Summary

December 6, 2024

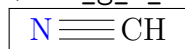# Contents

0.1 Loaded Graphs

0.1.1 g_{0}

$$N \equiv C \text{—} H$$

File: out/001_g_0_10300000

$$N \equiv CH$$

File: out/003_g_0_11310100

0.1.2 g_{1}

File: out/005_g_1_10300000

$$NH_3$$

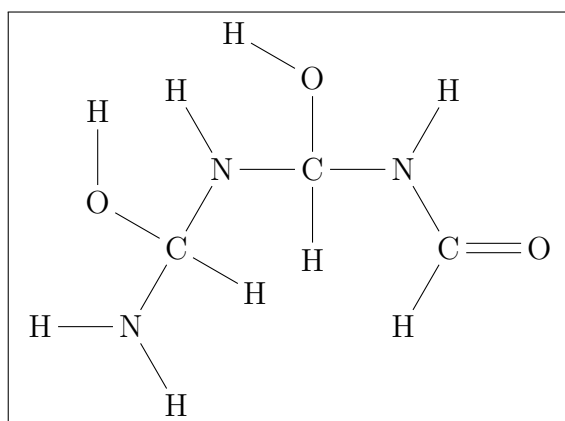File: out/007_g_1_11310100

0.1.3 g_{2}

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
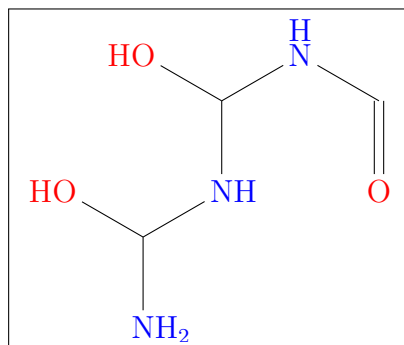
File: `out/015_g_1088_11310100`

0.3 Enumerated Flows

0.3.1 Solution 0

Overall Data

```
Objective value (non-integral): -0.101116
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  -3.000000 0
g_{2}        3  0   -5.068033  -3.000000 0
p_{0,13}     0  0   -21.240635 -3.000000 65
p_{0,1}      0  0   -10.610101 -3.000000 1
