Summary

December 6, 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}

$$H \quad N \quad H$$
$$H$$

File: out/005_g_1_10300000

$$NH_3$$

File: out/007_g_1_11310100

0.1.3 g_{2}

$$H \quad O \quad H$$

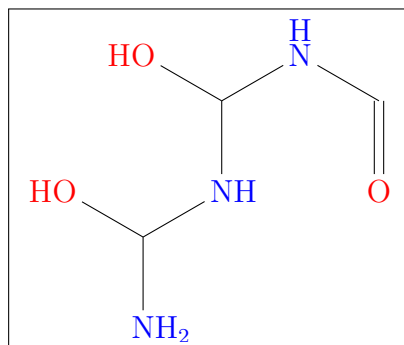File: out/009_g_2_10300000

$$H_2O$$

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
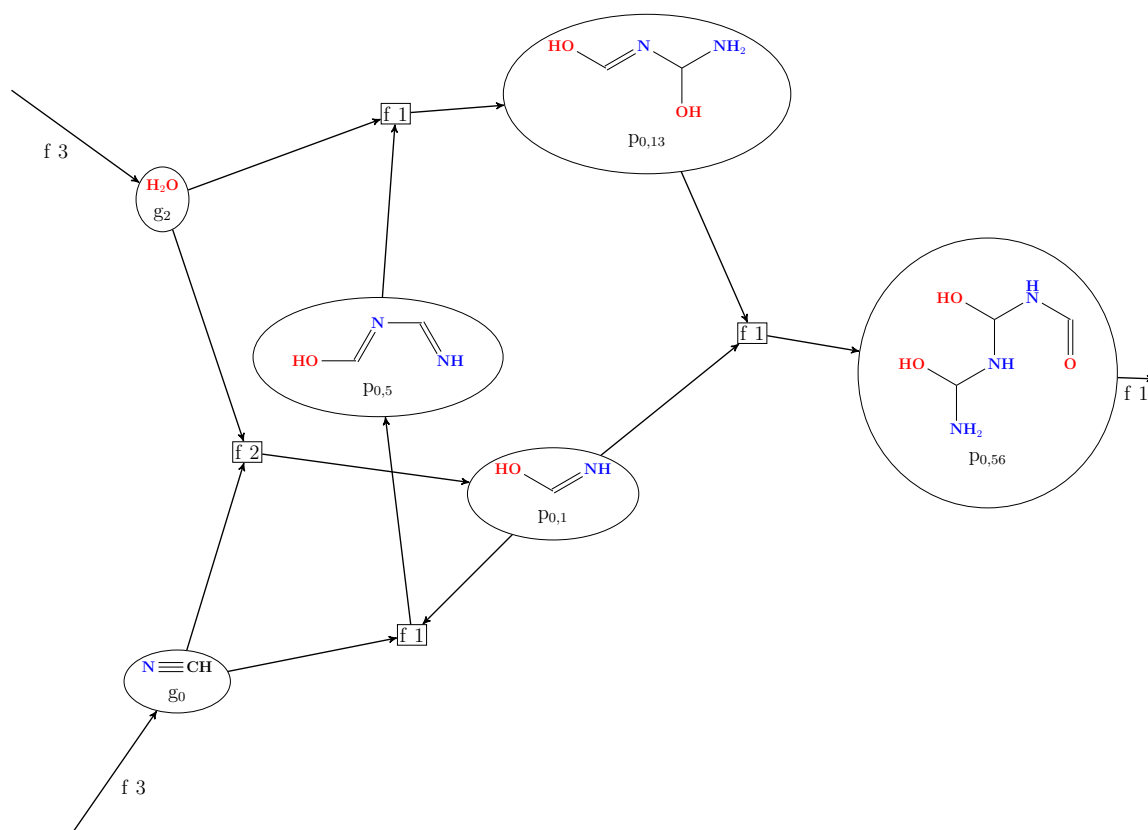
0.3.1 Solution 0

Overall Data

```
Objective value (non-integral): -0.0889455
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 -6.000000 65
p_{0,1}     0  0   -10.610101 -6.000000 1
p_{0,56}    0  1   -31.869324 -9.000000 67
p_{0,5}     0  0   -16.158965 -9.000000 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	-6.0	-14478.980288	0
g_2	3	0	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	1
$p_{0,5}$	0	0	-42425.357769	-9.0	-42455.289835	2
$p_{0,13}$	0	0	-55767.279594	-6.0	-55787.234305	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	-76.707095	-76.707095
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-102.032121	-102.032121
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-13.354427	-13.354427
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-41.319127	-41.319127
Sum					-233.52631952661258

ΔG = -31.011985862394866
ΔE = -0.08894547765882163
|E| = 5
|U| = 4

0.3.2 Solution 1

Overall Data

