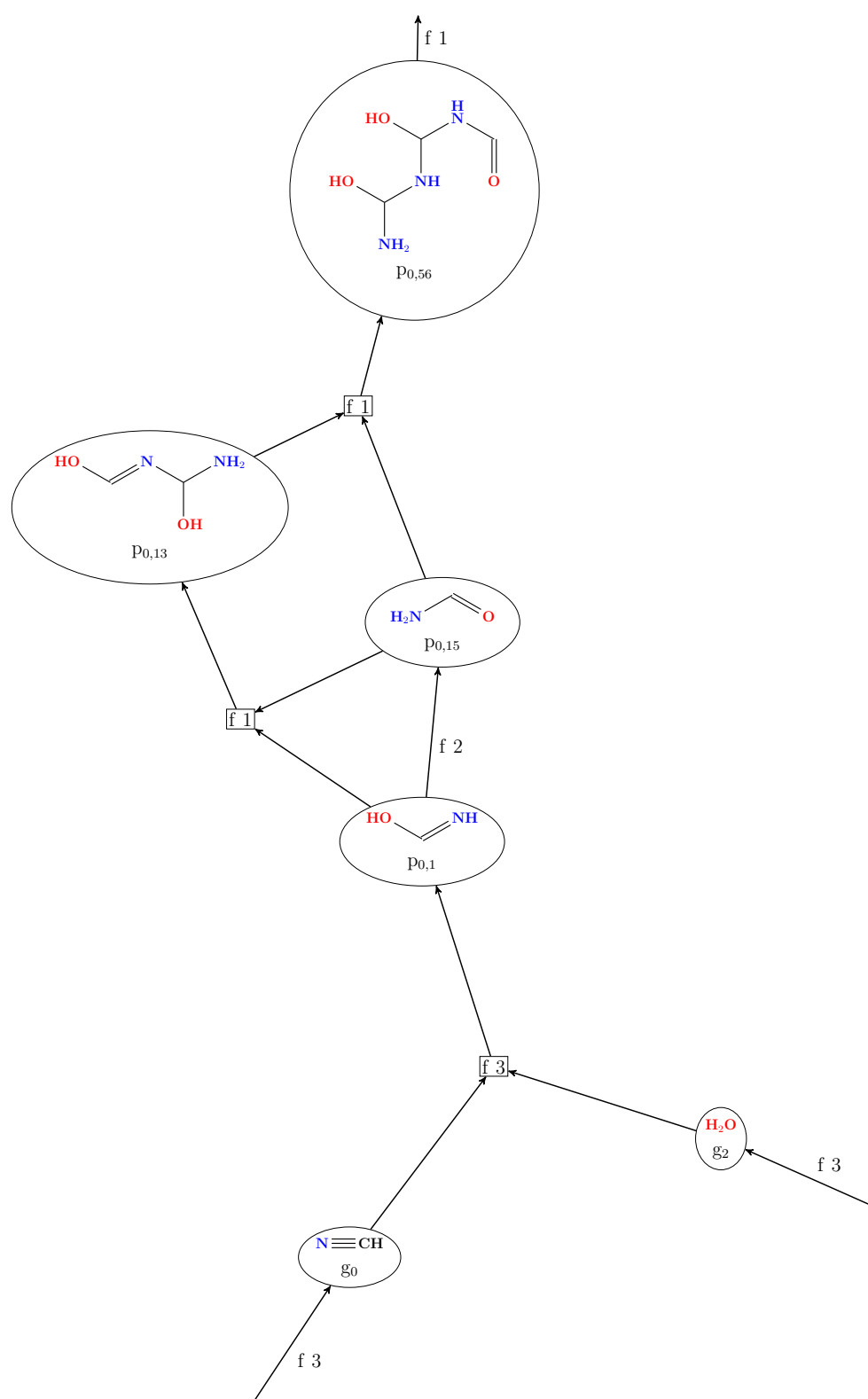|E| = 8

|U| = 5

## 0.3.22 Solution 21

**Overall Data**

```
Objective value (non-integral): -0.0794807
Vertex/Graph In Out G         logK      t_order
g_{0}         3  0   -5.507152  1.000000  0
g_{2}         3  0   -5.068043  1.000000  0
p_{0,13}      0  0   -21.240678 -9.000000 64
p_{0,15}      0  0   -10.625174 1.000000  2
p_{0,1}       0  0   -10.610080 1.000000  1
p_{0,56}      0  1   -31.869324 -9.000000 67
```