p_{0,56}     0  1   -31.869324 -6.000000 67
p_{0,5}      0  0   -16.158998 -6.000000 2
```

Filtered Graph
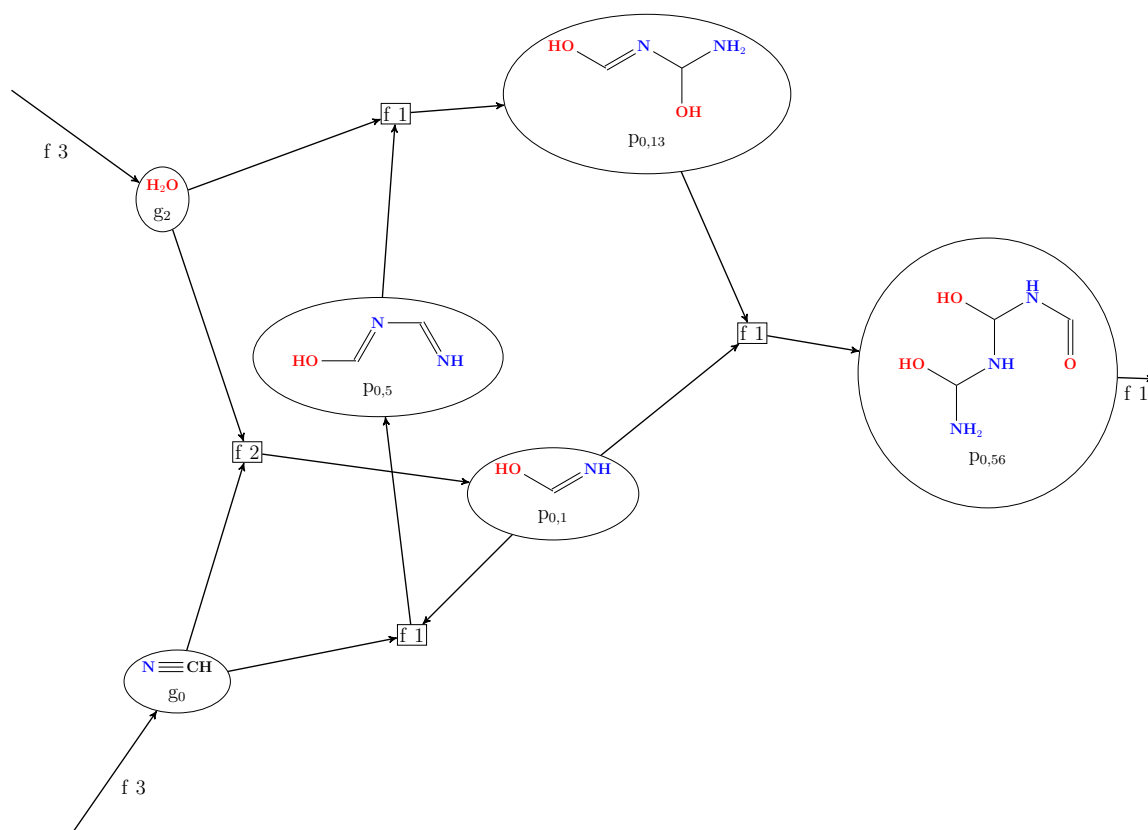
File: `out/027_dg_0_11100_f_0_0_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-3.0	-14469.002933	0
g_2	3	0	-13306.118349	-3.0	-13316.095704	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,5}$	0	0	-42425.44262	-6.0	-42445.397331	2
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	65
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-84.863583	-84.863583
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-109.599988	-109.599988
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-22.099535	-22.099535
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-48.802143	-48.802143
Sum					-265.4787993681657