```
Objective value (non-integral): -0.0889455
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   -21.240678 -9.000000 64
p_{0,17}     0  0   -21.248844 -9.000000 65
p_{0,1}      0  0   -10.610101 -9.000000 1
p_{0,56}     0  1   -31.869324 -7.073211 67
p_{0,5}      0  0   -16.158998 -9.000000 2
```

Filtered Graph
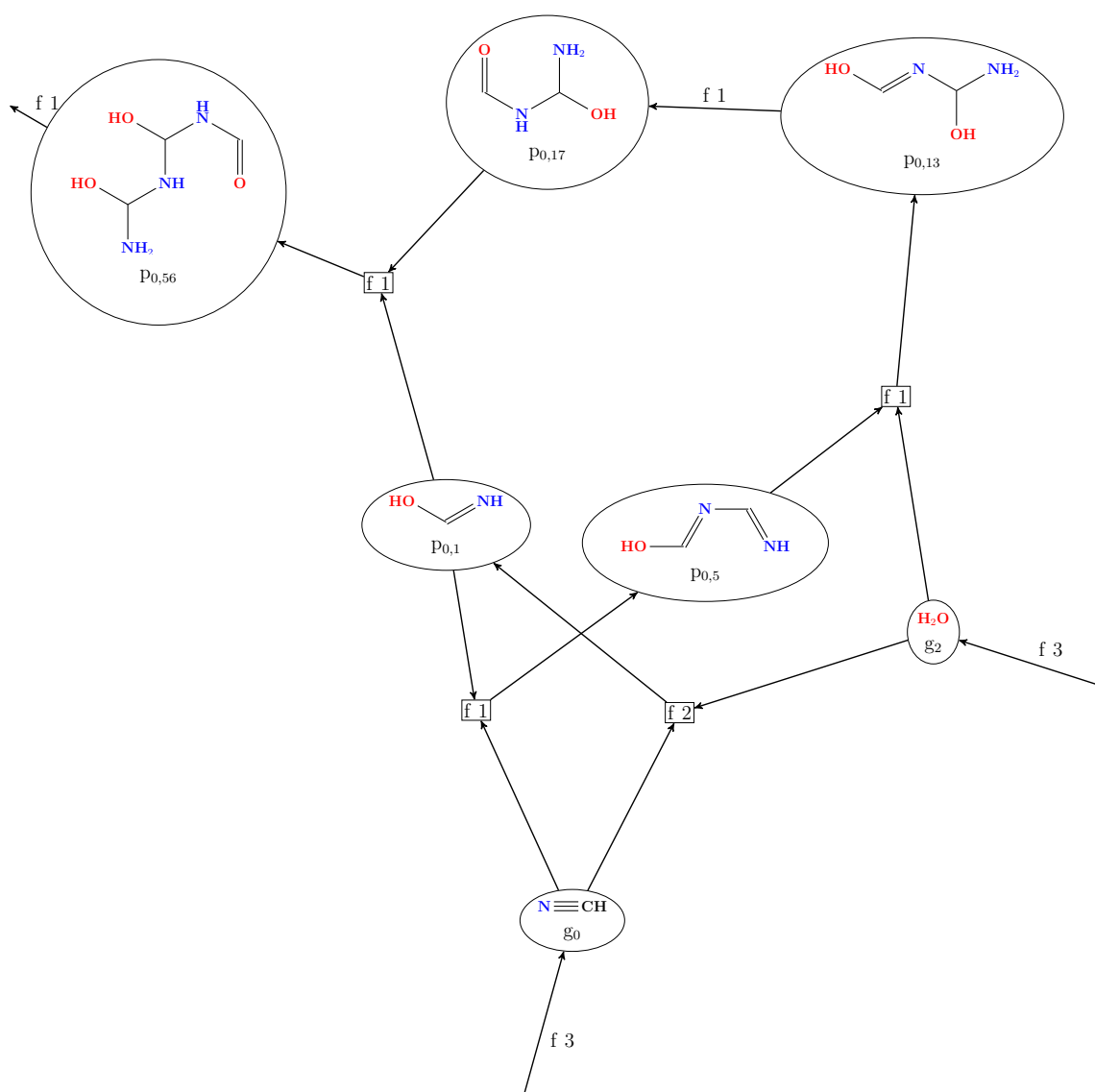
File: `out/038_dg_0_11100_f_0_1_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-6.0	-14478.980288	0
g_2	3	0	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.817054	-9.0	-27886.74912	1
$p_{0,5}$	0	0	-42425.44262	-9.0	-42455.374686	2
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	64
$p_{0,17}$	0	0	-55788.832737	-9.0	-55818.764803	65
$p_{0,56}$	0	1	-83672.898792	-7.073211	-83696.422772	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-84.190111	-84.190111
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-94.633956	-94.633956
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-20.864127	-20.864127
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	0.006113	0.006113
250	$p_{0,13},$	$p_{0,17},$	1	-21.441608	-21.441608
Sum					-233.5263195266147

$\Delta G = $ -30.531379489239242

$\Delta E = $ -0.08894547765882244

$|\text{E}| = 6$

$|\text{U}| = 5$

0.3.3 Solution 2

Overall Data

