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}

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

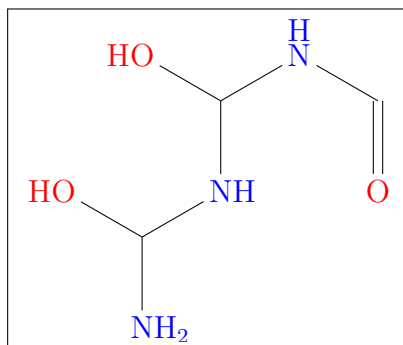File: out/009_g_2_10300000

$$H_2O$$

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): -0.125433
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507141  1.000000  0
g_{2}        3  0   -5.068033  1.000000  0
p_{0,13}     0  0   -21.240635 1.000000  10
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   -10.610080 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
p_{0,5}      0  0   -16.158998 -9.000000 9
```

Filtered Graph
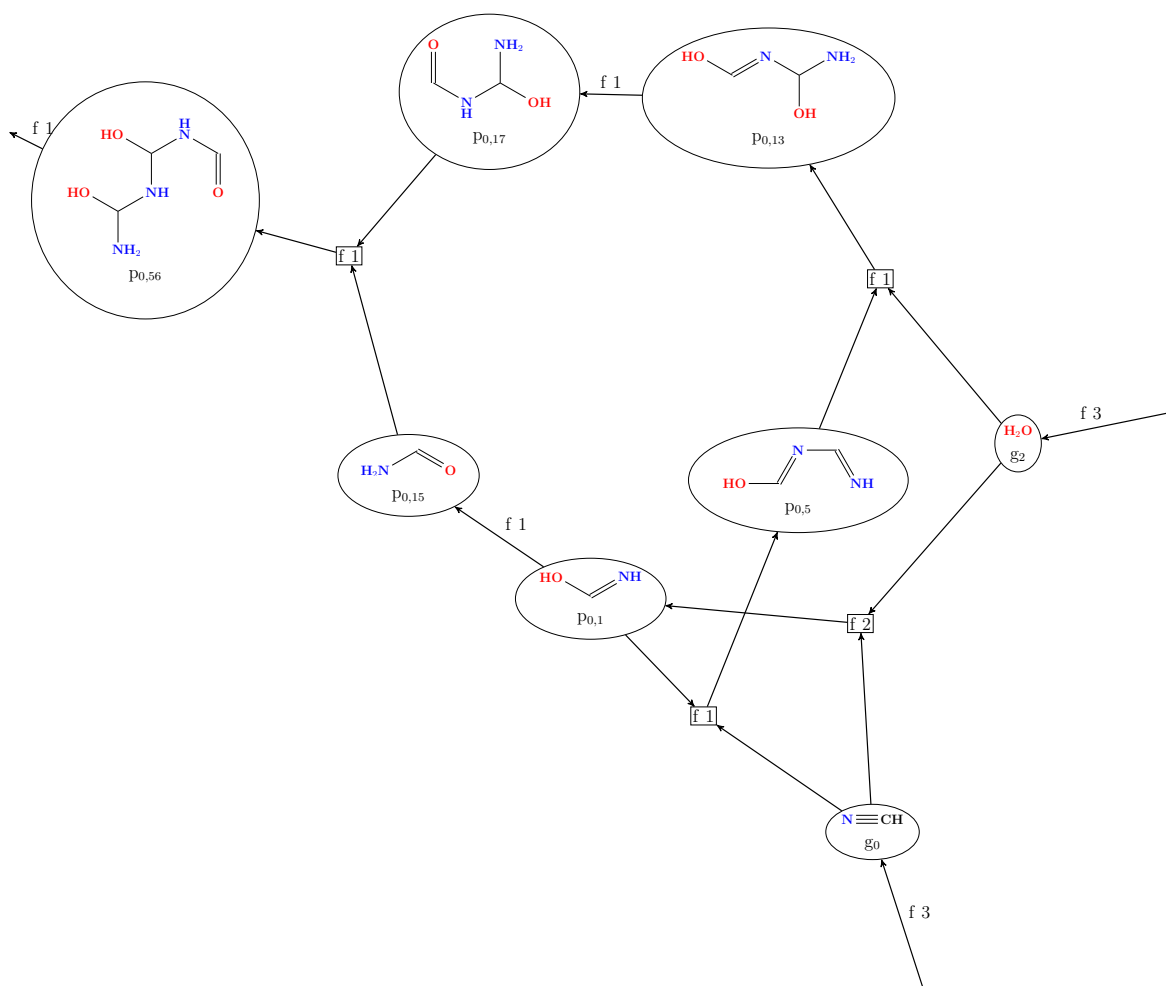
File: out/033_dg_0_11100_f_0_0_filt

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14458.99666	1.0	-14455.670875	0
g_2	3	0	-13306.118349	1.0	-13302.792564	0
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	1
$p_{0,5}$	0	0	-42425.44262	-9.0	-42455.374686	9
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	10
$p_{0,15}$	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	$g_0, g_2,$	$p_{0,1},$	2	-94.747627	-94.747627
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-143.79886	-143.79886
36	$p_{0,1},$	$p_{0,15},$	1	-39.628622	-39.628622
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-7.806974	-7.806974
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	-21.790332	-21.790332
250	$p_{0,13},$	$p_{0,17},$	1	-21.553143	-21.553143
Sum					-329.32555781296026

ΔG = -42.40731802404693
ΔE = -0.1254334804929494
|E| = 7
|U| = 6

0.3.2 Solution 1

Overall Data

```
Objective value (non-integral): -0.125433
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 -5.648103  3
p_{0,1}       0  0   -10.610101 -9.000000  1
p_{0,56}      0  1   -31.869260 1.000000   67
p_{0,5}       0  0   -16.158965 1.000000   2
```

Filtered Graph
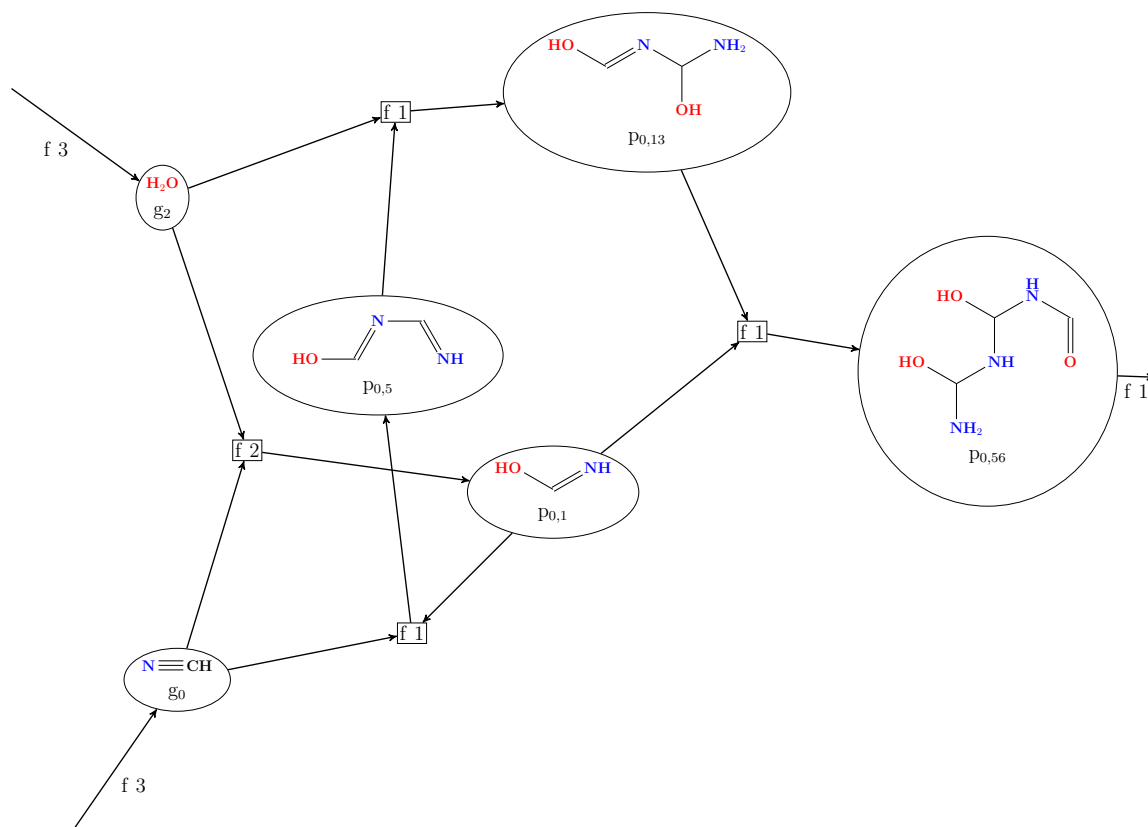
File: `out/042_dg_0_11100_f_0_1_filt`

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	-9.0	-27886.74912	1
$p_{0,5}$	0	0	-42425.357769	1.0	-42422.031984	2
$p_{0,13}$	0	0	-55767.391129	-5.648103	-55786.175505	3
$p_{0,56}$	0	1	-83672.731446	1.0	-83669.405661	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-94.74781	-94.74781
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-81.603486	-81.603486
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-28.594472	-28.594472
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-329.3255578129623

ΔG = -29.968745943597163
ΔE = -0.12543348049295017
|E| = 5
|U| = 4

### 0.3.3 Solution 2

Overall Data

```
Objective value (non-integral): -0.125433
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 -5.951710  64
p_{0,17}    0  0   -21.248887 1.000000   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   2
```

Filtered Graph
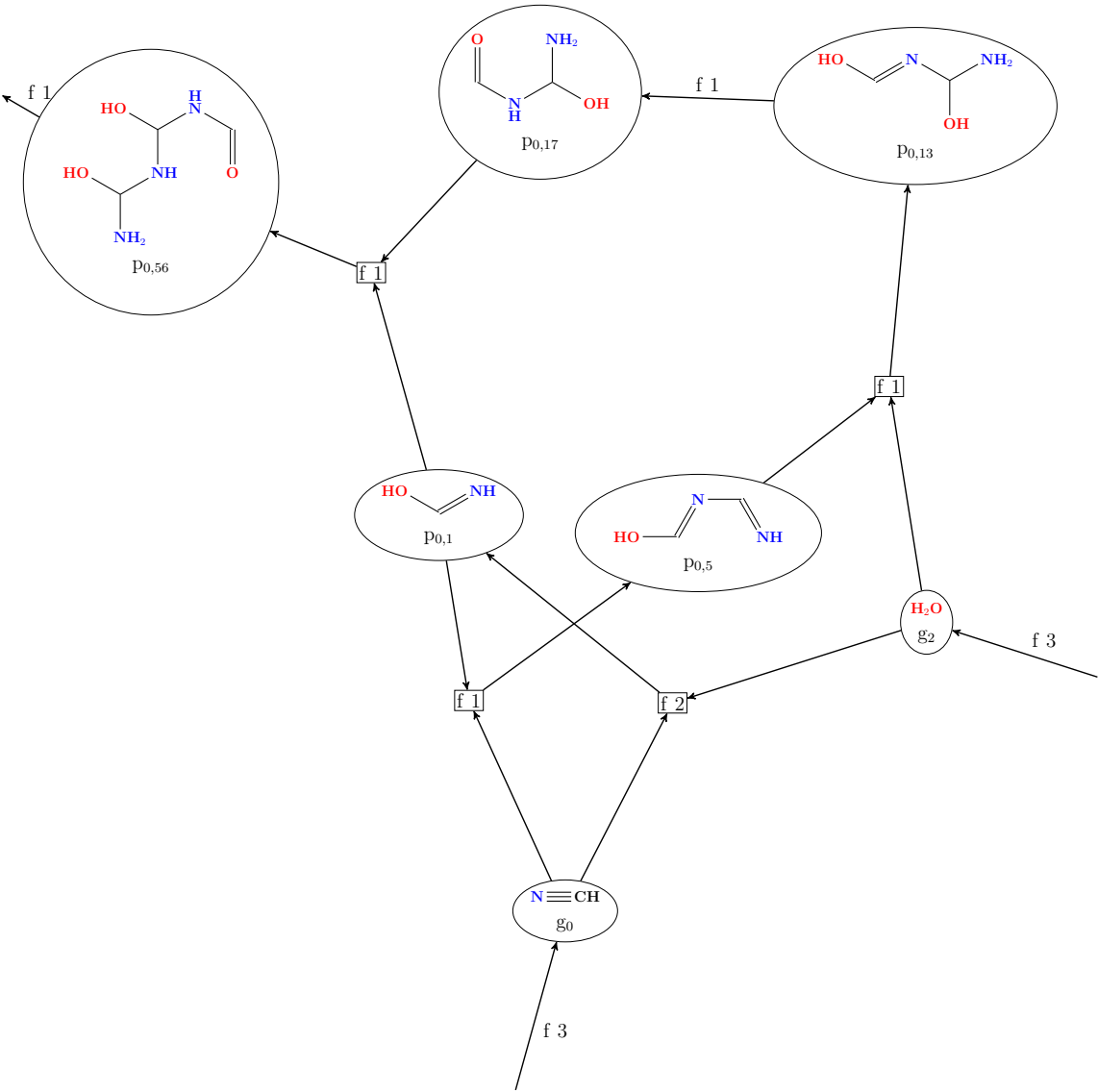
File: `out/051_dg_0_11100_f_0_2_filt`

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	1.0	-42422.116835	2
$p_{0,13}$	0	0	-55767.391129	-5.95171	-55787.185236	64
$p_{0,17}$	0	0	-55788.944315	1.0	-55785.61853	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	-94.74781	-94.74781
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-112.701283	-112.701283
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-60.464141	-60.464141
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-61.251663	-61.251663
250	$p_{0,13},$	$p_{0,17},$	1	0.006113	0.006113
Sum					-329.32555781295895

ΔG = -42.3906587037345
ΔE = -0.1254334804929489
|E| = 6
|U| = 5

0.3.4   Solution 3

Overall Data