ΔG = -35.02288237153935
ΔE = -0.10111553449717699
|E| = 5
|U| = 4

### 0.3.2 Solution 1

Overall Data

```
Objective value (non-integral): -0.101116
Vertex/Graph In Out G          logK       t_order
g_{0}         3  0   -5.507152  -3.000000 0
g_{2}         3  0   -5.068043  -6.000000 0
p_{0,13}      0  0   -21.240678 -6.000000 64
p_{0,15}      0  0   -10.625195 -3.000000 2
p_{0,1}       0  0   -10.610101 -3.000000 1
p_{0,56}      0  1   -31.869324 -6.000000 67
p_{0,5}       0  0   -16.158998 -3.000000 2
```

Filtered Graph
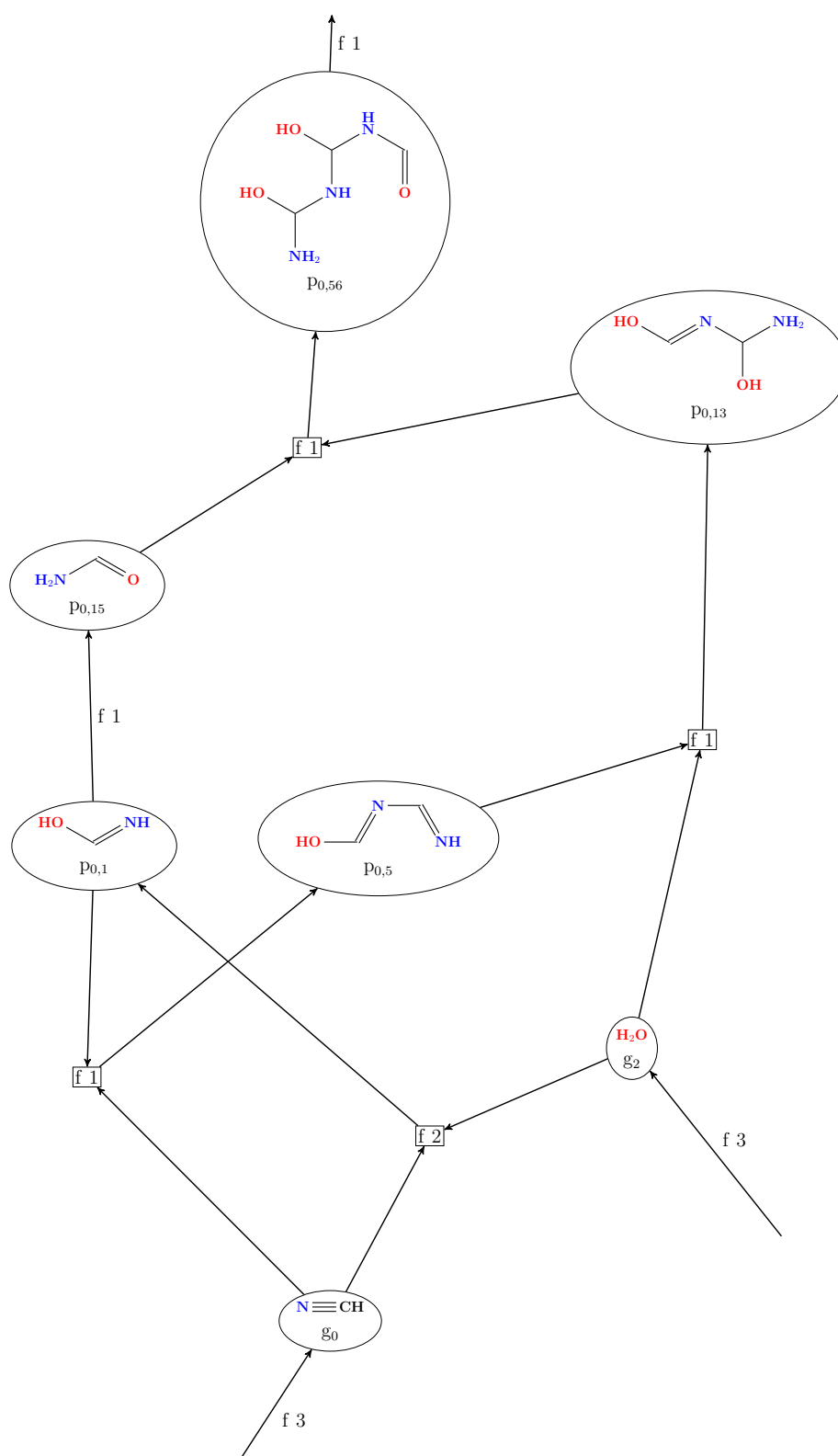
File: `out/038_dg_0_11100_f_0_1_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,5}$	0	0	-42425.44262	-3.0	-42435.419975	2
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	64
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-78.027426	-78.027426
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-102.790443	-102.790443
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-28.994003	-28.994003
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-2.252362	-2.252362
Sum					-265.47879936816463