```
Objective value (non-integral): -0.0889455
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  -6.000000 0
g_{2}        3  0   -5.068043  -6.000000 0
p_{0,13}     0  0   -21.240635 -6.000000 23
p_{0,15}     0  0   -10.625195 -6.680156 22
p_{0,1}      0  0   -10.610101 -6.000000 21
p_{0,56}     0  1   -31.869324 -9.000000 67
p_{0,5}      0  0   -16.158998 -9.000000 22
```

Filtered Graph
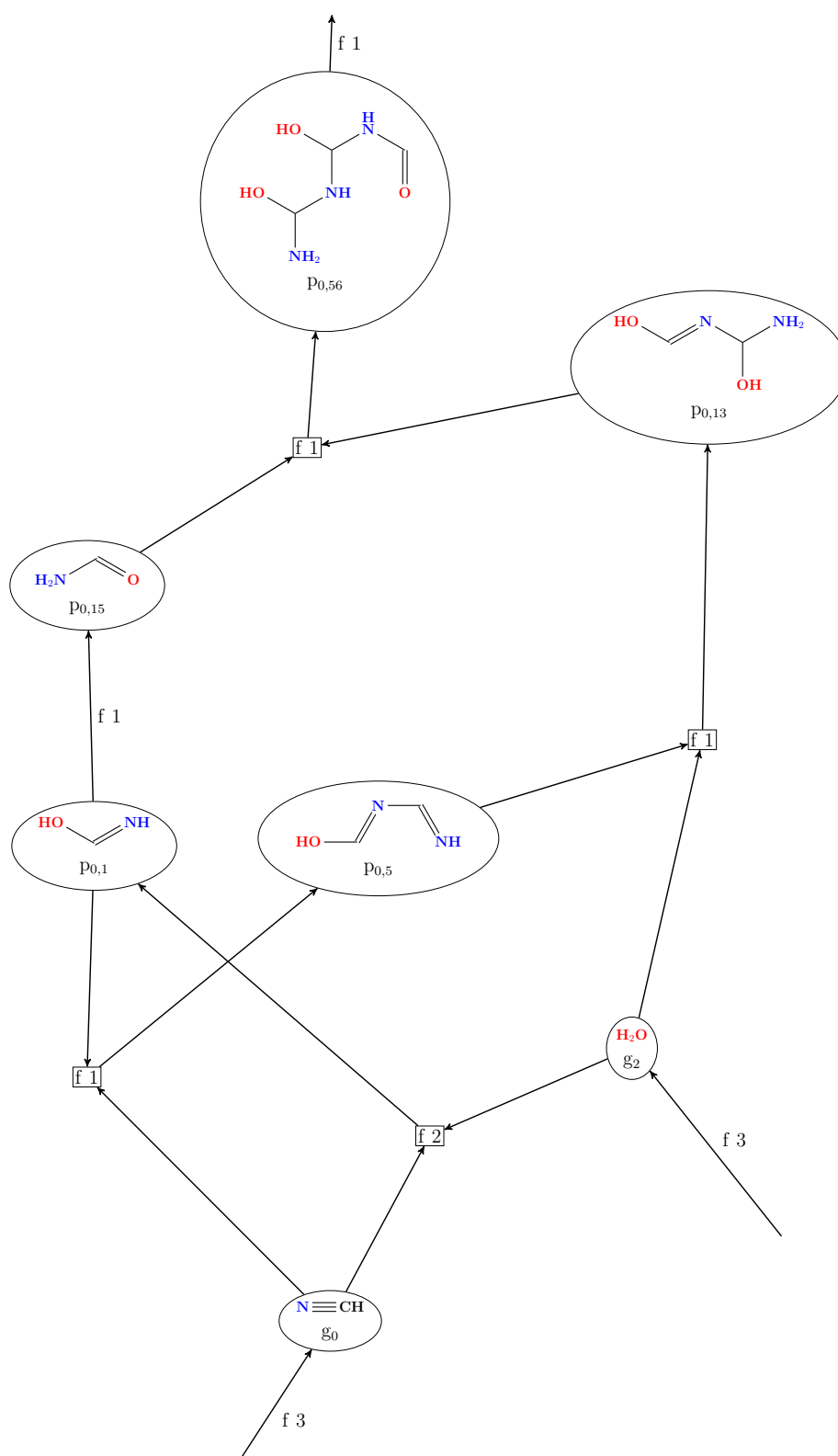
File: `out/049_dg_0_11100_f_0_2_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14459.025578	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	21
$p_{0,5}$	0	0	-42425.44262	-9.0	-42455.374686	22
$p_{0,13}$	0	0	-55767.279594	-6.0	-55787.234305	23
$p_{0,15}$	0	0	-27896.445756	-6.680156	-27918.662517	22
$p_{0,56}$	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	-76.680483	-76.680483
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-102.116972	-102.116972
36	$p_{0,1},$	$p_{0,15},$	1	-41.32524	-41.32524
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-13.242964	-13.242964
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-233.52631952661466

$\Delta G = $ -31.004002243091136
$\Delta E = $ -0.08894547765882242
$|E| = 6$
$|U| = 5$
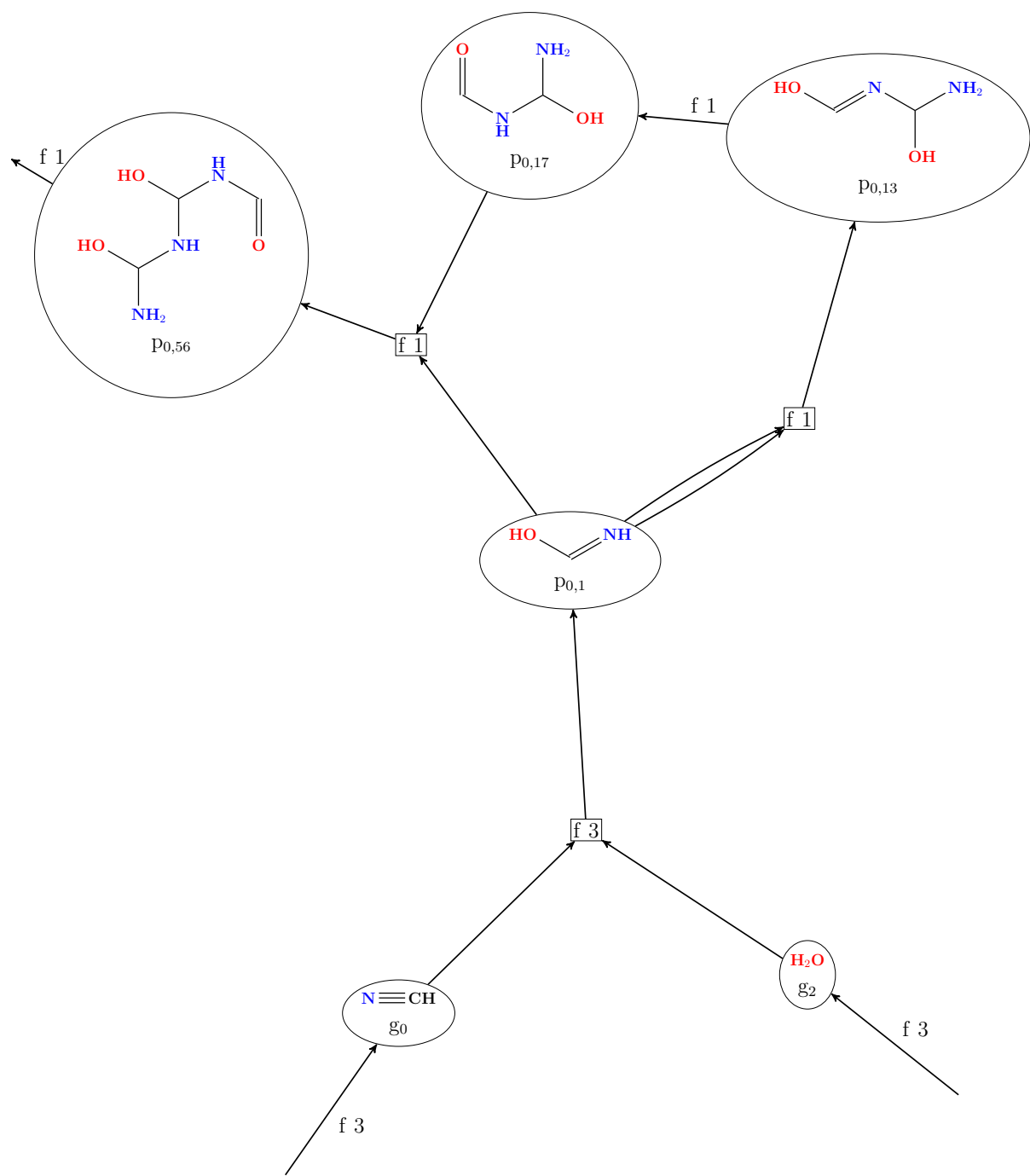
0.3.4   Solution 3

Overall Data