```
Objective value (non-integral): -0.125433
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  3
p_{0,15}     0  0   -10.625195 1.000000   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 1.000000   2
```

Filtered Graph

p_{0,56}

p_{0,13}

p_{0,15}

f 1

p_{0,1}

p_{0,5}

f 1

H_2O
g_2

f 1

f 2

f 3

N≡CH
g_0

f 3
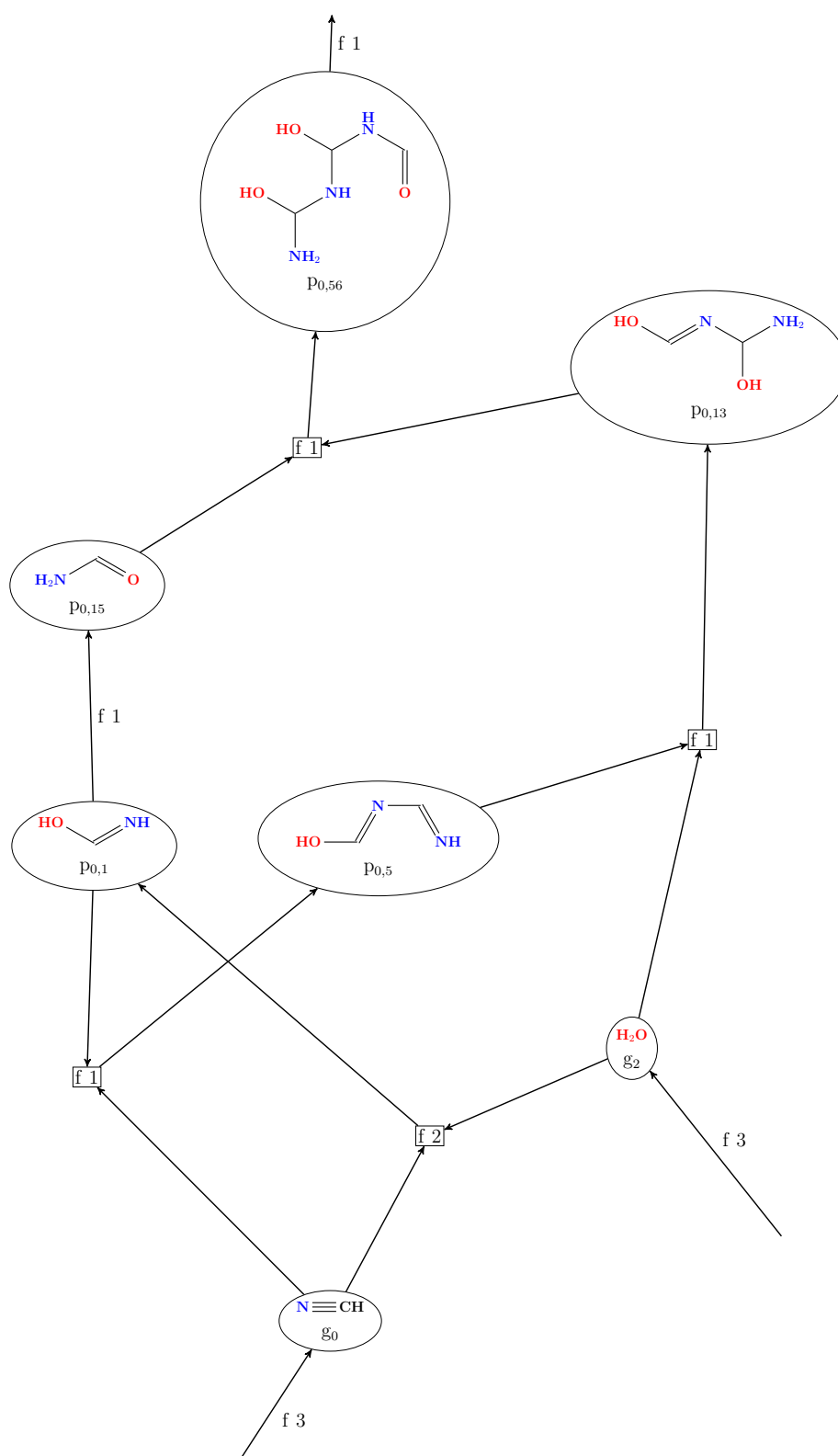
File: `out/060_dg_0_11100_f_0_3_filt`

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	-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	2
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	3
$p_{0,15}$	0	0	-27896.445756	1.0	-27893.119971	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	-63.734865	-63.734865
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-112.701283	-112.701283
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-38.904842	-38.904842
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-12.163202	-12.163202
Sum					-329.3255578129543

$\Delta G = -33.086774612645634$

$\Delta E = -0.1254334804929471$

$|E| = 6$

$|U| = 5$

0.3.5 Solution 4

Overall Data

```
Objective value (non-integral): -0.089346
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   -10.625195 1.000000   2
p_{0,17}      0  0   -21.248887 1.000000   3
p_{0,1}       0  0   -10.610101 1.000000   1
p_{0,56}      0  1   -31.869324 -9.000000  67
```

Filtered Graph

HO

H
N

HO
NH

O

NH₂

p₀,₅₆

O
NH₂

N
H
OH

p₀,₁₇

f 1

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/069_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	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	-27896.445756	1.0	-27893.119971	2
$p_{0,17}$	0	0	-55788.944315	1.0	-55785.61853	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-78.411501	-78.411501
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	-21.622961	-21.622961
Sum					-234.57793100918383

ΔG = -42.390658441184534
ΔE = -0.08934601531906657
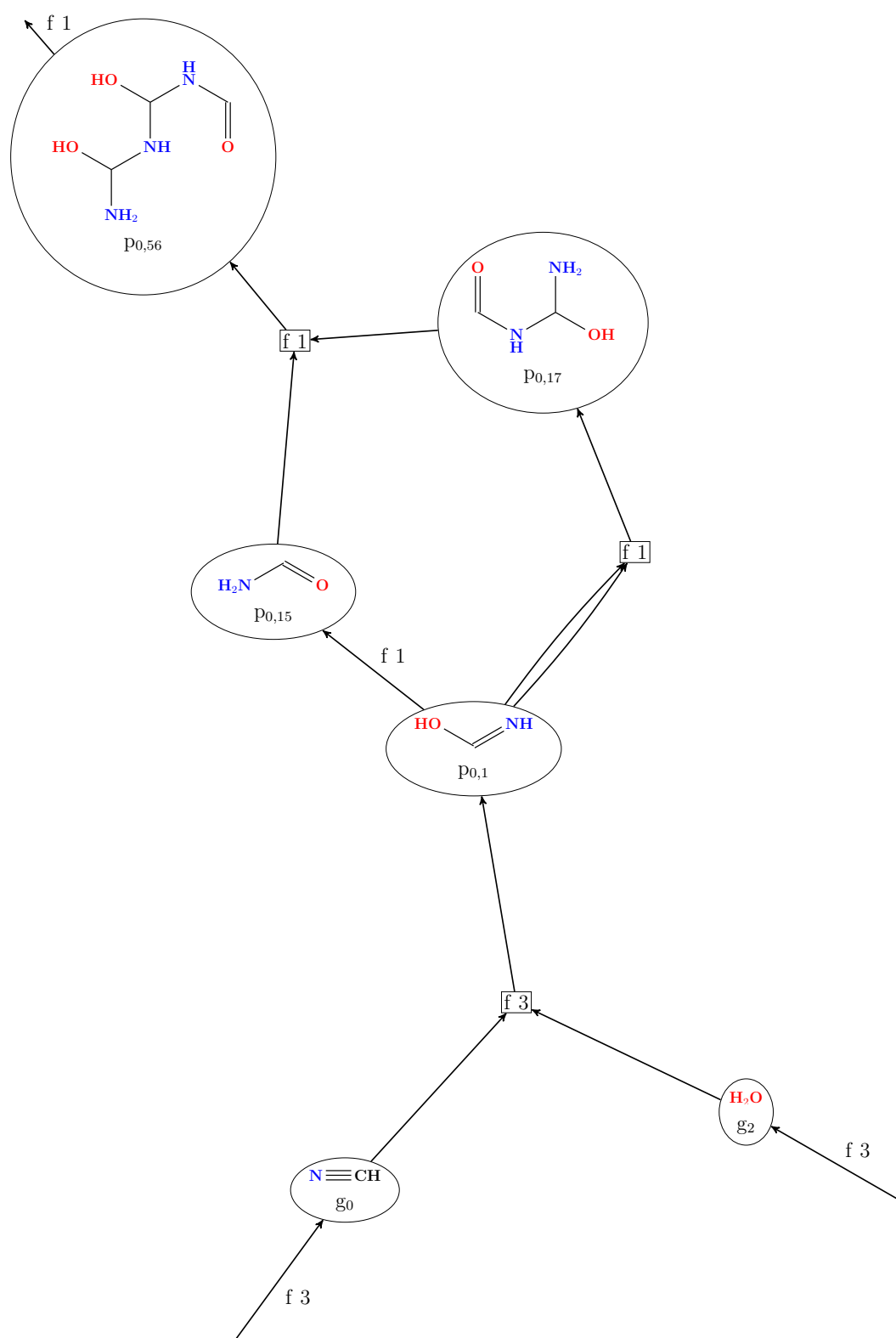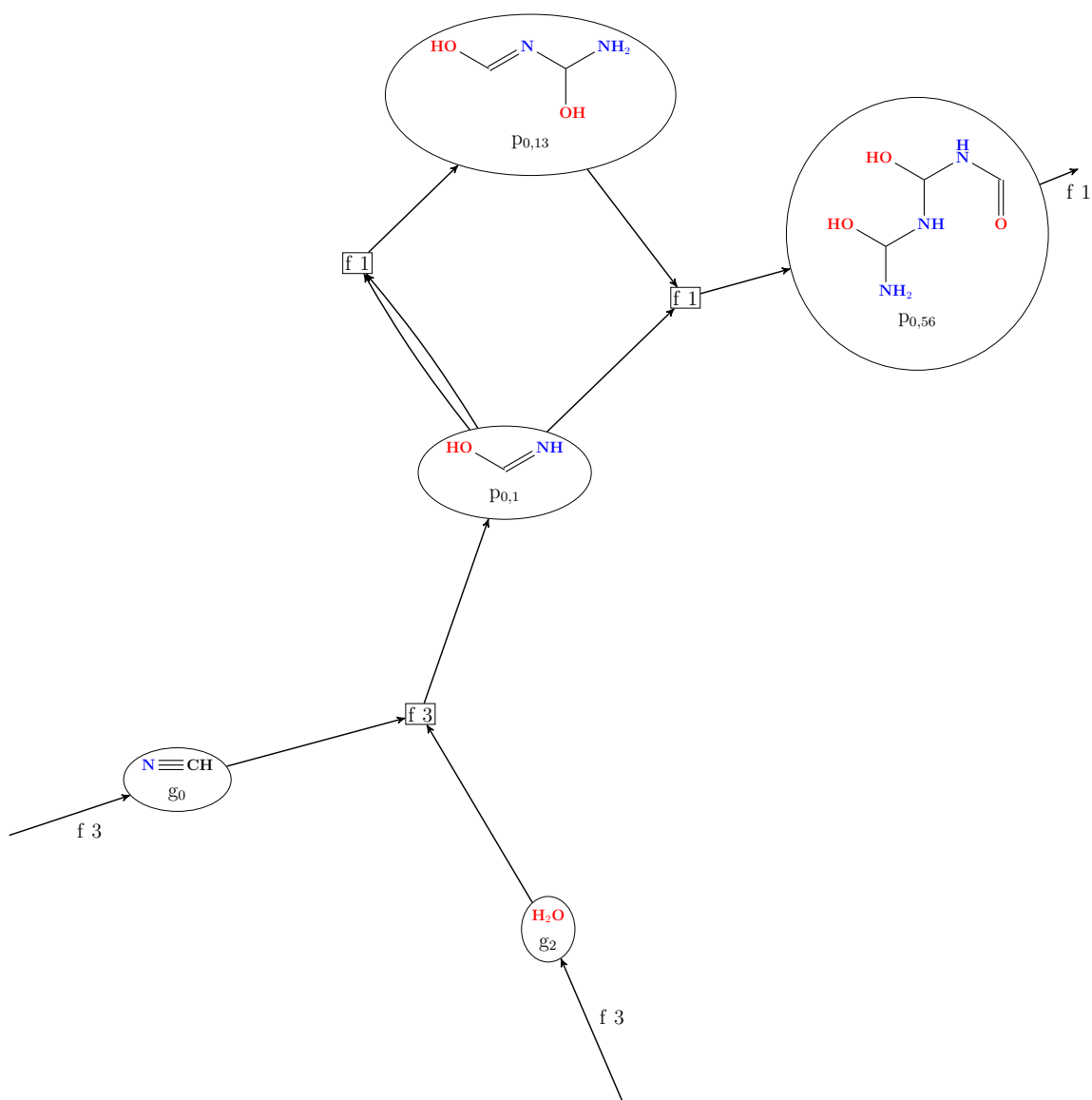|E| = 6
|U| = 4

0.3.6   Solution 5

Overall Data