ΔG = -32.97203528995104
ΔE = -0.10111553449717658
|E| = 6
|U| = 5

0.3.3 Solution 2

Overall Data

```
Objective value (non-integral): -0.0688029
Vertex/Graph In Out G          logK       t_order
g_{0}       3  0   -5.507152  -3.000000 0
g_{2}       3  0   -5.068043  -3.000000 0
p_{0,13}    0  0   -21.240635 -3.000000 34
p_{0,15}    0  0   -10.625195 -6.000000 32
p_{0,17}    0  0   -21.248887 -3.000000 3
p_{0,1}     0  0   -10.610101 -3.000000 1
p_{0,56}    0  1   -31.869324 -6.000000 67
```

Filtered Graph
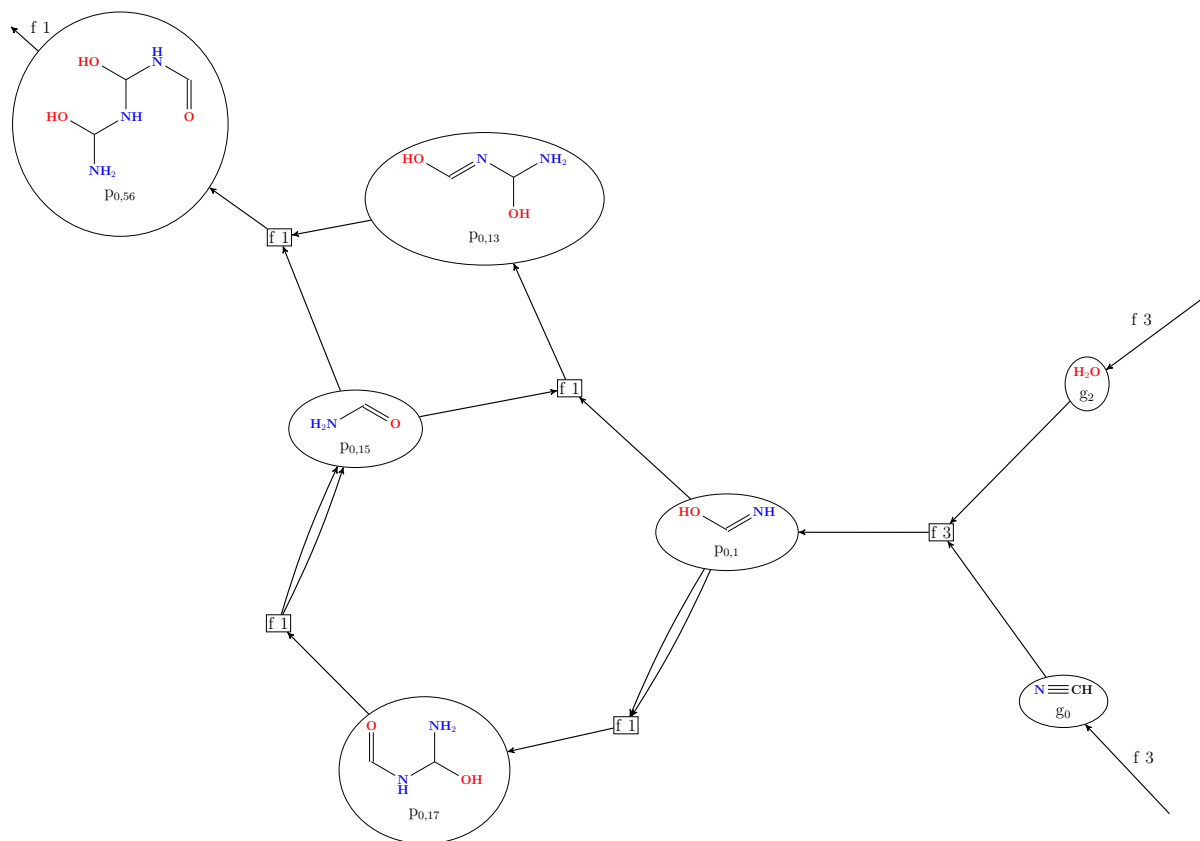
File: `out/049_dg_0_11100_f_0_2_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	34
$p_{0,15}$	0	0	-27896.445756	-6.0	-27916.400466	32
$p_{0,17}$	0	0	-55788.944315	-3.0	-55798.92167	3
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.836971	-84.836971
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-68.500661	-68.500661
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-2.363897	-2.363897
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-0.397694	-0.397694
237	$p_{0,17},$	$p_{0,15}, p_{0,15},$	1	-24.375831	-24.375831
Sum					-180.6420120052131