```
Objective value (non-integral): -0.0597395
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 -6.000000 3
p_{0,17}     0  0   -21.248844 -6.000000 65
p_{0,1}      0  0   -10.610080 -6.000000 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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	1
$p_{0,13}$	0	0	-55767.279594	-6.0	-55787.234305	3
$p_{0,17}$	0	0	-55788.832737	-6.0	-55808.787447	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	-61.658737	-61.658737
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-38.79088	-38.79088
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-19.821698	-19.821698
250	$p_{0,13},$	$p_{0,17},$	1	-21.553143	-21.553143
Sum					-156.8460199920717

ΔG = -26.5141920204086

ΔE = -0.05973949401232301

$|\text{E}| = 6$

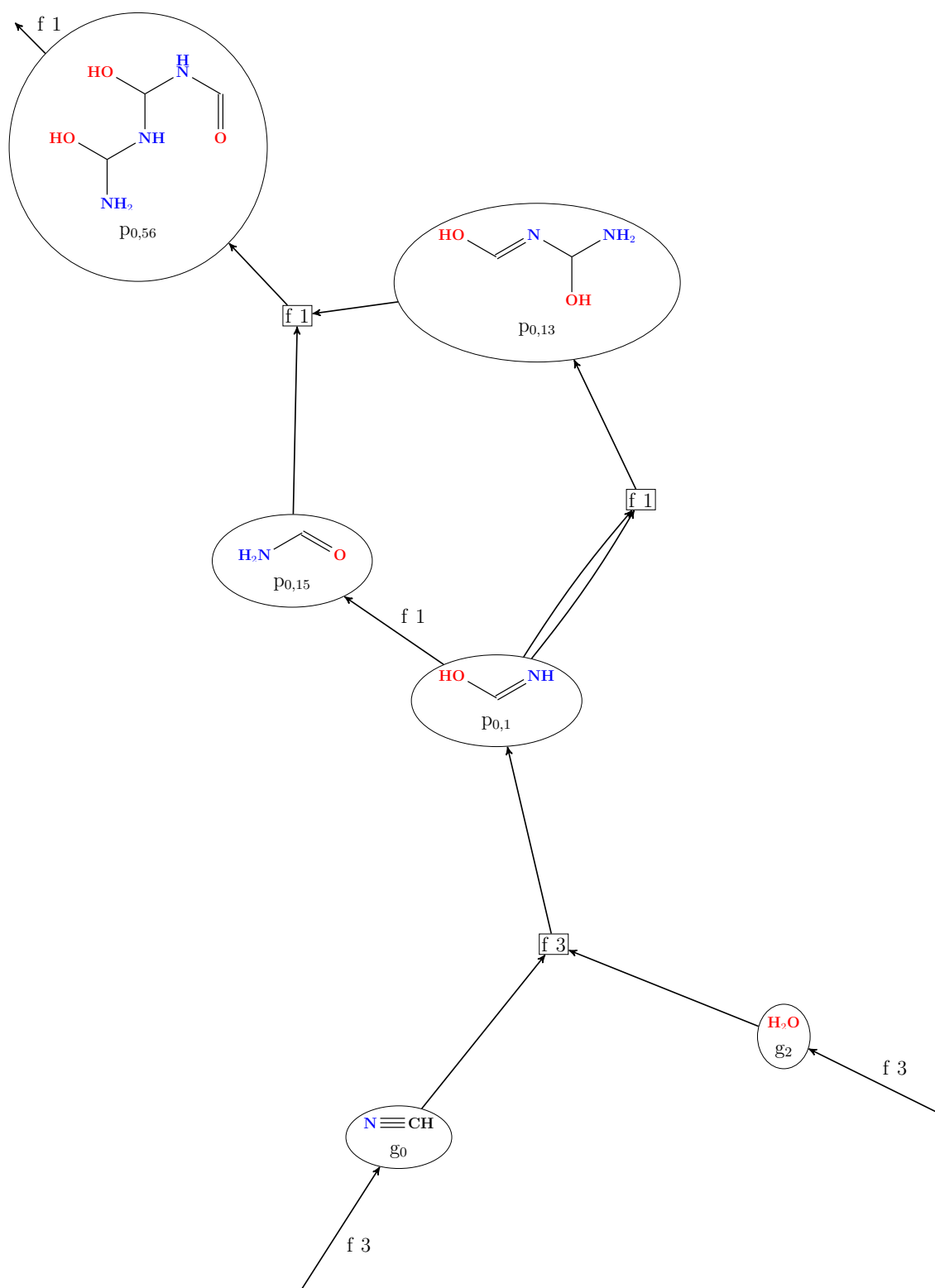$|\text{U}| = 4$

0.3.5 Solution 4

Overall Data

```
Objective value (non-integral): -0.0597395
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 -6.000000 3
p_{0,15}      0   0   -10.625195 -6.635441 2
p_{0,1}       0   0   -10.610101 -6.000000 1
p_{0,56}      0   1   -31.869324 -9.000000 67
```

Filtered Graph

f 1

HO—NH
HO—NH
NH₂
O

p₀,₅₆

f 1

HO—N—NH₂
OH

p₀,₁₃

f 1

H₂N—O

p₀,₁₅

f 1

HO—NH

p₀,₁

f 1

f 3

H₂O

g₂

f 3

N≡CH

g₀

f 3

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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	1
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	3
$p_{0,15}$	0	0	-27896.445756	-6.635441	-27918.513805	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	-61.71445	-61.71445
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-38.790987	-38.790987
36	$p_{0,1},$	$p_{0,15},$	1	-41.213705	-41.213705
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-156.8460199920717