**Filtered Graph**



f 1

HO  
HO  
NH  
NH$_2$  
N  
H  
O  
$p_{0,56}$

f 1

HO  
N  
NH$_2$  
OH  
$p_{0,13}$

f 1

H$_2$N  
O  
$p_{0,15}$

f 2

HO  
NH  
$p_{0,1}$

f 3

H$_2$O  
$g_2$

f 3

N≡CH  
$g_0$

f 3

File: `out/222_dg_0_11100_f_0_21_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|---------|---------|---------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.761341$ | $1.0$ | $-27853.435556$ | 1 |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | 64 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | 2 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|---------|---------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.748033$ | $-95.748033$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 2 | $-39.628622$ | $-39.628622$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $-13.274931$ | $-13.274931$ |
| 192 | $p_{0,1}, p_{0,15},$ | $p_{0,13},$ | 1 | $-59.96937$ | $-59.96937$ |
| Sum | | | | | $-208.67648668794948$ |

$\Delta G$ = -43.97456356249089
$\Delta E$ = -0.0794806761920864
|E| = 7
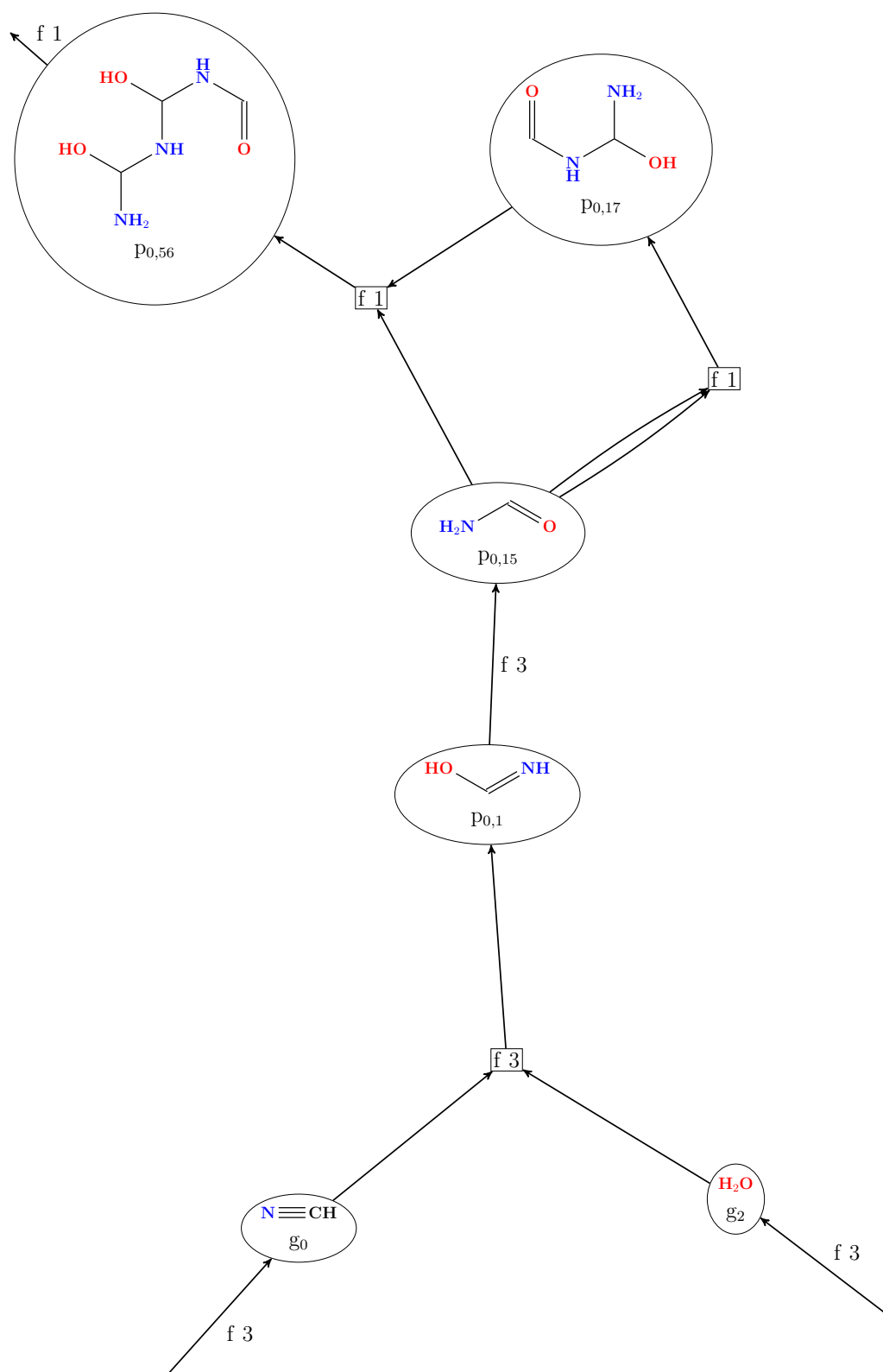|U| = 4