ΔG = -35.01489822713569

ΔE = -0.06880290870692735

|E| = 7

|U| = 5

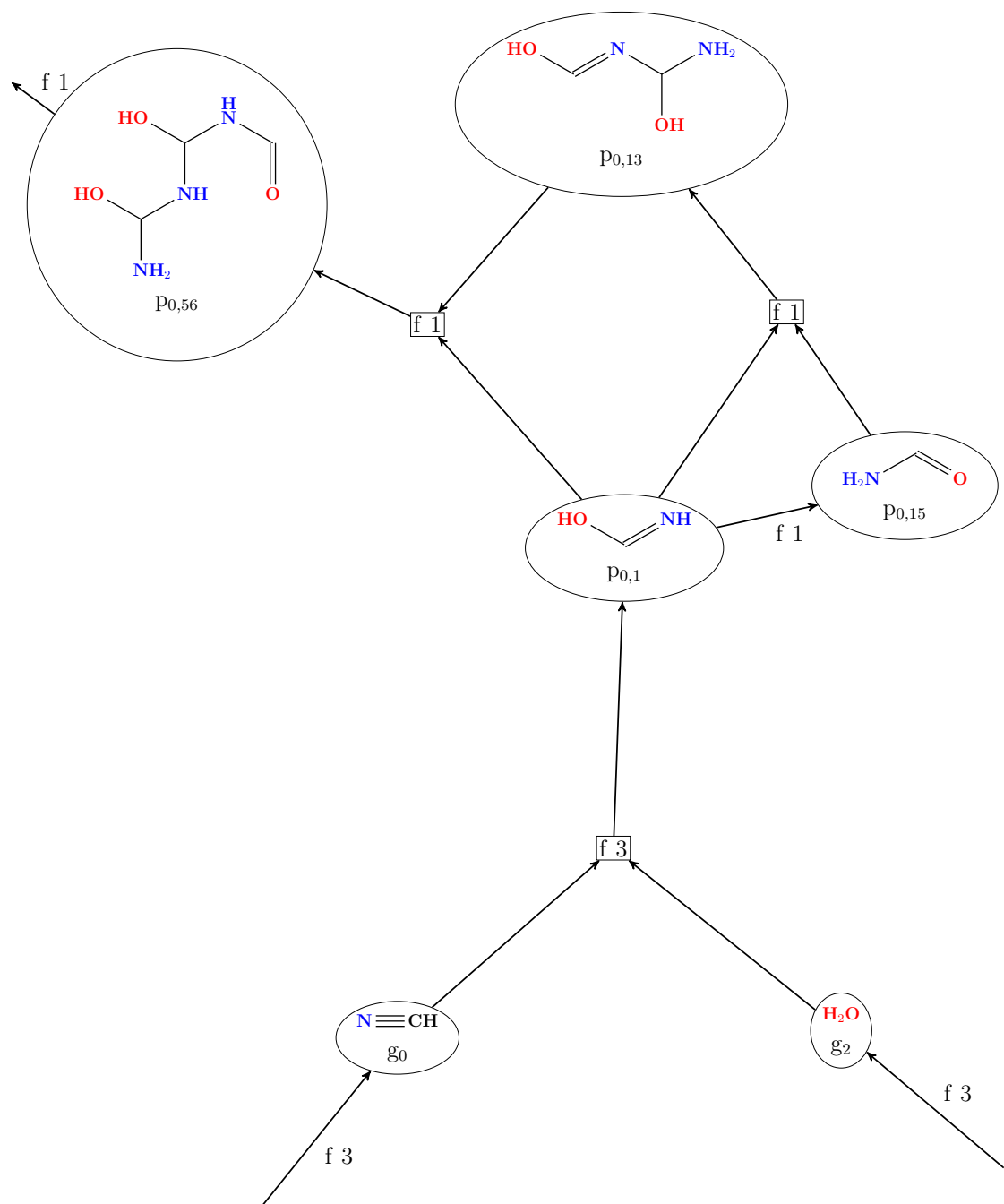### 0.3.4   Solution 3

Overall Data

```
Objective value (non-integral): -0.0688029
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  -3.000000 0
g_{2}        3  0   -5.068033  -6.000000 0
p_{0,13}     0  0   -21.240678 -6.000000 46
p_{0,15}     0  0   -10.625174 -6.000000 22
p_{0,1}      0  0   -10.610101 -6.000000 20
p_{0,56}     0  1   -31.869260 -3.000000 67
```

Filtered Graph

File: out/058_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	-3.0	-14469.002933	0
g_2	3	0	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	20
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	46
$p_{0,15}$	0	0	-27896.389963	-6.0	-27916.344673	22
$p_{0,56}$	0	1	-83672.731446	-3.0	-83682.708802	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.863583	-84.863583
36	$p_{0,1},$	$p_{0,15},$	1	-39.572909	-39.572909
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-0.565022	-0.565022
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-28.094628	-28.094628
Sum					-180.64201200521208