ΔG = -26.514192282958568
ΔE = -0.05973949401232301
|E| = 6
|U| = 4

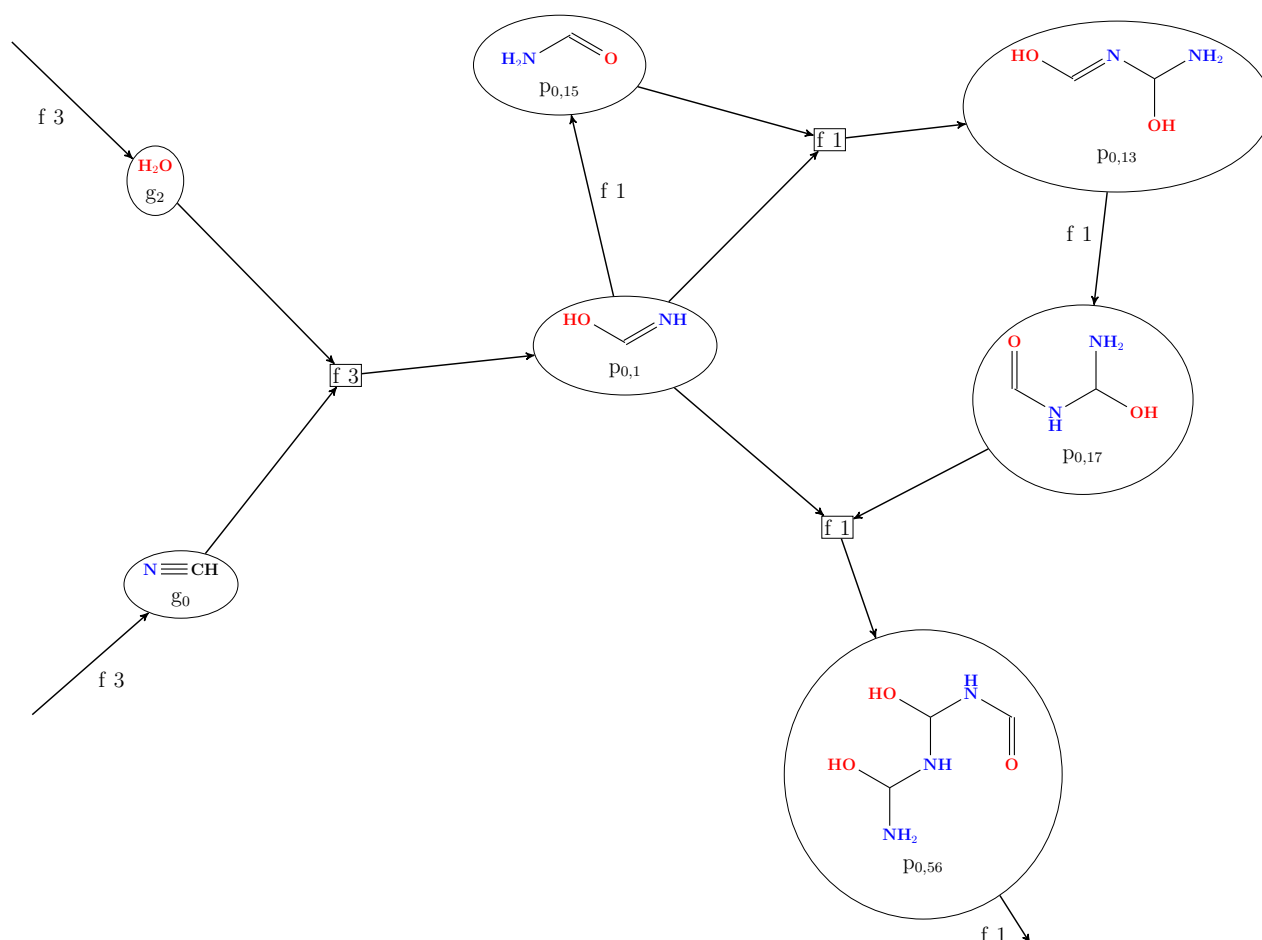### 0.3.6 Solution 5

Overall Data

```
Objective value (non-integral): -0.0597395
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 -6.335857 4
p_{0,15}     0  0   -10.625174 -6.000000 2
p_{0,17}     0  0   -21.248887 -9.000000 5
p_{0,1}      0  0   -10.610080 -6.000000 1
p_{0,56}     0  1   -31.869324 -9.000000 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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	1
$p_{0,13}$	0	0	-55767.279594	-6.335857	-55788.351294	4
$p_{0,15}$	0	0	-27896.389963	-6.0	-27916.344673	2
$p_{0,17}$	0	0	-55788.944315	-9.0	-55818.87638	5
$p_{0,56}$	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	-61.658737	-61.658737
36	$p_{0,1},$	$p_{0,15},$	1	-39.628622	-39.628622
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	0.0	0.0
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-12.227104	-12.227104
250	$p_{0,13},$	$p_{0,17},$	1	-28.309995	-28.309995
Sum					-156.8460199920696

ΔG = -26.514192282958568

ΔE = -0.059739494012322224
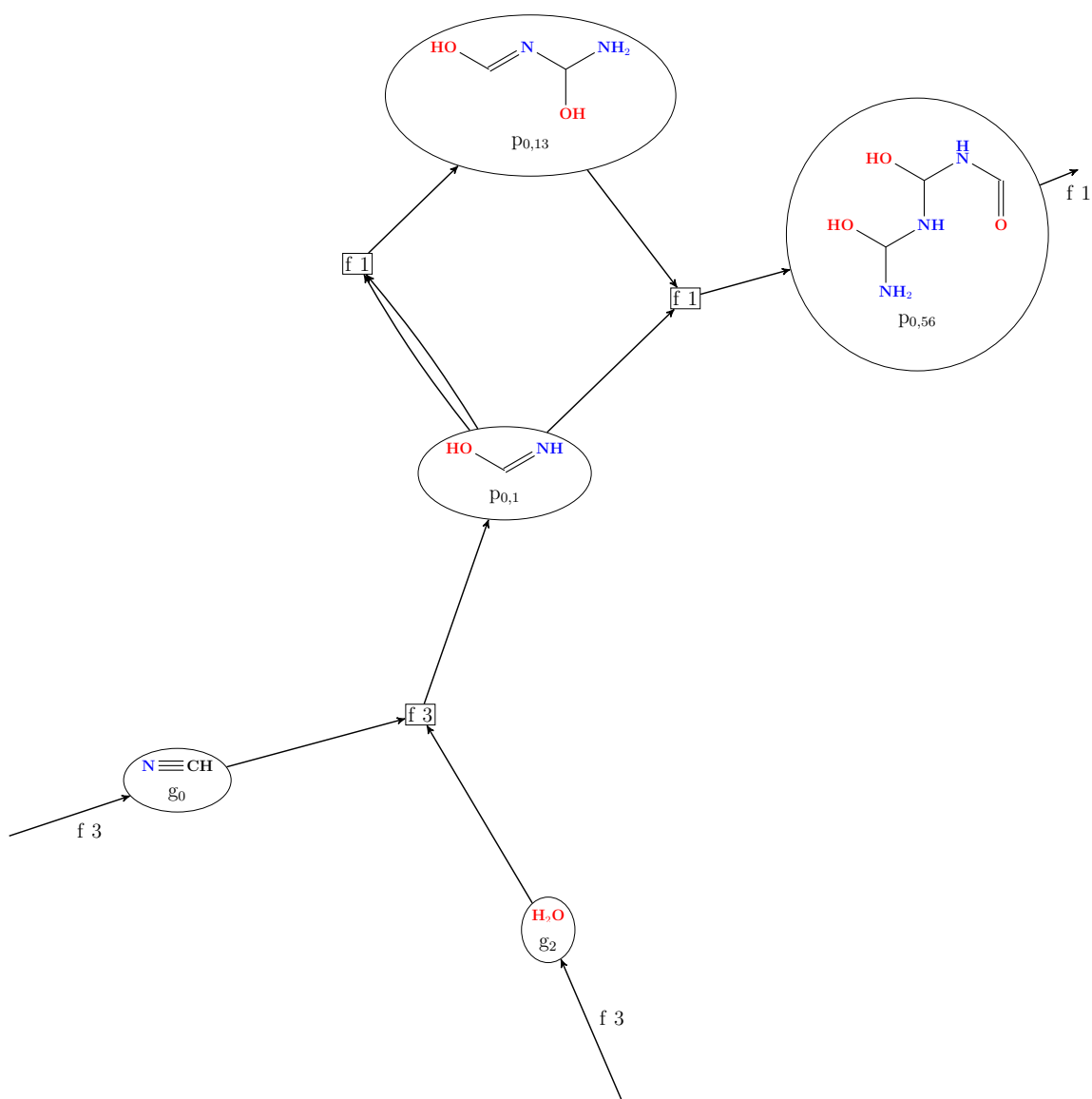
$|E| = 7$
$|U| = 5$

0.3.7 Solution 6

Overall Data

```
Objective value (non-integral): -0.0597395
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152 -6.000000 0
g_{2}        3  0   -5.068033 -9.000000 0
p_{0,13}     0  0   -21.240635 -6.000000 3
p_{0,1}      0  0   -10.610080 -6.000000 1
p_{0,56}     0  1   -31.869324 -9.000000 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	-6.0	-14478.980288	0
g_2	3	0	-13306.118349	-9.0	-13336.050414	0
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	1
$p_{0,13}$	0	0	-55767.279594	-6.0	-55787.234305	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	-69.168365	-69.168365
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-38.79088	-38.79088
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-41.374841	-41.374841
Sum					-156.8460199920696