```
Objective value (non-integral): -0.089346
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   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/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	-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	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	-63.679151	-63.679151
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.858207	-56.858207
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-82.972097	-82.972097
Sum					-234.57793100918255

ΔG = -33.086774875195594

ΔE = -0.08934601531906608
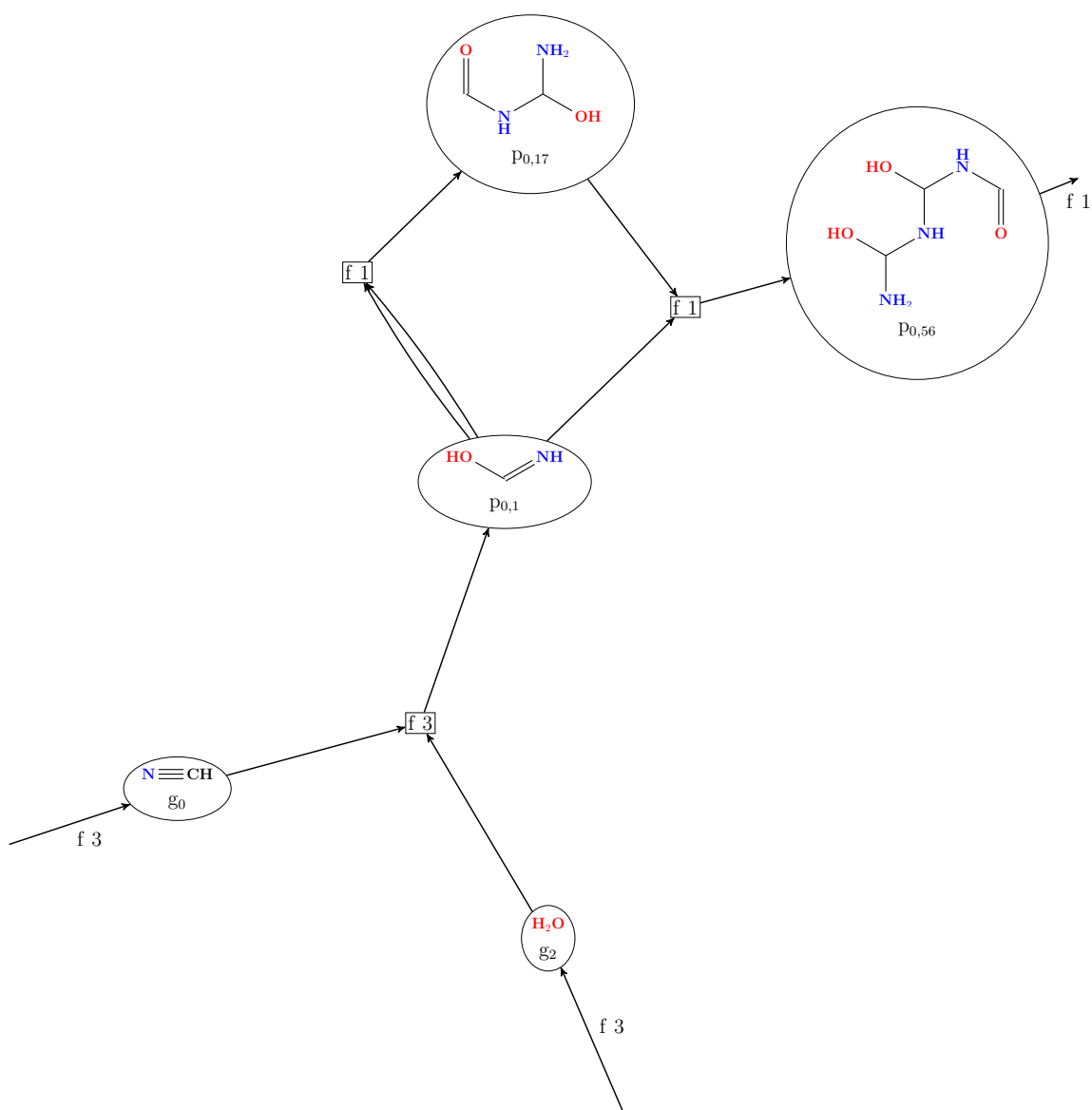
|E| = 5
|U| = 3

0.3.7 Solution 6

Overall Data

```
Objective value (non-integral): -0.089346
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_{0,17}     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/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	-9.0	-13336.077027	0
$p_{0,1}$	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	-63.679151	-63.679151
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-78.41135	-78.41135
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-61.418954	-61.418954
Sum					-234.57793100918255

ΔG = -33.086774875195594

ΔE = -0.08934601531906608
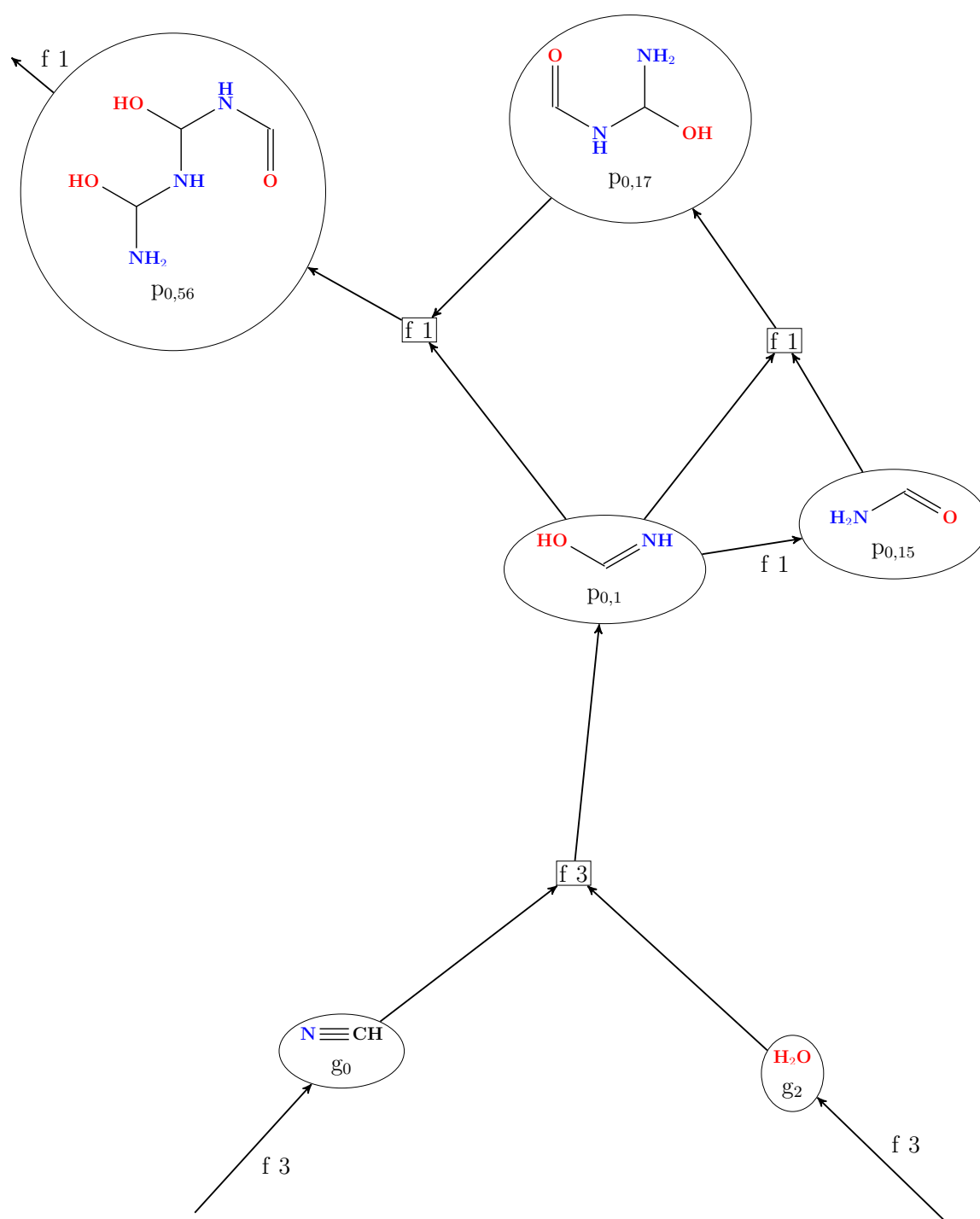
$|E| = 5$

$|U| = 3$

0.3.8 Solution 7

Overall Data

```
Objective value (non-integral): -0.089346
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 -9.000000 23
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/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	-9.0	-13336.077027	20
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	21
$p_{0,15}$	0	0	-27896.445756	-9.0	-27926.377821	23
$p_{0,17}$	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	-63.679151	-63.679151
36	$p_{0,1},$	$p_{0,15},$	1	-70.697361	-70.697361
183	$p_{0,1}, p_{0,15},$	$p_{0,17},$	1	-7.71399	-7.71399
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-61.418954	-61.418954
Sum					-234.57793100918383

ΔG = -33.086774875195594
ΔE = -0.08934601531906657
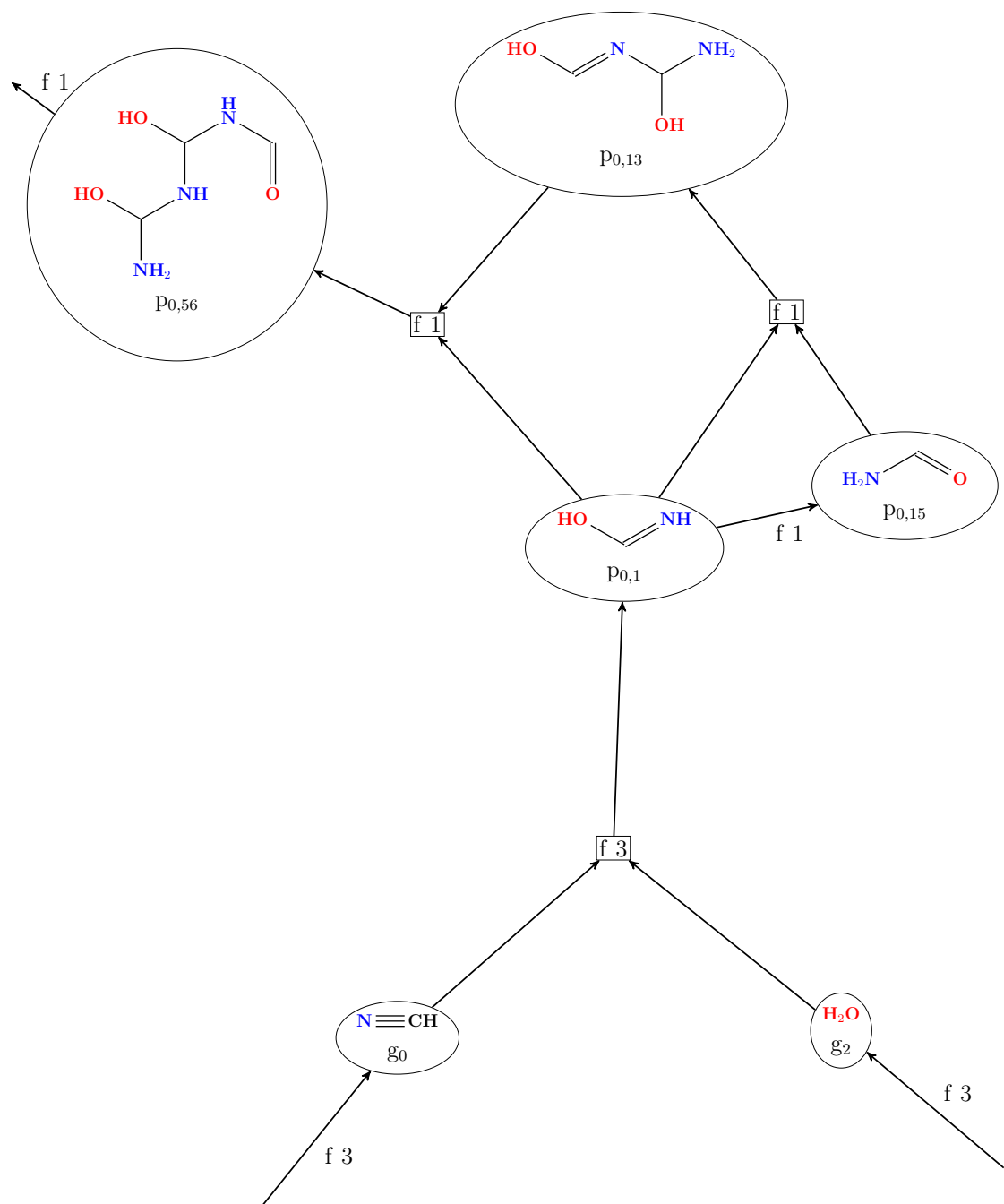|E| = 6
|U| = 4