$\Delta G = -32.28232966215784$
$\Delta E = -0.06880290870692696$
$|E| = 6$
$|U| = 4$
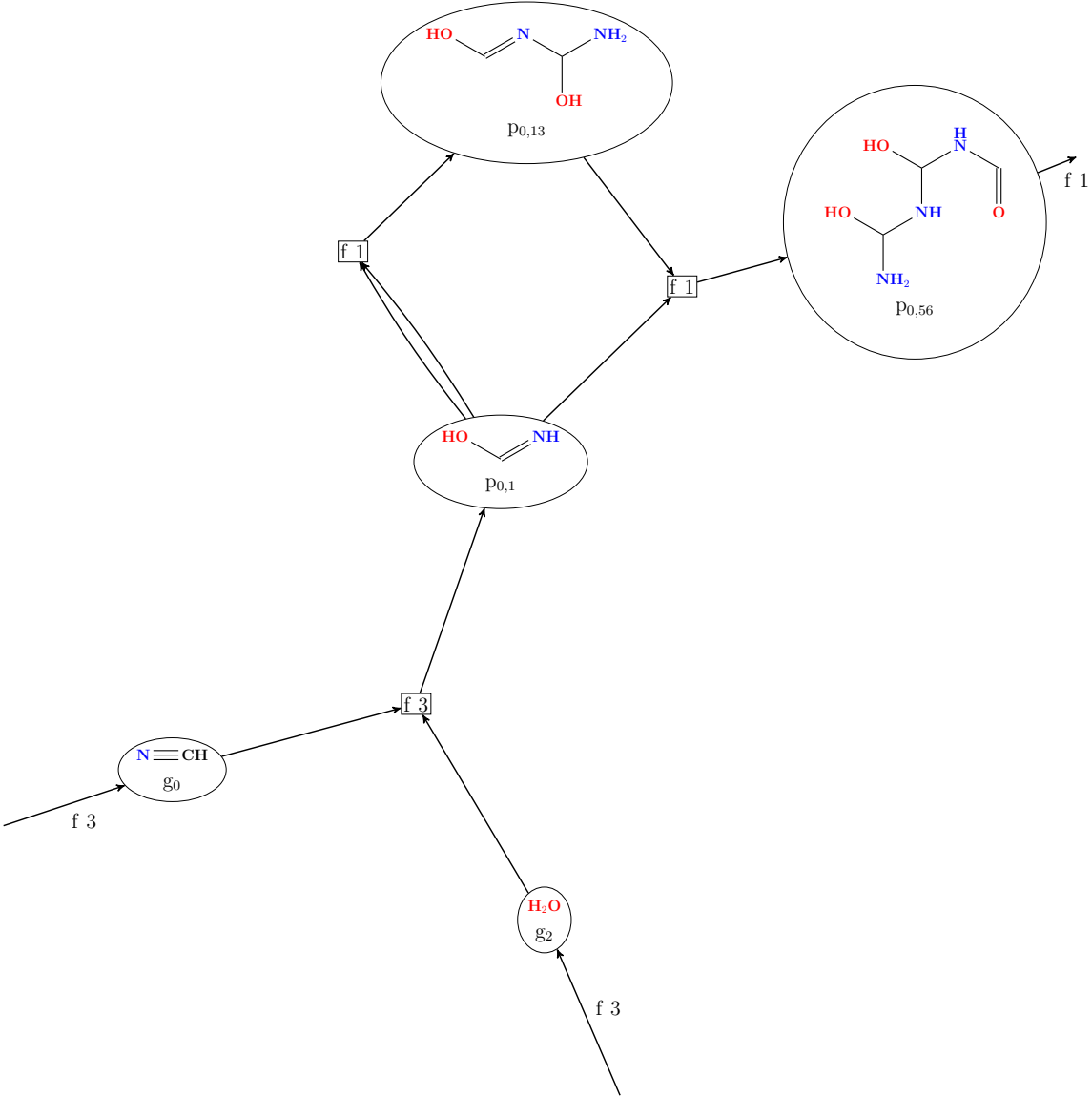
0.3.5   Solution 4

Overall Data

```
Objective value (non-integral): -0.0688029
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  -6.000000 0
g_{2}        3  0   -5.068033  -6.000000 0
p_{0,13}     0  0   -21.240635 -3.000000 3
p_{0,1}      0  0   -10.610080 -3.000000 1
p_{0,56}     0  1   -31.869324 -6.000000 67
```

Filtered Graph

File: `out/067_dg_0_11100_f_0_4_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-6.0	-14478.980288	0
g_2	3	0	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	1
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	3
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-71.18878	-71.18878
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-46.947368	-46.947368
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-48.857857	-48.857857
Sum					-180.642012005211