ΔG = -28.767080488503638
ΔE = -0.059739494012322224
|E| = 5
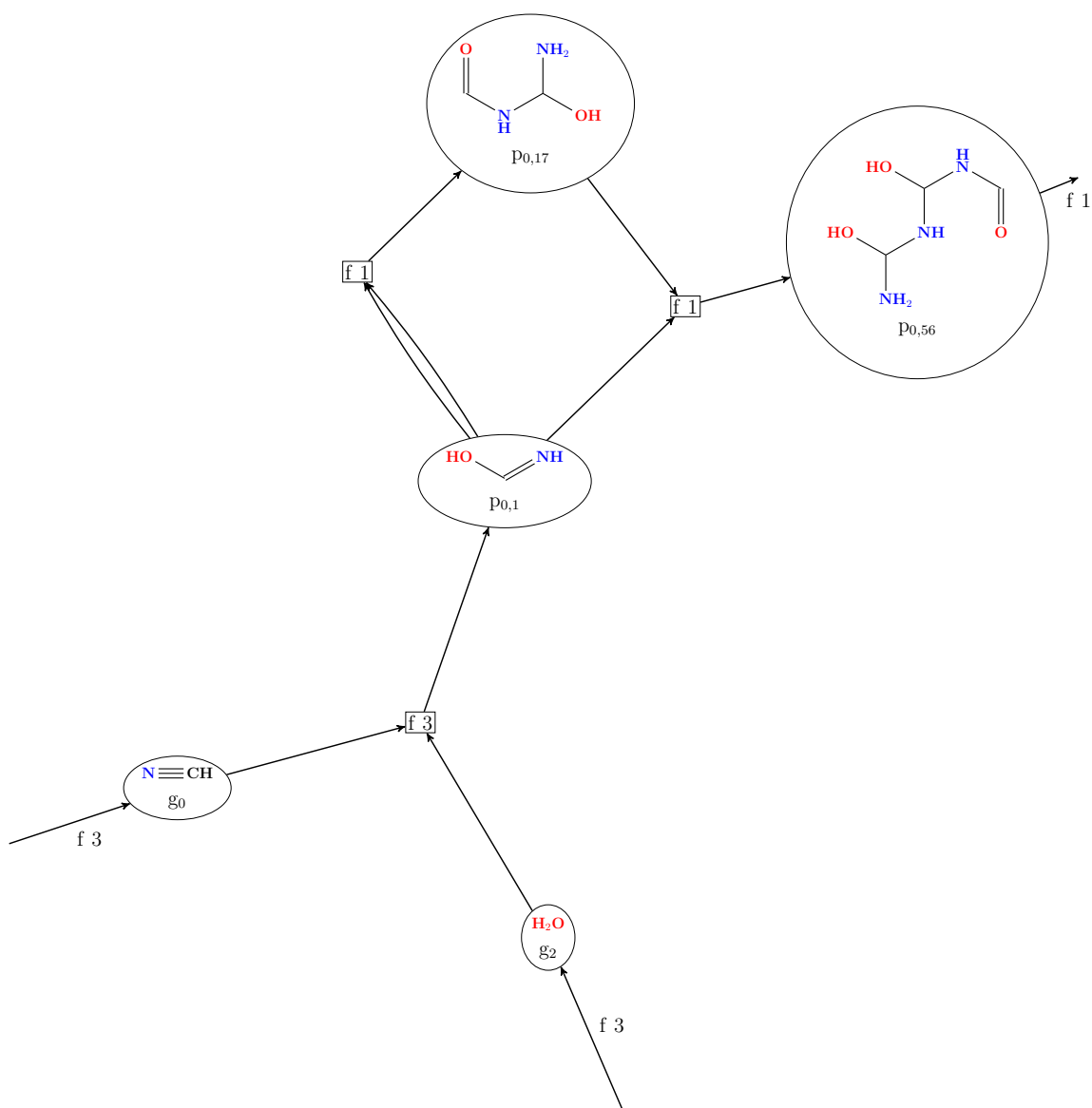|U| = 3

0.3.8 Solution 7

Overall Data

```
Objective value (non-integral): -0.0597395
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507152  -6.000000 0
g_{2}        3  0   -5.068043  -9.000000 20
p_{0,17}     0  0   -21.248844 -6.000000 43
p_{0,1}      0  0   -10.610080 -6.000000 21
p_{0,56}     0  1   -31.869324 -9.000000 67
```

Filtered Graph

File: `out/094_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	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	20
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	21
$p_{0,17}$	0	0	-55788.832737	-6.0	-55808.787447	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	-69.141753	-69.141753
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-60.344023	-60.344023
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-19.821698	-19.821698
Sum					-156.8460199920696

$\Delta G = -28.759096869199908$

$\Delta E = -0.059739494012322224$
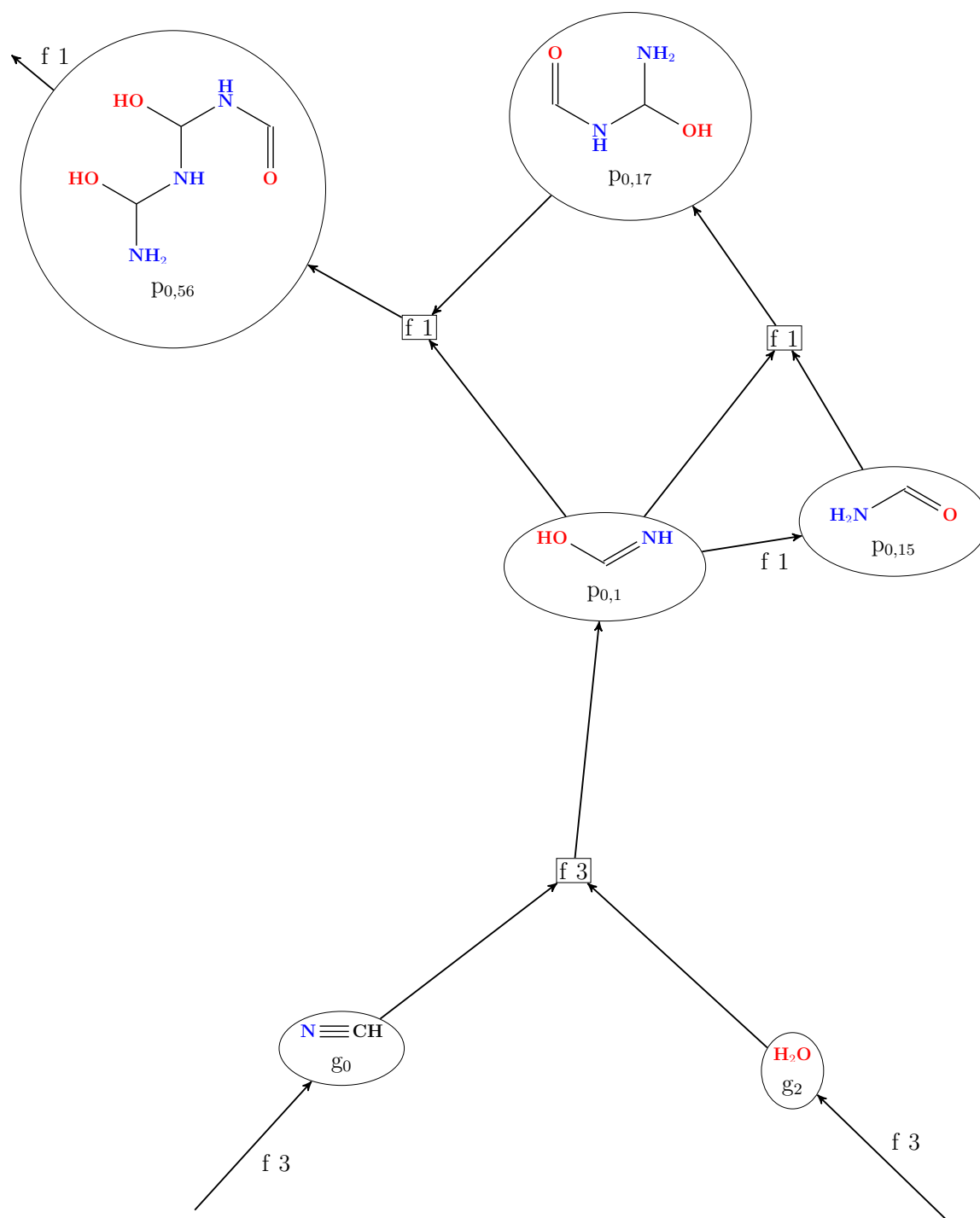
|E| = 5
|U| = 3

0.3.9 Solution 8

Overall Data

```
Objective value (non-integral): -0.0597395
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_{0,15}      0   0   -10.625195 -6.000000 2
p_{0,17}      0   0   -21.248844 -6.000000 4
p_{0,1}       0   0   -10.610080 -6.000000 1
p_{0,56}      0   1   -31.869324 -9.000000 67
```