0.3.9 Solution 8

Overall Data

```
Objective value (non-integral): -0.089346
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   45
p_{0,15}      0   0  -10.625174 -4.557582  22
p_{0,1}       0   0  -10.610080 1.000000   21
p_{0,56}      0   1  -31.869324 -9.000000  67
```

Filtered Graph

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	-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	45
$p_{0,15}$	0	0	-27896.389963	-4.557582	-27911.5475	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	-63.679151	-63.679151
36	$p_{0,1},$	$p_{0,15},$	1	-56.86432	-56.86432
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	-82.972097	-82.972097
Sum					-234.57793100918127

ΔG = -33.086774875195594
ΔE = -0.0893460153190656
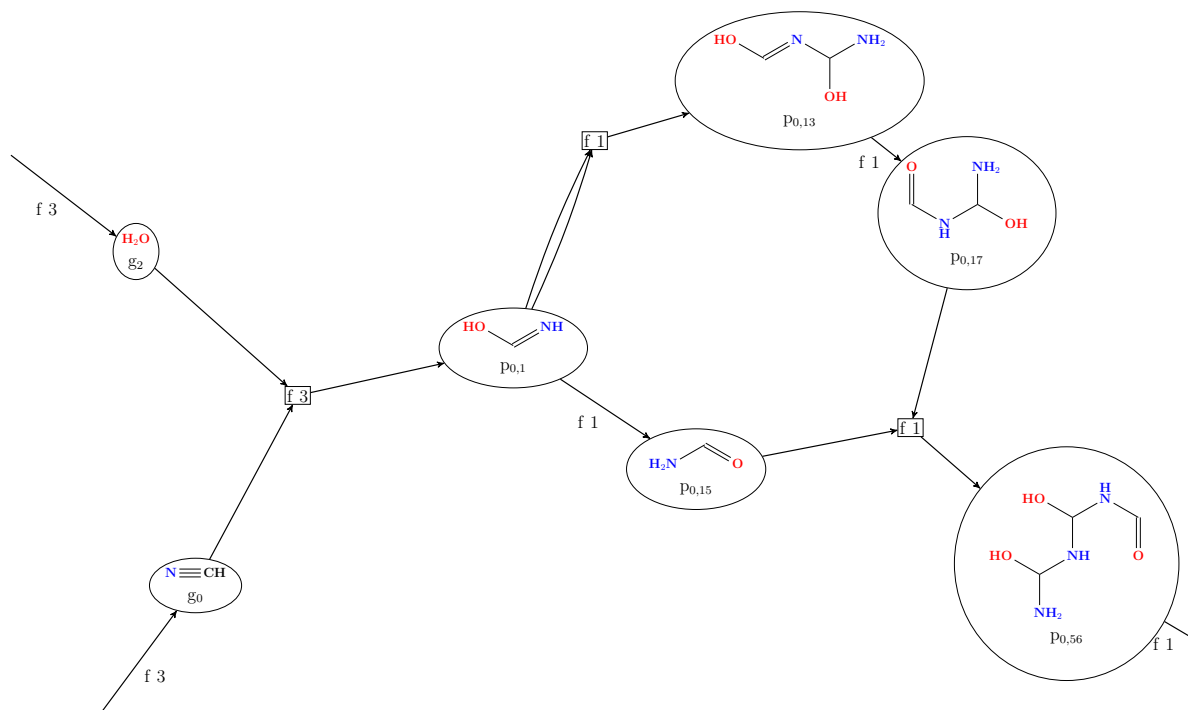|E| = 6
|U| = 4

0.3.10 Solution 9

Overall Data

```
Objective value (non-integral): -0.089346
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   44
p_{0,15}     0  0   -10.625174 1.000000   21
p_{0,17}     0  0   -21.248844 -6.026205  45
p_{0,1}      0  0   -10.610101 1.000000   20
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	20
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	44
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	21
$p_{0,17}$	0	0	-55788.832737	-6.026205	-55808.8746	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	-63.734865	-63.734865
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.74678	-56.74678
36	$p_{0,1},$	$p_{0,15},$	1	-39.572909	-39.572909
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	0.0	0.0
250	$p_{0,13},$	$p_{0,17},$	1	-43.343475	-43.343475
Sum					-234.57793100918045

ΔG = -33.086774612645634
ΔE = -0.08934601531906528
|E| = 7
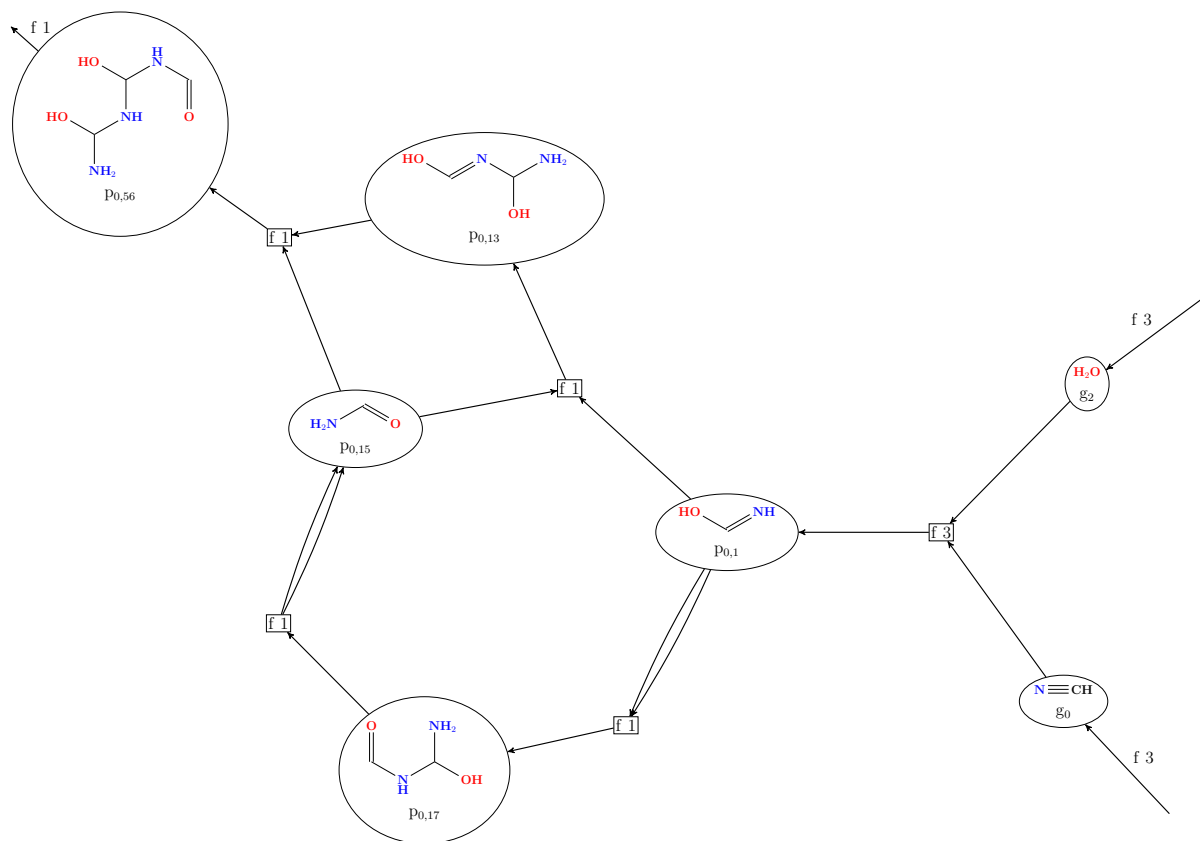|U| = 5

0.3.11 Solution 10

Overall Data

```
Objective value (non-integral): -0.089346
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 -8.061311  34
p_{0,15}     0  0   -10.625174 -3.880626  32
p_{0,17}     0  0   -21.248887 -9.000000  31
p_{0,1}      0  0   -10.610101 -8.756266  1
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	0
$p_{0,1}$	0	0	-27856.817054	-8.756266	-27885.938515	1
$p_{0,13}$	0	0	-55767.391129	-8.061311	-55794.201317	34
$p_{0,15}$	0	0	-27896.389963	-3.880626	-27909.29609	32
$p_{0,17}$	0	0	-55788.944315	-9.0	-55818.87638	31
$p_{0,56}$	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	-93.991921	-93.991921
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-48.910334	-48.910334
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	0.006113	0.006113
Sum					-234.57793100918

ΔG = -33.086775137745555
ΔE = -0.08934601531906511
|E| = 7
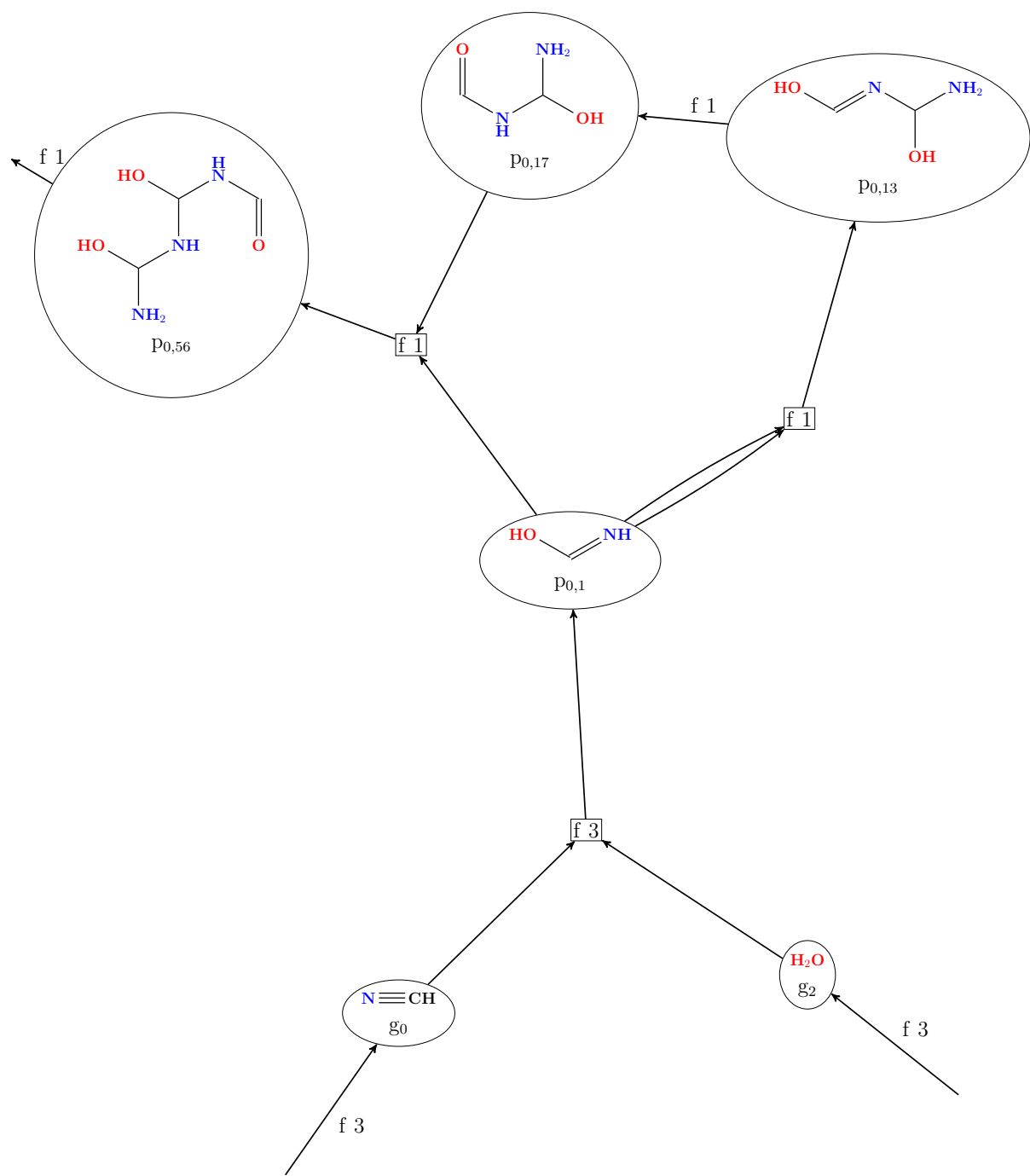|U| = 5