### 0.3.23 Solution 22

**Overall Data**

```
Objective value (non-integral): -0.0643869
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  1.000000   0
p_{0,15}     0  0   -10.625174 1.000000   2
p_{0,17}     0  0   -21.248887 -7.008710  64
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

**Filtered Graph**

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | 0 |
| $g_2$ | 3 | 0 | $-13306.144961$ | $1.0$ | $-13302.819176$ | 0 |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | 1 |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | 2 |
| $p_{0,17}$ | 0 | 0 | $-55788.944315$ | $-7.00871$ | $-55812.253777$ | 64 |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | 67 |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|-----------|--------|--------|------|------------------|-----------------------------|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-95.803747$ | $-95.803747$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 3 | $-39.572909$ | $-39.572909$ |
| 180 | $p_{0,15}, p_{0,15},$ | $p_{0,17},$ | 1 | $-33.615679$ | $-33.615679$ |
| 181 | $p_{0,15}, p_{0,17},$ | $p_{0,56},$ | 1 | $0.0$ | $0.0$ |
| Sum | | | | | $-169.04786458416666$ |

$\Delta G$ = -43.97456356249089
$\Delta E$ = -0.06438693117384997
$|E| = 8$
$|U| = 4$

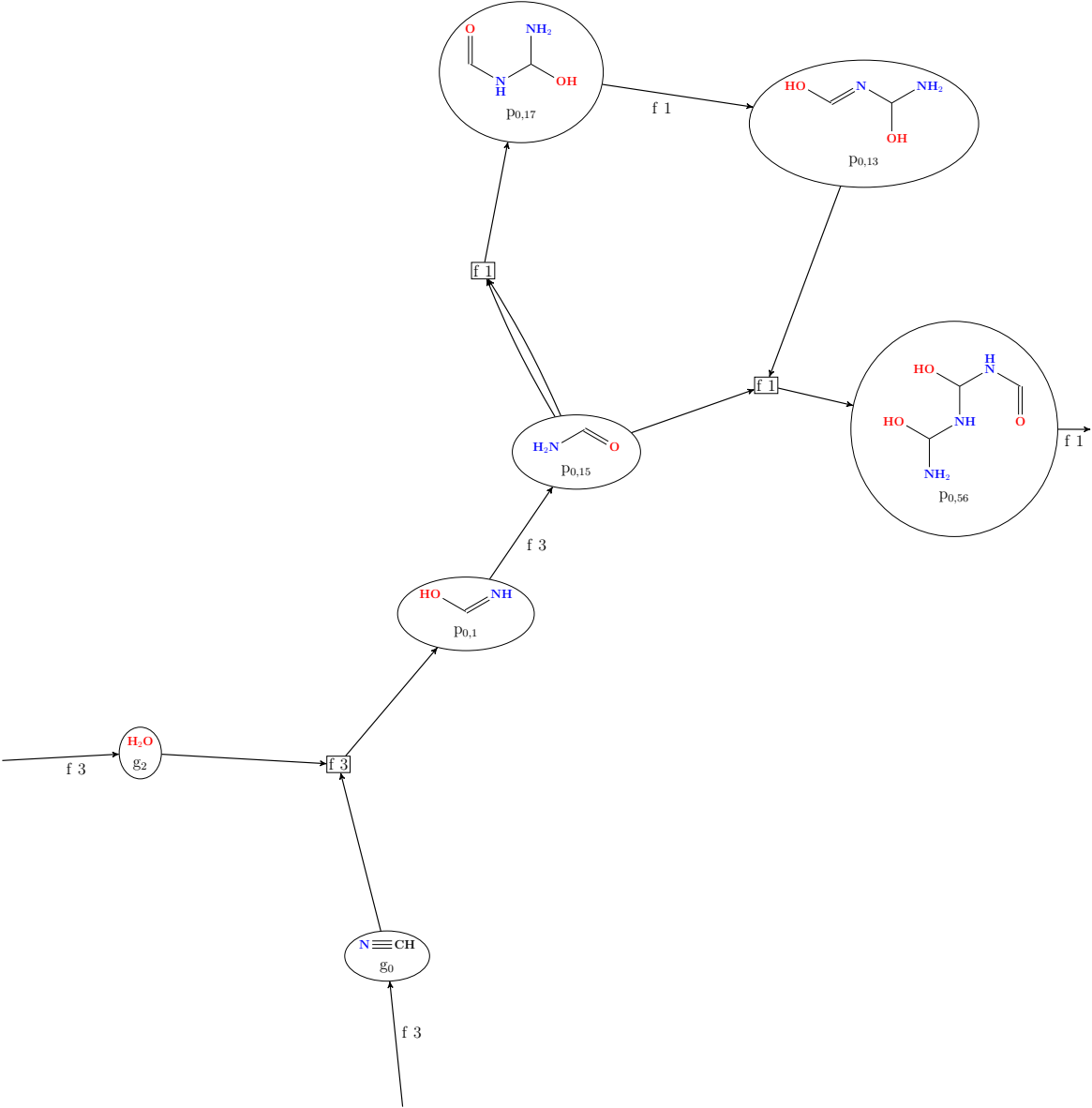### 0.3.24    Solution 23

**Overall Data**