ΔG = -30.93715597207012

ΔE = -0.06880290870692654
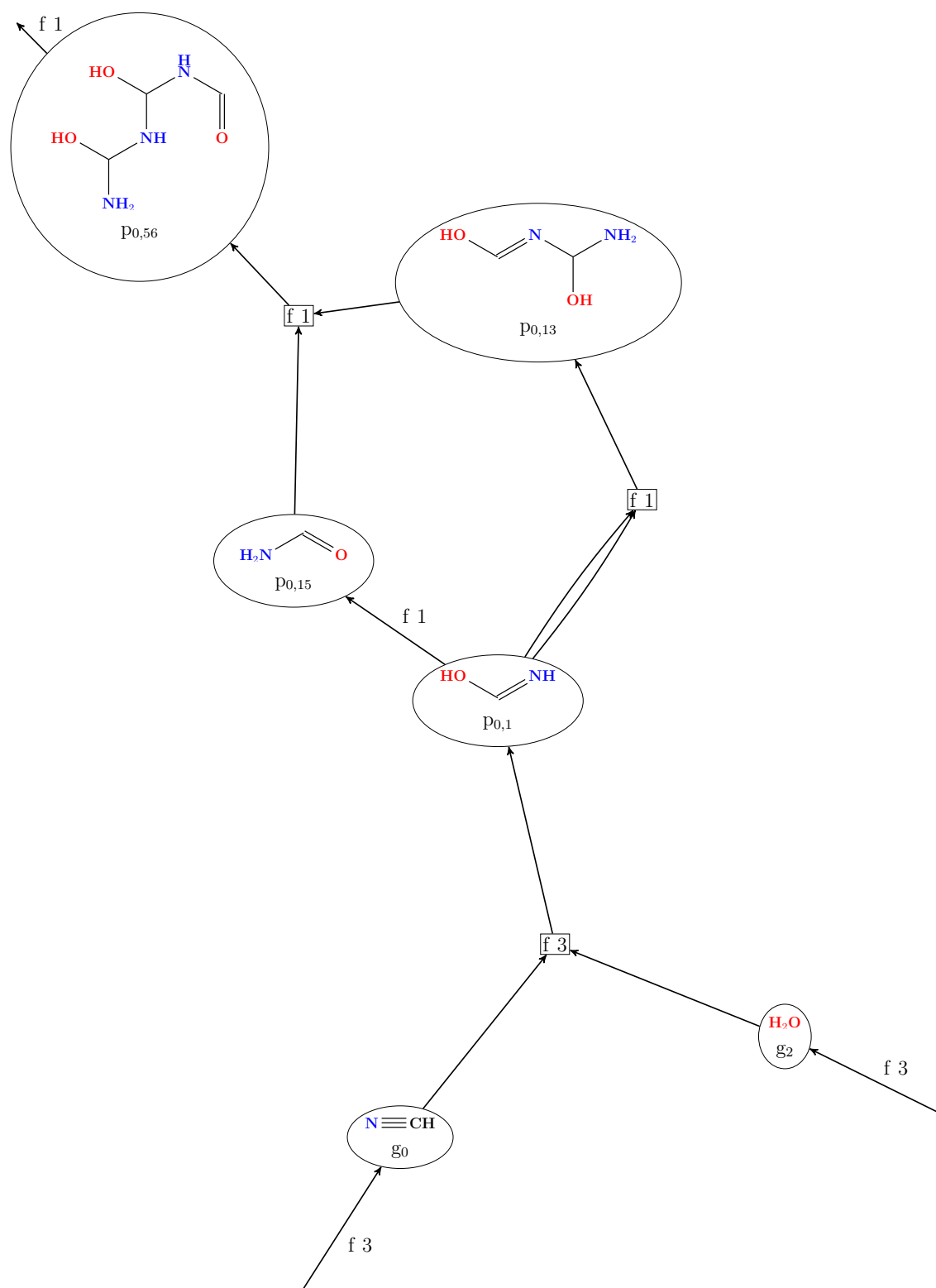
|E| = 5
|U| = 3

0.3.6 Solution 5

Overall Data

```
Objective value (non-integral): -0.0688029
Vertex/Graph In Out G           logK      t_order
g_{0}        3  0   -5.507152  -3.000000 0
g_{2}        3  0   -5.068043  -3.000000 0
p_{0,13}     0  0   -21.240678 -6.000000 3
p_{0,15}     0  0   -10.625195 -3.000000 2
p_{0,1}      0  0   -10.610101 -3.000000 1
p_{0,56}     0  1   -31.869324 -6.000000 67
```

Filtered Graph

File: out/076_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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	3
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.836971	-84.836971
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-53.75702	-53.75702
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-2.252362	-2.252362
Sum					-180.64201200520992