0.3.12 Solution 11

Overall Data

```
Objective value (non-integral): -0.089346
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  44
p_{0,17}     0  0   -21.248844 -9.000000 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/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	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	44
$p_{0,17}$	0	0	-55788.832737	-9.0	-55818.764803	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	-94.692097	-94.692097
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.858207	-56.858207
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-30.406009	-30.406009
250	$p_{0,13},$	$p_{0,17},$	1	-52.566088	-52.566088
Sum					-234.57793100917917

ΔG = -42.390658441184534
ΔE = -0.08934601531906479
|E| = 6
|U| = 4
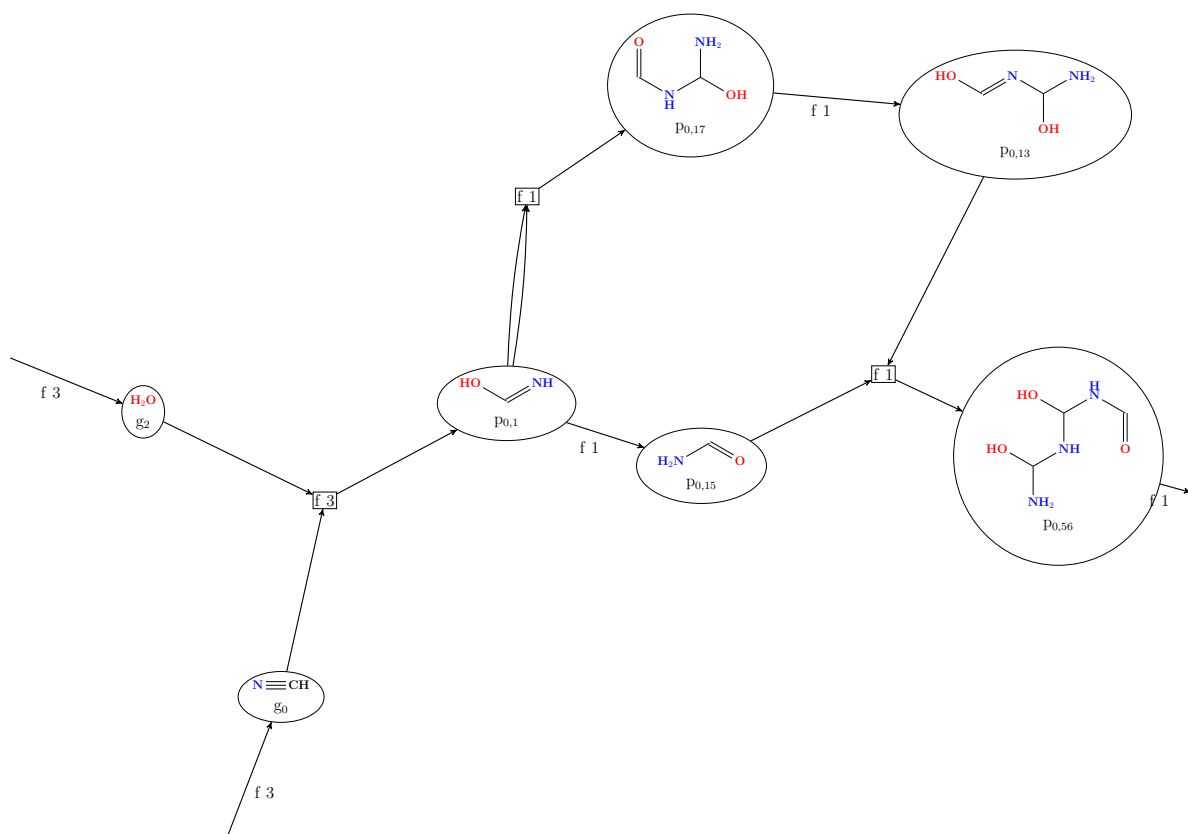
0.3.13   Solution 12

Overall Data

```
Objective value (non-integral): -0.089346
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 -5.911790  11
p_{0,15}     0  0   -10.625174 -6.030147  54
p_{0,17}     0  0   -21.248844 1.000000   10
p_{0,1}      0  0   -10.610101 1.000000   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	1.0	-13302.819176	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,13}$	0	0	-55767.391129	-5.91179	-55787.05247	11
$p_{0,15}$	0	0	-27896.389963	-6.030147	-27916.444937	54
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	10
$p_{0,56}$	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	1	-61.375467	-61.375467
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-78.299923	-78.299923
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
253	$p_{0,17},$	$p_{0,13},$	1	0.006113	0.006113
Sum					-234.5779310091779

ΔG = -42.390658441184534
ΔE = -0.0893460153190643
|E| = 7
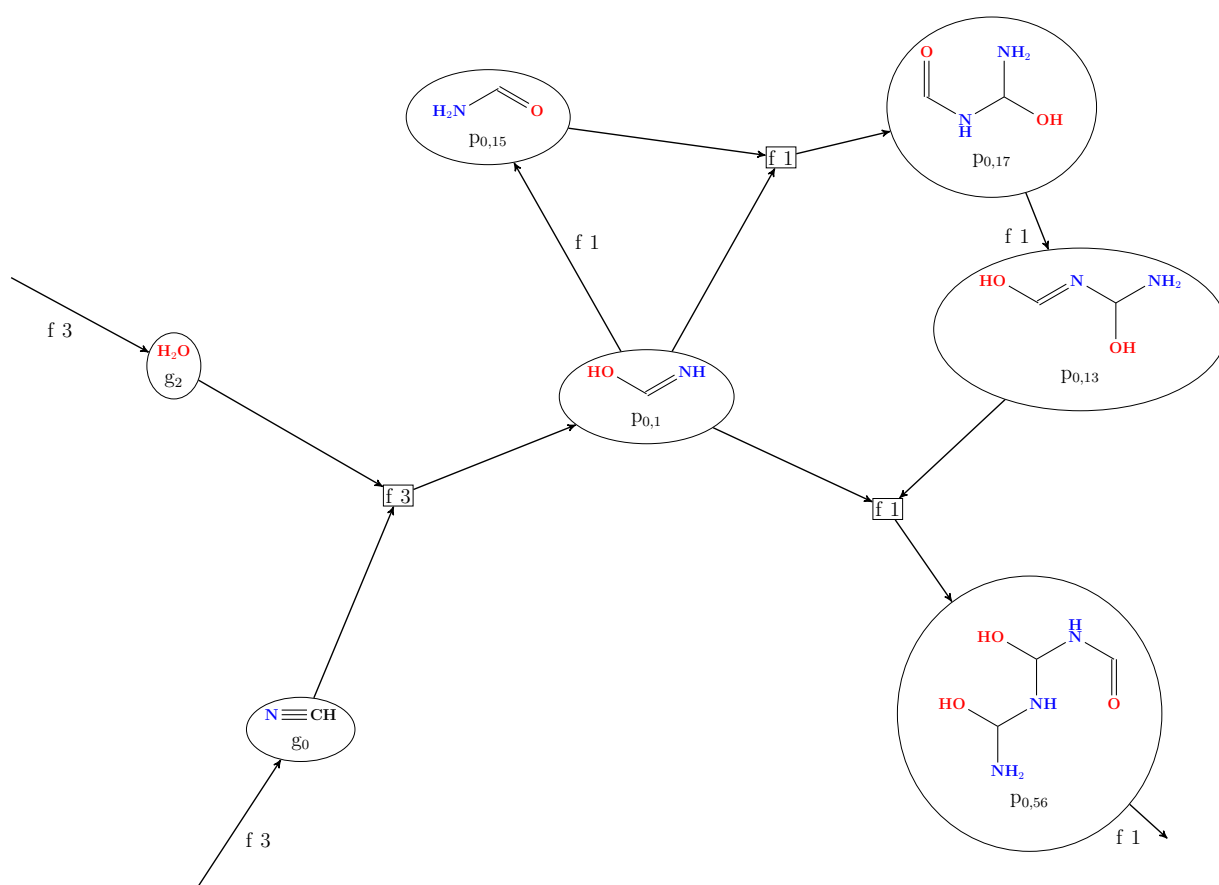|U| = 5

0.3.14 Solution 13

Overall Data

```
Objective value (non-integral): -0.089346
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 -1.471351 2
p_{0,17}   0  0   -21.248844 1.000000  4
p_{0,1}    0  0   -10.610101 -9.000000 1
p_{0,56}   0  1   -31.869324 -2.297937 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	-27856.817054	-9.0	-27886.74912	1
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	65
$p_{0,15}$	0	0	-27896.445756	-1.471351	-27901.339155	2
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	4
$p_{0,56}$	0	1	-83672.898792	-2.297937	-83680.541237	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-125.760756	-125.760756
36	$p_{0,1},$	$p_{0,15},$	1	-16.280145	-16.280145
183	$p_{0,1}, p_{0,15},$	$p_{0,17},$	1	0.006113	0.006113
253	$p_{0,17},$	$p_{0,13},$	1	-9.571337	-9.571337
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-234.5779310091872

ΔG = -40.31215198344427

ΔE = -0.08934601531906786

$|E| = 7$

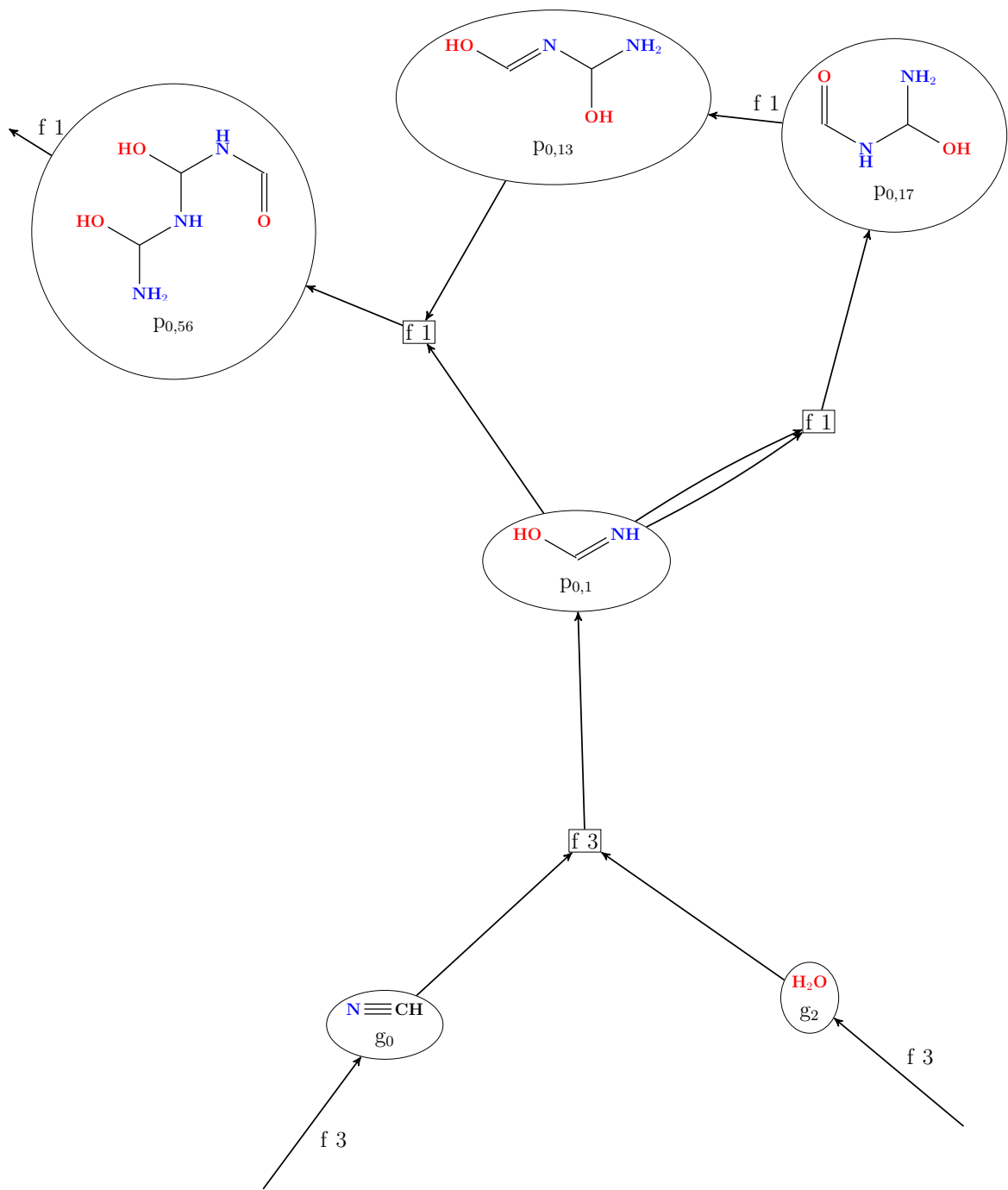$|U| = 5$

0.3.15 Solution 14

Overall Data