```
Objective value (non-integral): -0.0643869
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -9.000000  0
p_{0,13}     0  0   -21.240678 -9.000000  64
p_{0,15}     0  0   -10.625174 1.000000   2
p_{0,17}     0  0   -21.248844 1.000000   63
p_{0,1}      0  0   -10.610101 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

**Filtered Graph**



File: `out/240_dg_0_11100_f_0_23_filt`

| Vertex | InFlow | OutFlow | $x_v^{\Delta G^0}$ | $x_v^K$ | $x_v^{\Delta G}$ | $t_v$ |
|--------|--------|---------|--------------------|---------|------------------|-------|
| $g_0$ | 3 | 0 | $-14459.025578$ | $1.0$ | $-14455.699793$ | $0$ |
| $g_2$ | 3 | 0 | $-13306.144961$ | $-9.0$ | $-13336.077027$ | $0$ |
| $p_{0,1}$ | 0 | 0 | $-27856.817054$ | $1.0$ | $-27853.491269$ | $1$ |
| $p_{0,13}$ | 0 | 0 | $-55767.391129$ | $-9.0$ | $-55797.323194$ | $64$ |
| $p_{0,15}$ | 0 | 0 | $-27896.389963$ | $1.0$ | $-27893.064178$ | $2$ |
| $p_{0,17}$ | 0 | 0 | $-55788.832737$ | $1.0$ | $-55785.506952$ | $63$ |
| $p_{0,56}$ | 0 | 1 | $-83672.898792$ | $-9.0$ | $-83702.830857$ | $67$ |

| Hyperedge | Source | Target | Flow | $x_e^{\Delta G}$ | $\overline{x}_e^{\Delta G}$ |
|---|---|---|---|---|---|
| 6 | $g_0, g_2,$ | $p_{0,1},$ | 3 | $-54.231434$ | $-54.231434$ |
| 36 | $p_{0,1},$ | $p_{0,15},$ | 3 | $-39.572909$ | $-39.572909$ |
| 169 | $p_{0,13}, p_{0,15},$ | $p_{0,56},$ | 1 | $-13.274931$ | $-13.274931$ |
| 180 | $p_{0,15}, p_{0,15},$ | $p_{0,17},$ | 1 | $-0.210043$ | $-0.210043$ |
| 253 | $p_{0,17},$ | $p_{0,13},$ | 1 | $-20.130705$ | $-20.130705$ |
| Sum | | | | | $-169.04786458416052$ |

$\Delta G$ = -31.502869228789308
$\Delta E$ = -0.06438693117384763
|E| = 9
|U| = 5