Filtered Graph

File: `out/103_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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	1
$p_{0,15}$	0	0	-27896.445756	-6.0	-27916.400466	2
$p_{0,17}$	0	0	-55788.832737	-6.0	-55808.787447	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	-61.658737	-61.658737
36	$p_{0,1},$	$p_{0,15},$	1	-39.684415	-39.684415
183	$p_{0,1}, p_{0,15},$	$p_{0,17},$	1	-20.659608	-20.659608
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-19.821698	-19.821698
Sum					-156.8460199920717

ΔG = -26.514192282958568
ΔE = -0.05973949401232301
|E| = 6
|U| = 4
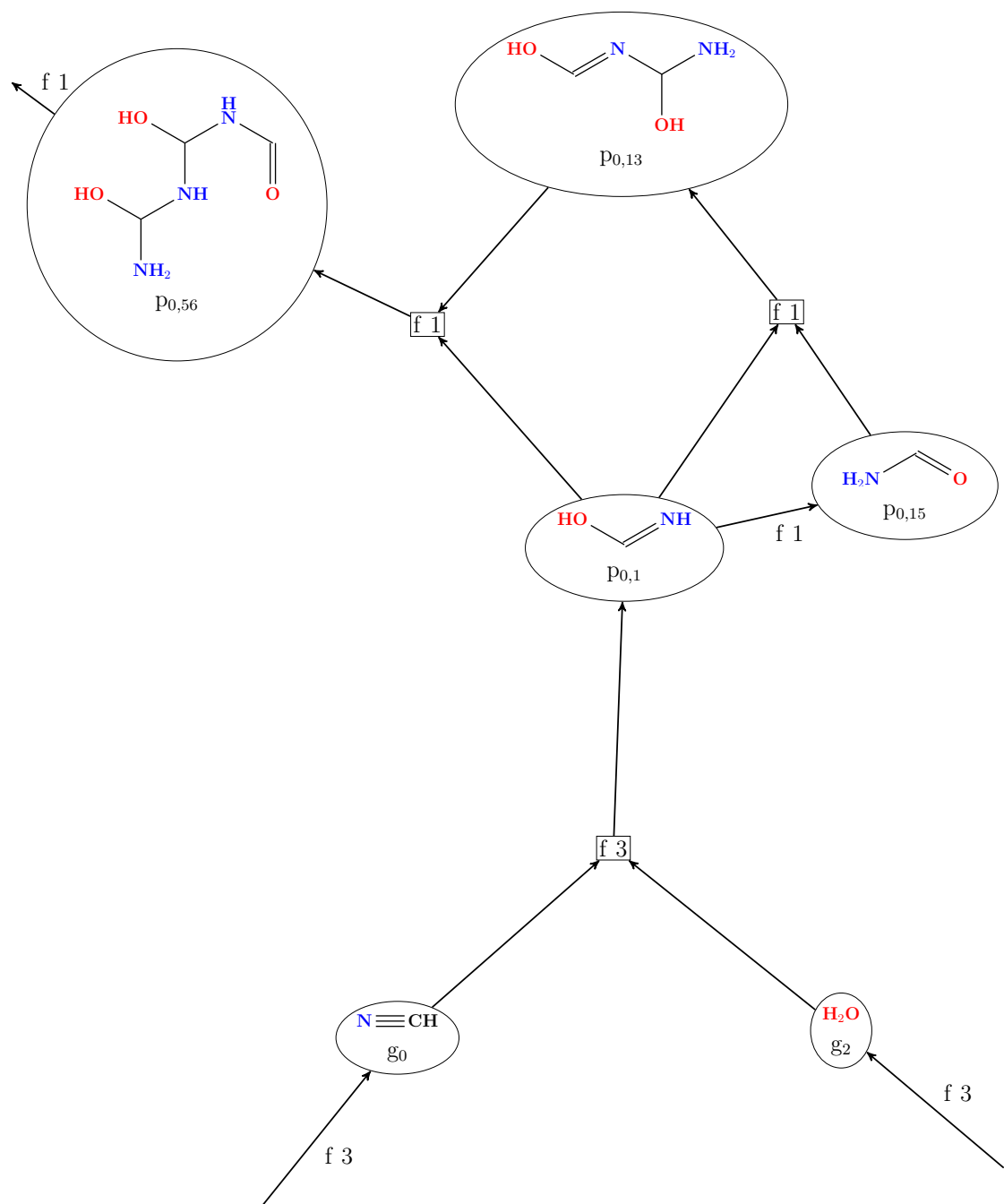
0.3.10 Solution 9

Overall Data

```
Objective value (non-integral): -0.0597395
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 65
p_{0,15}      0  0   -10.625174 -8.688972 63
p_{0,1}       0  0   -10.610101 -6.000000 1
p_{0,56}      0  1   -31.869260 -6.000000 67
```

Filtered Graph

File: out/112_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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	1
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	65
$p_{0,15}$	0	0	-27896.389963	-8.688972	-27925.287618	63
$p_{0,56}$	0	1	-83672.731446	-6.0	-83692.686157	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-61.71445	-61.71445
36	$p_{0,1},$	$p_{0,15},$	1	-46.280117	-46.280117
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	-26.074214	-26.074214
Sum					-156.84601999206757