```
Objective value (non-integral): -0.089346
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  65
p_{0,17}     0  0   -21.248844 1.000000   64
p_{0,1}      0  0   -10.610080 1.000000   1
p_{0,56}     0  1   -31.869324 -9.000000  67
```

Filtered Graph

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	1.0	-14455.699793	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	-55767.391129	-9.0	-55797.323194	65
$p_{0,17}$	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	-63.679151	-63.679151
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-78.41135	-78.41135
253	$p_{0,17},$	$p_{0,13},$	1	-9.571337	-9.571337
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-51.847617	-51.847617
Sum					-234.57793100918593

ΔG = -33.086774612645634
ΔE = -0.08934601531906737
|E| = 6
|U| = 4

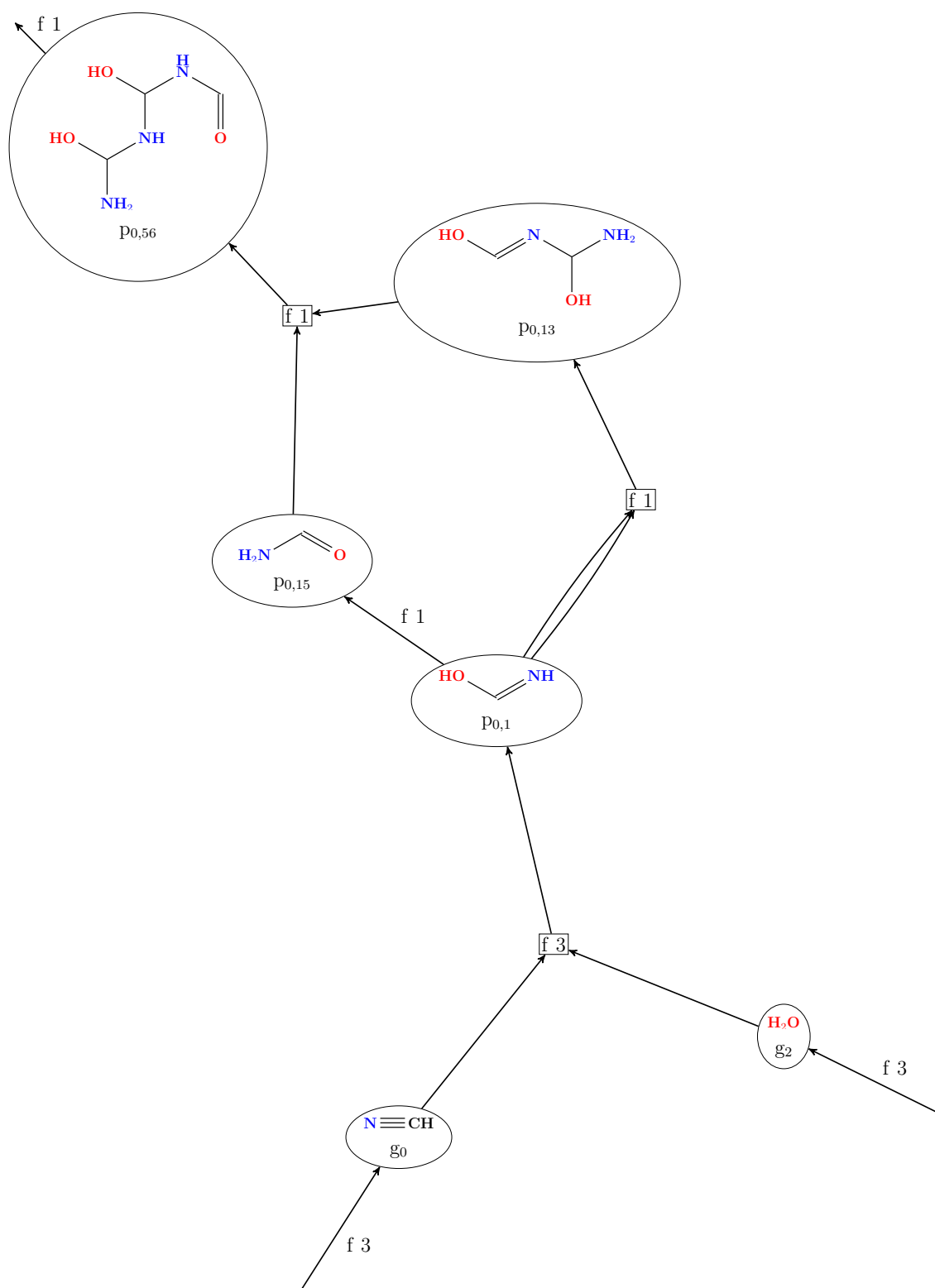## 0.3.16 Solution 15

Overall Data

```
Objective value (non-integral): -0.089346
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   -21.240678 -9.000000  44
p_{0,15}     0  0   -10.625195 1.000000   22
p_{0,1}      0  0   -10.610101 1.000000   21
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	20
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	21
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	44
$p_{0,15}$	0	0	-27896.445756	1.0	-27893.119971	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	-63.734865	-63.734865
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-87.87126	-87.87126
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-12.163202	-12.163202
Sum					-234.5779310091745

ΔG = -33.086774612645634
ΔE = -0.08934601531906301
|E| = 6
|U| = 4

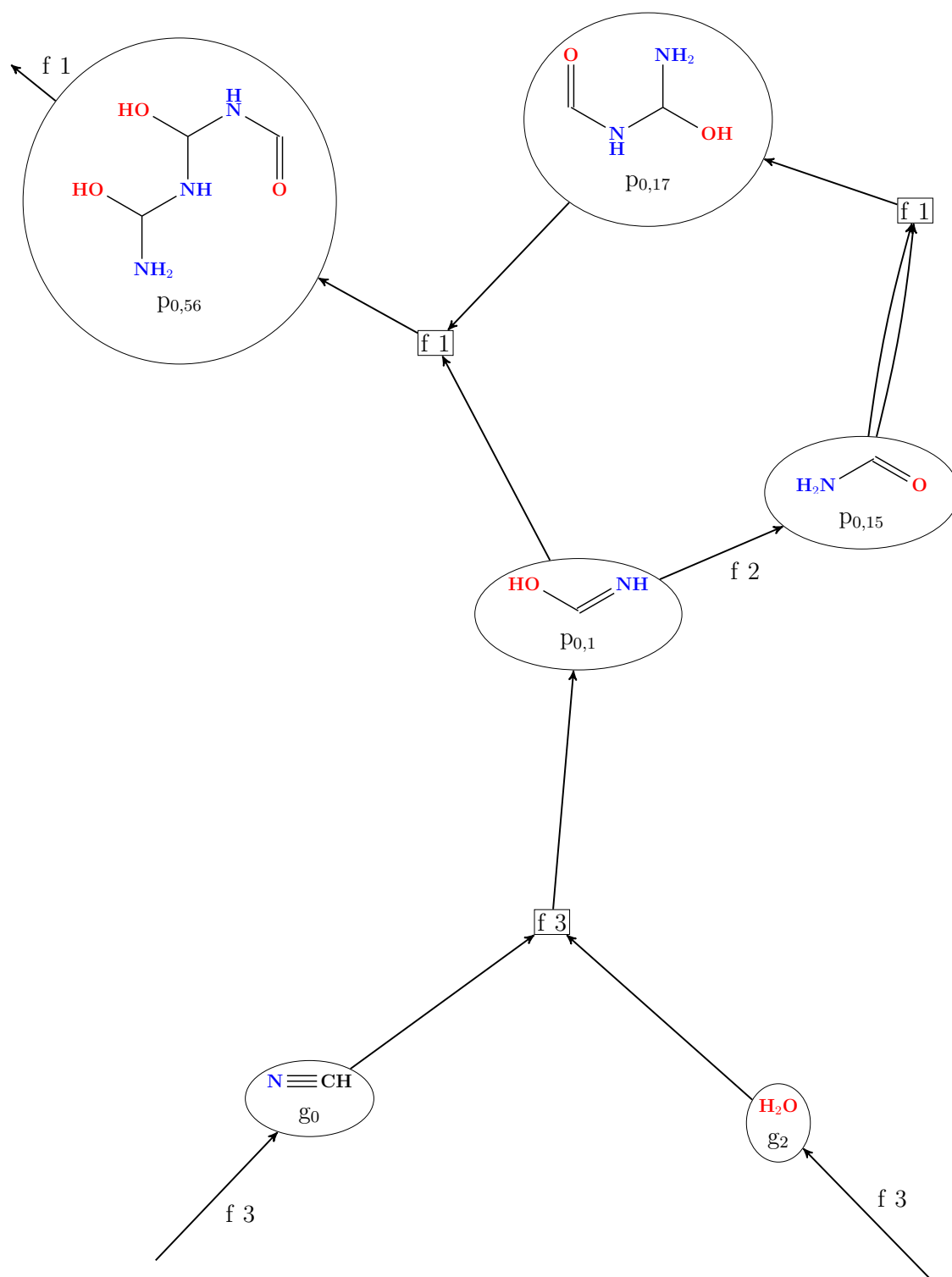### 0.3.17 Solution 16

Overall Data

```
Objective value (non-integral): -0.0742523
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  22
p_{0,17}      0  0   -21.248844 0.727245  45
p_{0,1}       0  0   -10.610080 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	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
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	22
$p_{0,17}$	0	0	-55788.832737	0.727245	-55786.414077	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	-94.692097	-94.692097
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
180	$p_{0,15}, p_{0,15},$	$p_{0,17},$	1	0.0	0.0
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-60.57306	-60.57306
Sum					-194.94930890539212

ΔG = -42.3906587037345
ΔE = -0.07425227030082673
|E| = 7
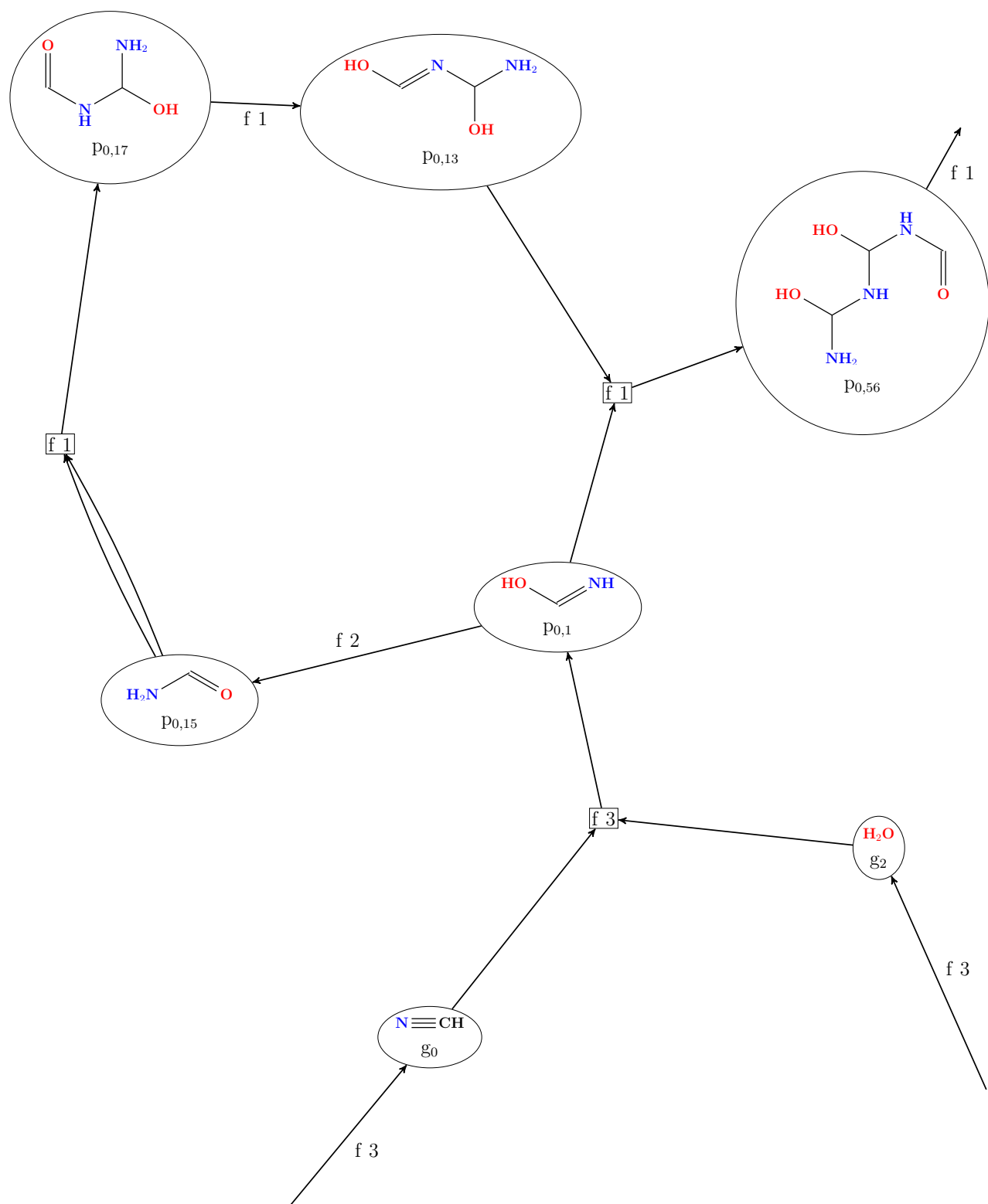|U| = 4

0.3.18   Solution 17

Overall Data

```
Objective value (non-integral): -0.0742523
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 -6.182574 46
p_{0,15}      0  0   -10.625174 1.000000  22
p_{0,17}      0  0   -21.248887 0.765194  45
p_{0,1}       0  0   -10.610101 1.000000  1
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	1.0	-13302.819176	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,13}$	0	0	-55767.391129	-6.182574	-55787.95304	46
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	22
$p_{0,17}$	0	0	-55788.944315	0.765194	-55786.399445	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	2	-39.572909	-39.572909
180	$p_{0,15}, p_{0,15},$	$p_{0,17},$	1	0.006113	0.006113
253	$p_{0,17},$	$p_{0,13},$	1	0.006113	0.006113
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-60.529572	-60.529572
Sum					-194.94930890539212