ΔG = -35.014898752235624

ΔE = -0.06880290870692614

|E| = 6

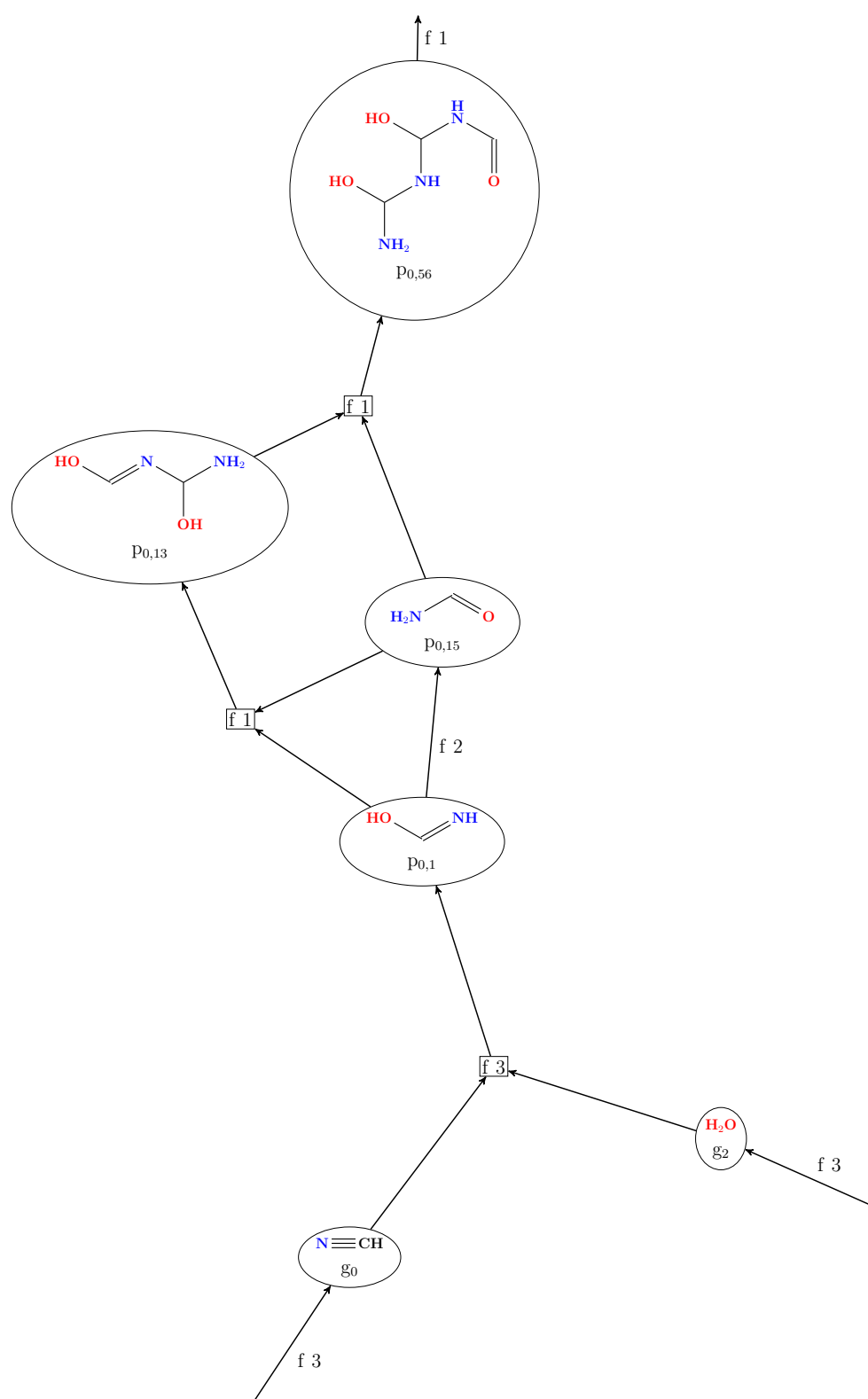|U| = 4

0.3.7 Solution 6

Overall Data

```
Objective value (non-integral): -0.0537092
Vertex/Graph In Out G          logK      t_order
g_{0}         3  0   -5.507152  -3.000000 0
g_{2}         3  0   -5.068043  -3.000000 0
p_{0,13}      0  0   -21.240678 -6.000000 64
p_{0,15}      0  0   -10.625174 -3.000000 2
p_{0,1}       0  0   -10.610080 -3.000000 1
p_{0,56}      0  1   -31.869324 -6.000000 67
```

Filtered Graph

File: `out/085_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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	1
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	64
$p_{0,15}$	0	0	-27896.389963	-3.0	-27906.367318	2
$p_{0,56}$	0	1	-83672.898792	-6.0	-83692.853502	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.781257	-84.781257
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-2.308155	-2.308155
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-14.239825	-14.239825
Sum					-141.01338990141696

ΔG = -35.014898752235624

ΔE = -0.05370916368868583

|E| = 7

|U| = 4