ΔG = -25.74915608205937

ΔE = -0.05973949401232144

|E| = 6

|U| = 4

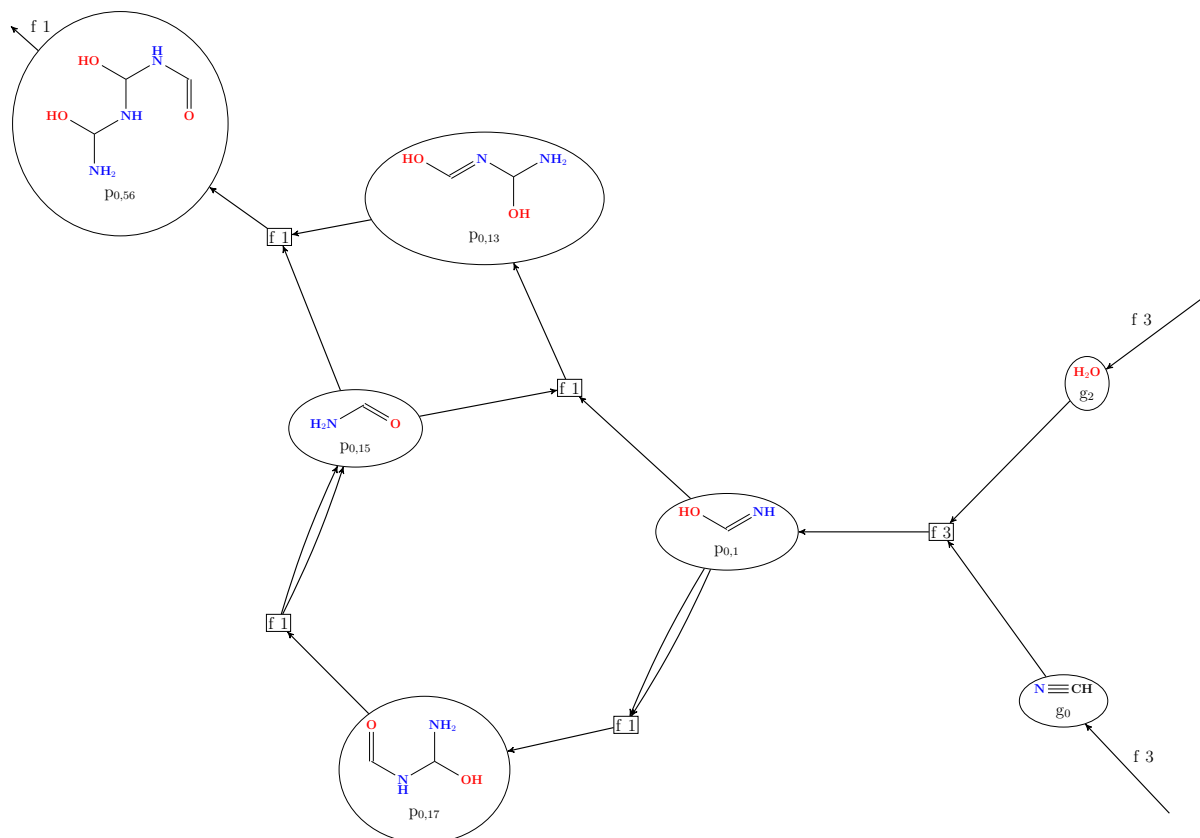## 0.3.11   Solution 10

Overall Data

```
Objective value (non-integral): -0.0597395
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  -6.000000 0
g_{2}        3  0   -5.068043  -6.000000 11
p_{0,13}     0  0   -21.240678 -6.484418 40
p_{0,15}     0  0   -10.625174 -6.173390 26
p_{0,17}     0  0   -21.248887 -6.000000 25
p_{0,1}      0  0   -10.610101 -6.000000 12
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	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	11
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	12
$p_{0,13}$	0	0	-55767.391129	-6.484418	-55788.956909	40
$p_{0,15}$	0	0	-27896.389963	-6.17339	-27916.921332	26
$p_{0,17}$	0	0	-55788.944315	-6.0	-55808.899025	25
$p_{0,56}$	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	-76.680483	-76.680483
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-60.344173	-60.344173
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	0.006113	0.006113
237	$p_{0,17},$	$p_{0,15}, p_{0,15},$	1	-19.666632	-19.666632
Sum					-156.8460199920655

ΔG = -31.004002243091136

ΔE = -0.059739494012320656
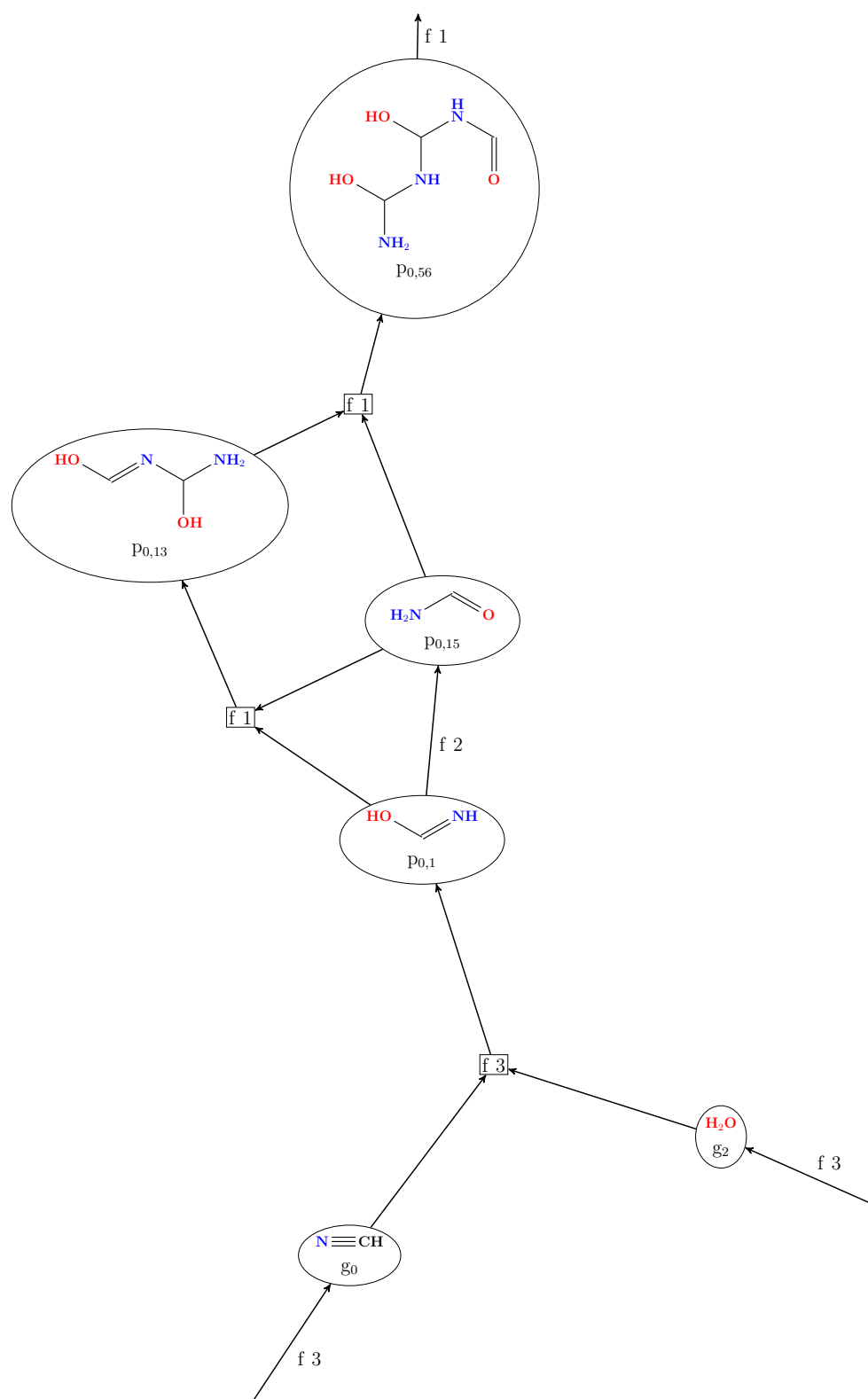
|E| = 7

|U| = 5

0.3.12 Solution 11

Overall Data

```
Objective value (non-integral): -0.0446457
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 20
p_{0,13}      0  0   -21.240678 -6.655358 44
p_{0,15}      0  0   -10.625174 -6.000000 22
p_{0,1}       0  0   -10.610080 -6.000000 21
p_{0,56}      0  1   -31.869324 -9.000000 67
```

Filtered Graph

File: `out/130_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	20
$p_{0,1}$	0	0	-27856.761341	-6.0	-27876.716051	21
$p_{0,13}$	0	0	-55767.391129	-6.655358	-55789.525418	44
$p_{0,15}$	0	0	-27896.389963	-6.0	-27916.344673	22
$p_{0,56}$	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	-61.658737	-61.658737
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
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	-0.908476	-0.908476
Sum					-117.21739788827244

ΔG = -26.51419254550853

ΔE = -0.04464574899408032

|E| = 7

|U| = 4