$\Delta G = -42.390658178634574$

$\Delta E = -0.07425227030082673$

$|E| = 8$

$|U| = 5$

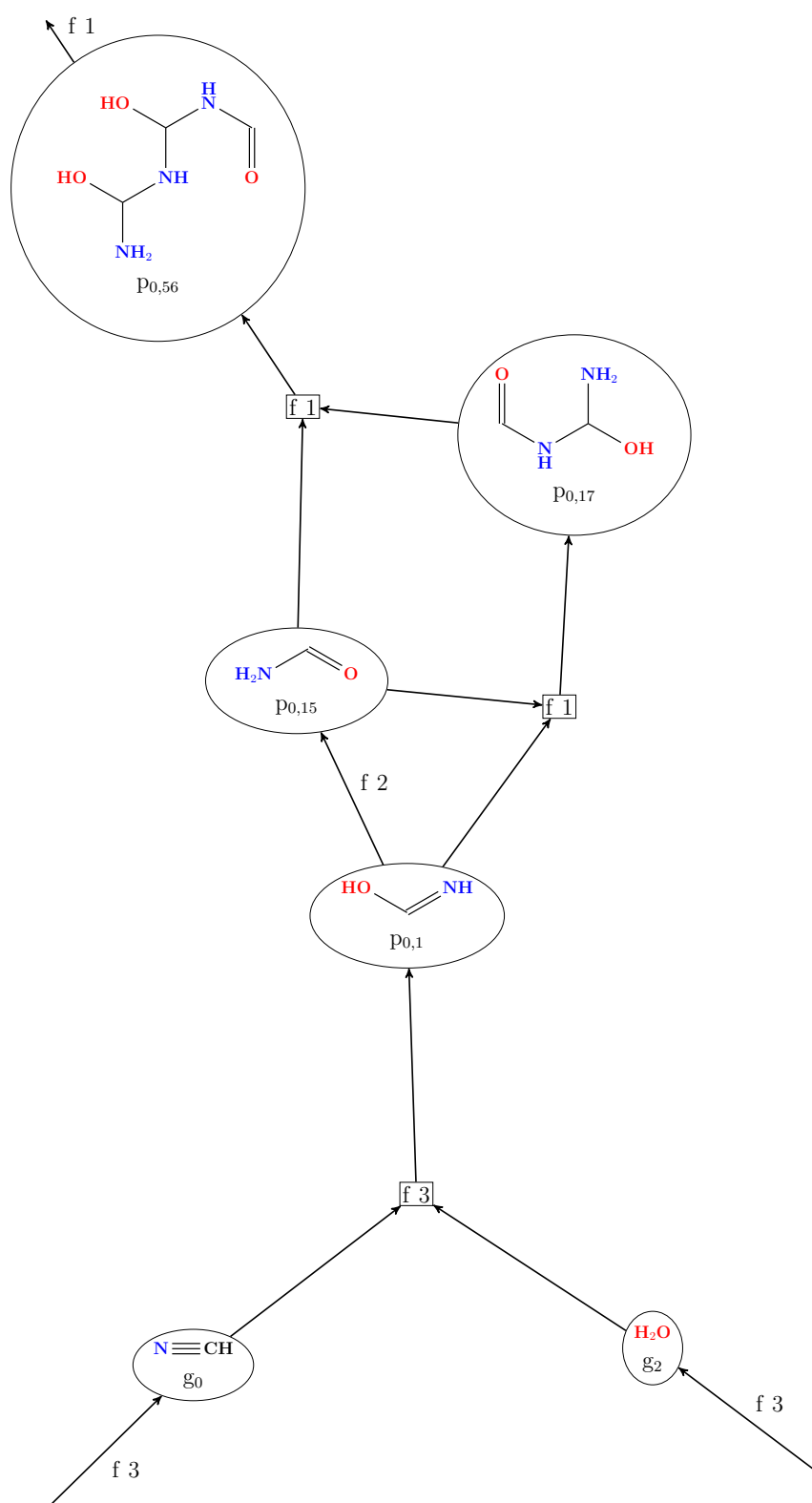## 0.3.19 Solution 18

Overall Data

```
Objective value (non-integral): -0.0742523
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 1.000000   22
p_{0,17}     0  0   -21.248887 -5.974208  44
p_{0,1}      0  0   -10.610101 1.000000   21
p_{0,56}     0  1   -31.869324 -9.000000  67
```

Filtered Graph

f 1

HO   **H**
    N

HO   NH   O

NH₂

p₀,₅₆

O   NH₂

N
H   OH

p₀,₁₇

f 1

H₂N   O

p₀,₁₅

f 1

f 2

HO   NH

p₀,₁

f 3

N≡CH
g₀

H₂O
g₂

f 3

f 3

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	-9.0	-13336.077027	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	21
$p_{0,15}$	0	0	-27896.445756	1.0	-27893.119971	22
$p_{0,17}$	0	0	-55788.944315	-5.974208	-55808.813248	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	-63.734865	-63.734865
36	$p_{0,1},$	$p_{0,15},$	2	-39.628701	-39.628701
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	-60.411874	-60.411874
Sum					-194.9493089053887

ΔG = -33.086774875195594
ΔE = -0.07425227030082544
|E| = 7
|U| = 4
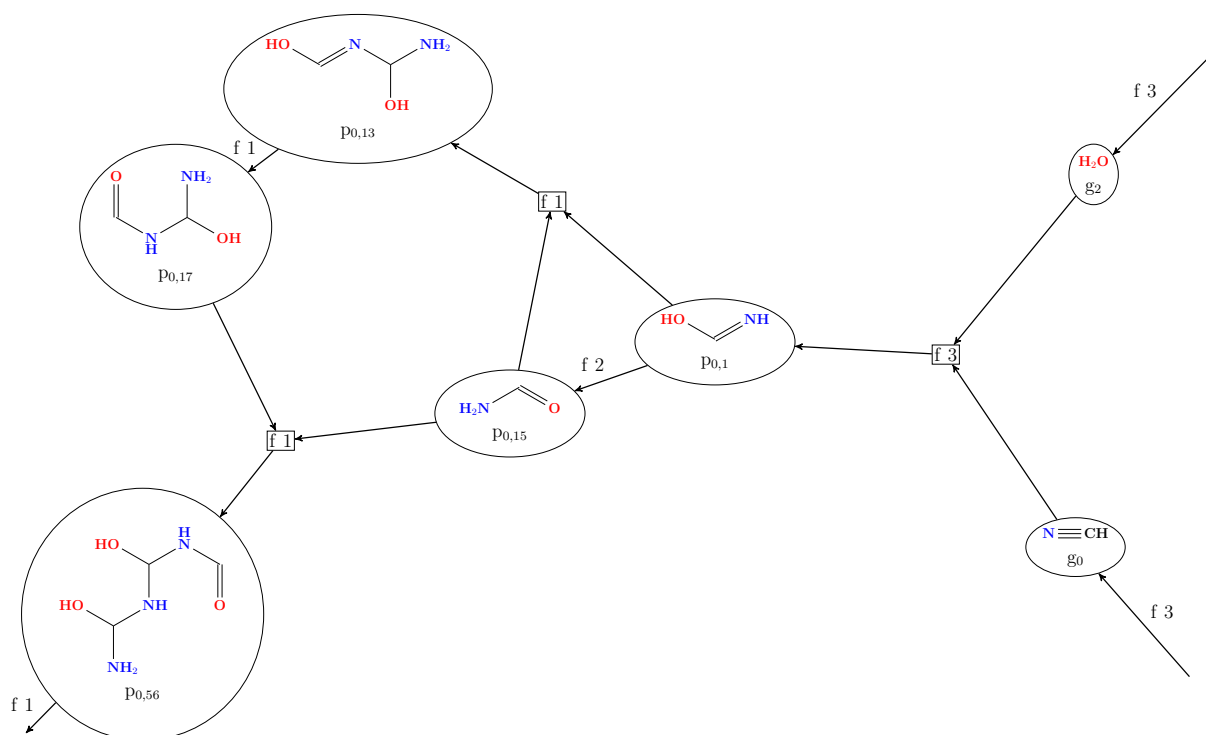
0.3.20   Solution 19

Overall Data

```
Objective value (non-integral): -0.0742523
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  33
p_{0,15}      0  0   -10.625174 1.000000  31
p_{0,17}      0  0   -21.248887 -5.990227 35
p_{0,1}       0  0   -10.610080 1.000000  1
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	-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	33
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	31
$p_{0,17}$	0	0	-55788.944315	-5.990227	-55808.866524	35
$p_{0,56}$	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	-32.666205	-32.666205
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
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	-17.229585	-17.229585
250	$p_{0,13},$	$p_{0,17},$	1	-43.343475	-43.343475
Sum					-194.94930890538276

ΔG = -23.782891309206658
ΔE = -0.07425227030082318
|E| = 8
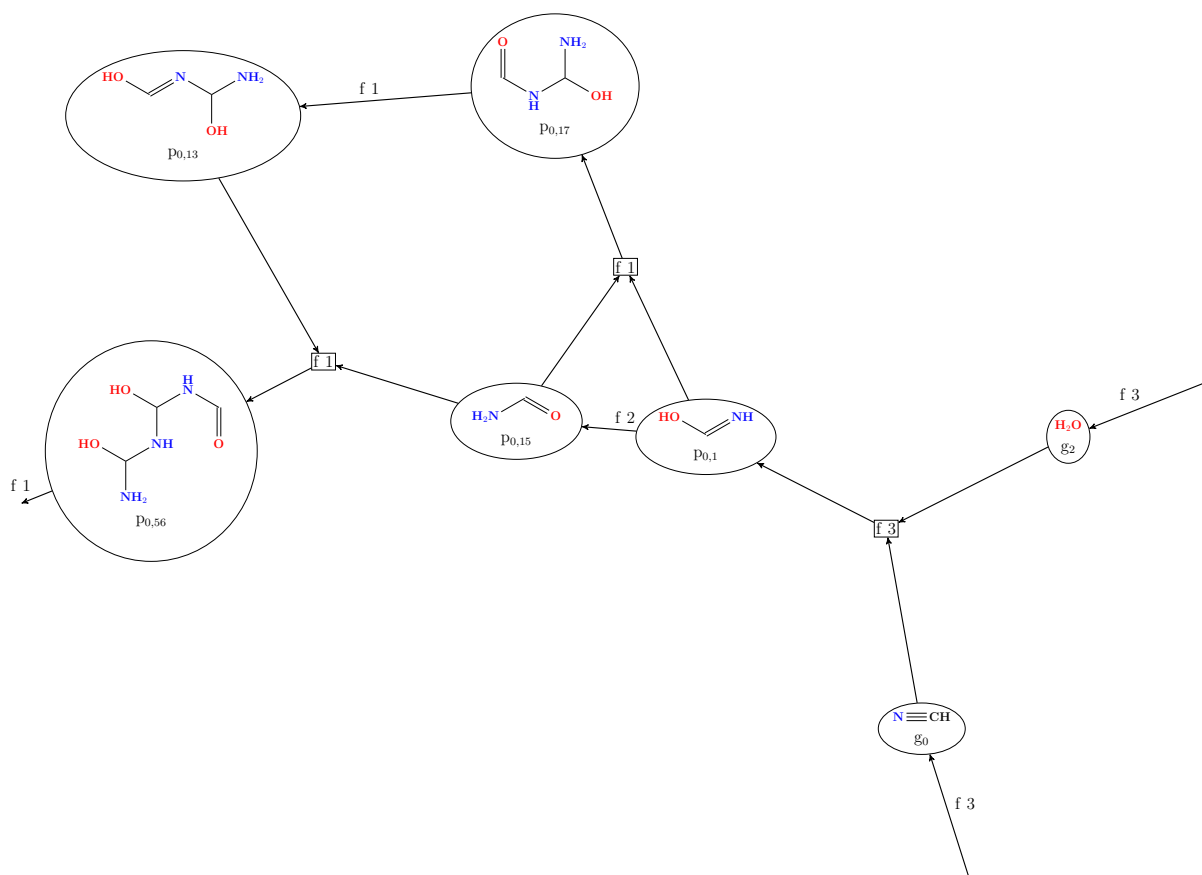|U| = 5

0.3.21 Solution 20

Overall Data

```
Objective value (non-integral): -0.0742523
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   -10.625195 -2.923947 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	-27896.445756	-2.923947	-27906.170174	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	2	-51.798016	-51.798016
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
183	$p_{0,1}, p_{0,15},$	$p_{0,17},$	1	-26.501907	-26.501907
253	$p_{0,17},$	$p_{0,13},$	1	-9.571337	-9.571337
Sum					-194.94930890538276

ΔG = -42.390658178634574

ΔE = -0.0742527030082318

|E| = 8

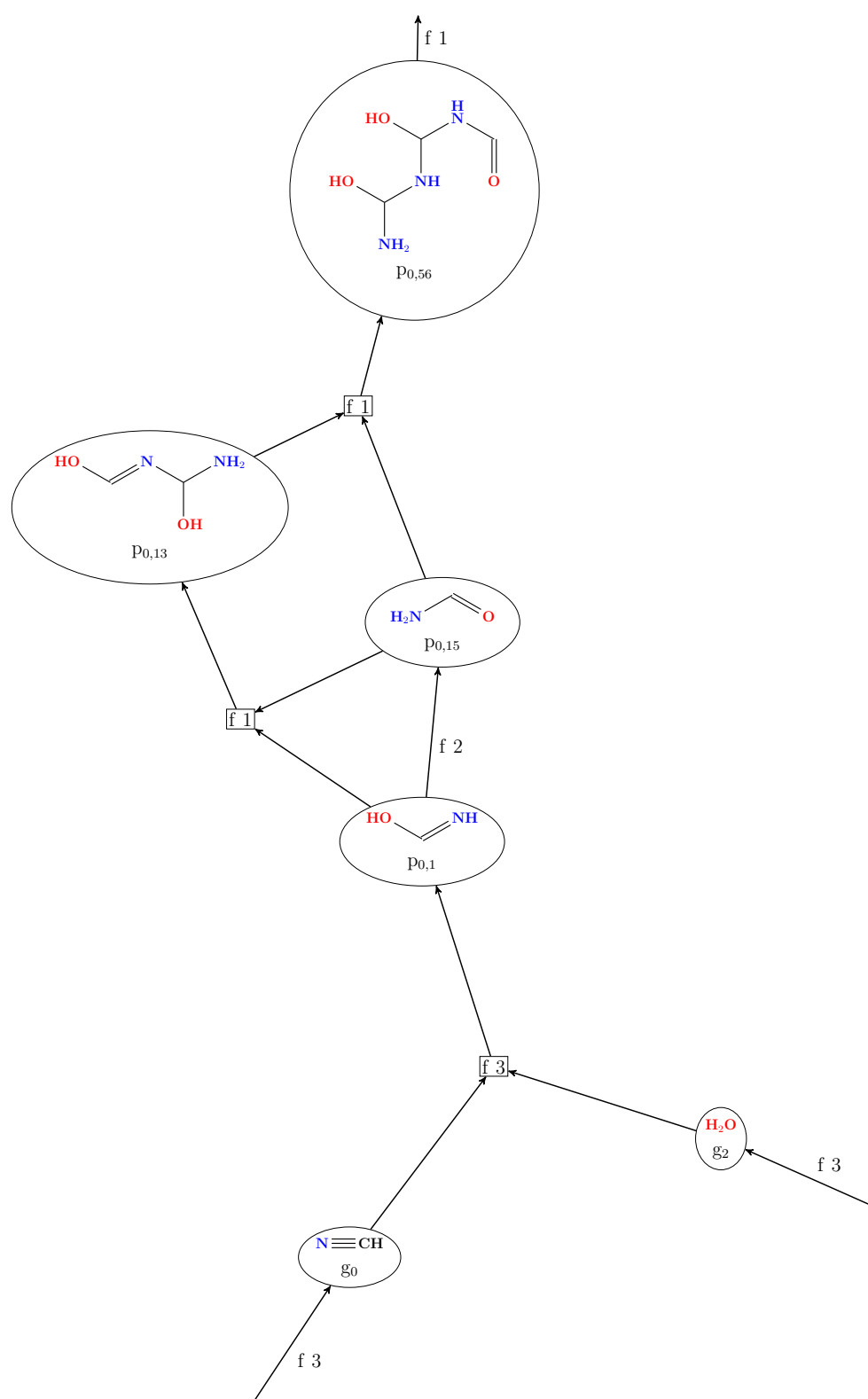|U| = 5

0.3.22   Solution 21

Overall Data

```
Objective value (non-integral): -0.0742523
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   -21.240678 -9.000000 44
p_{0,15}      0  0   -10.625174 1.000000  22
p_{0,1}       0  0   -10.610080 1.000000  21
p_{0,56}      0  1   -31.869324 -9.000000 67
```

f 1

HO

H
N

HO

NH

NH₂

O

p_{0,56}

f 1

HO

N

NH₂

OH

p_{0,13}

H₂N

O

p_{0,15}

f 1

f 2

HO

NH

p_{0,1}

f 3

H₂O

g₂

f 3

N≡CH

g₀

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	20
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	21
$p_{0,13}$	0	0	-55767.391129	-9.0	-55797.323194	44
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	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	-94.692097	-94.692097
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-12.218995	-12.218995
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-48.354065	-48.354065
Sum					-194.94930890537682

ΔG = -42.390658441184534
ΔE = -0.07425227030082092
|E| = 7
|U| = 4
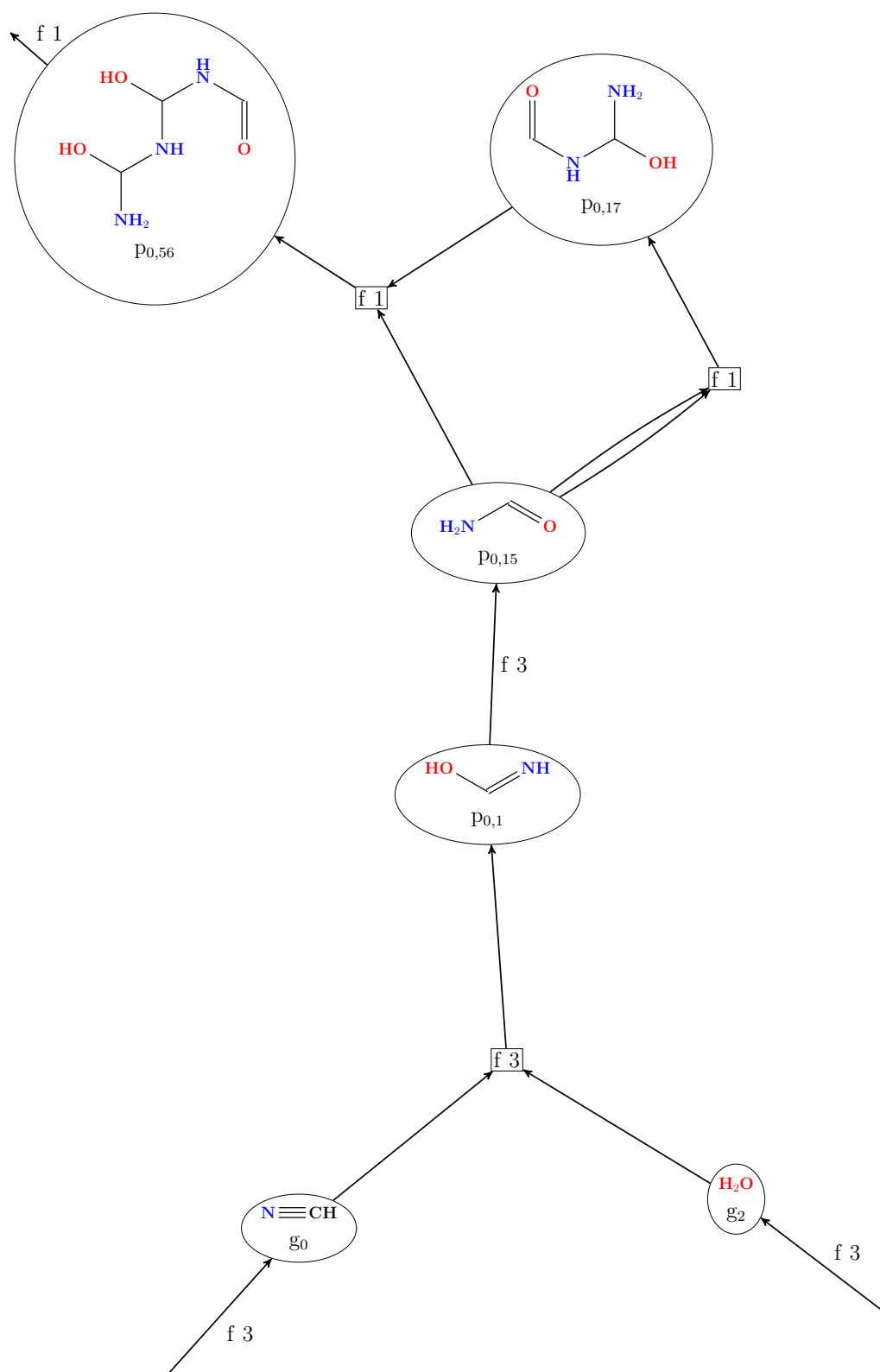
0.3.23   Solution 22

Overall Data

```
Objective value (non-integral): -0.0591585
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  21
p_{0,17}     0  0   -21.248887 -5.990227 44
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -9.000000 67
```

Filtered Graph

File: `out/231_dg_0_11100_f_0_22_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
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	21
$p_{0,17}$	0	0	-55788.944315	-5.990227	-55808.866524	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	3	-39.572909	-39.572909
180	$p_{0,15}, p_{0,15},$	$p_{0,17},$	1	-20.944438	-20.944438
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	0.0	0.0
Sum					-155.320686801597

ΔG = -42.390657916084606
ΔE = -0.05915852528258561
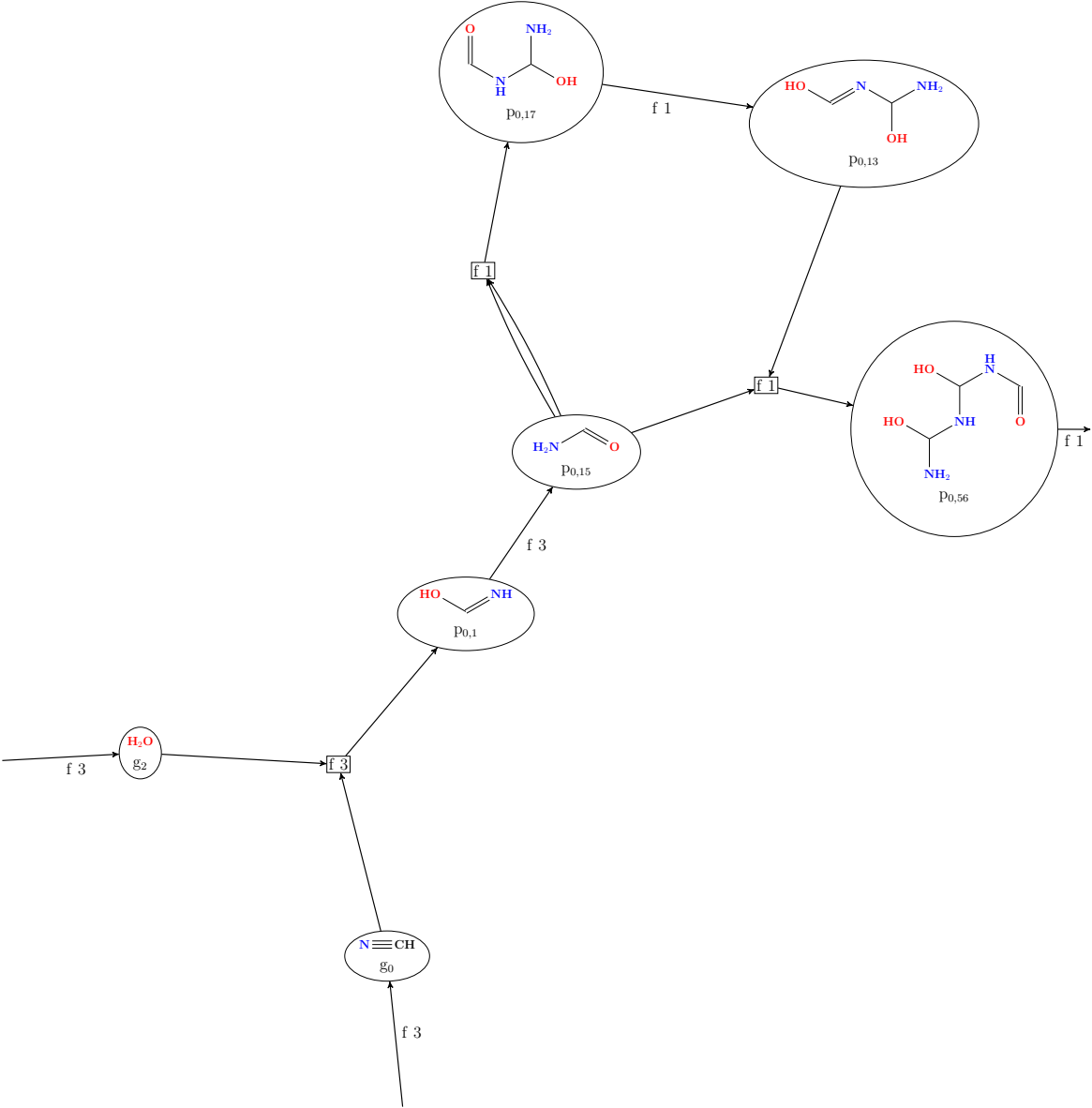$|E| = 8$
$|U| = 4$

0.3.24 Solution 23

Overall Data

```
Objective value (non-integral): -0.0591585
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  -9.000000 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 0.727245  63
p_{0,1}      0  0   -10.610101 -9.000000 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	-9.0	-14488.957643	0
g_2	3	0	-13306.144961	1.0	-13302.819176	0
$p_{0,1}$	0	0	-27856.817054	-9.0	-27886.74912	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	0.727245	-55786.414077	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	-94.74781	-94.74781
36	$p_{0,1},$	$p_{0,15},$	3	-8.559963	-8.559963
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-12.218995	-12.218995
180	$p_{0,15}, p_{0,15},$	$p_{0,17},$	1	0.0	0.0
253	$p_{0,17},$	$p_{0,13},$	1	-8.725443	-8.725443
Sum					-155.32068680158767

ΔG = -33.086774087545706

ΔE = -0.05915852528258206

|E| = 9

|U| = 5