Summary

December 6, 2024

Contents

0.1 Loaded Graphs

0.1.1 g_{0}

$$N \equiv C - H$$

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}

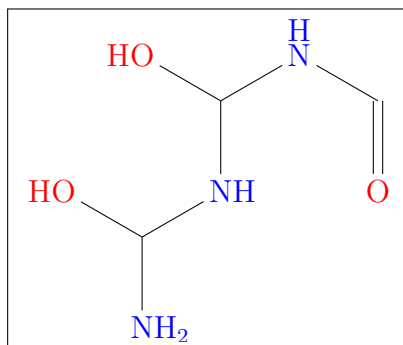File: out/009_g_2_10300000

$$H_2O$$

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): -0.116497
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 -3.000000 3
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 -3.000000 67
p_{0,5}      0  0   -16.158998 -3.000000 2
```
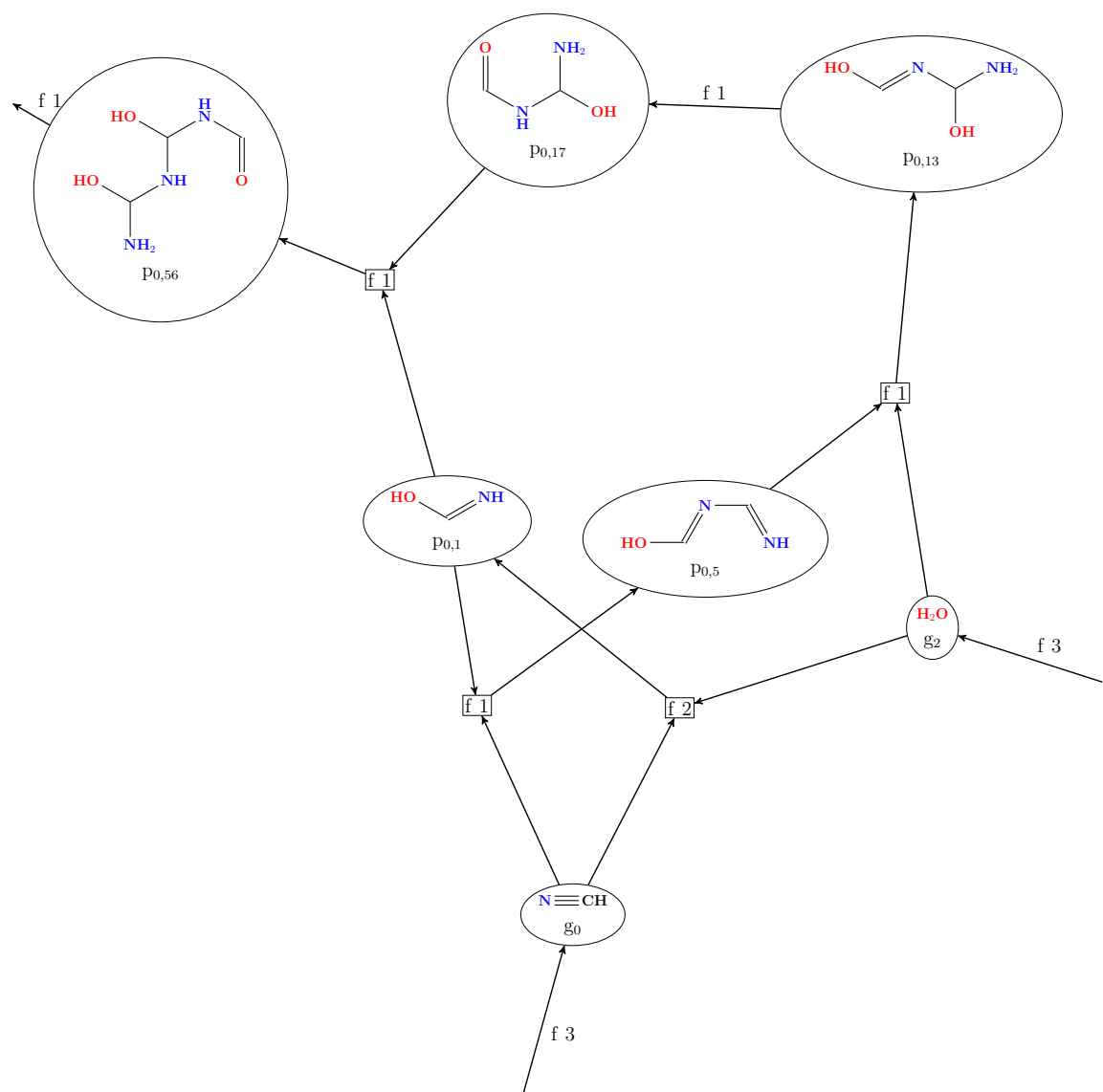
Filtered Graph

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	-27856.761341	1.0	-27853.435556	1
$p_{0,5}$	0	0	-42425.44262	-3.0	-42435.419975	2
$p_{0,13}$	0	0	-55767.391129	-3.0	-55777.368484	3
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	4
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-94.085141	-94.085141
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-122.127396	-122.127396
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-38.297886	-38.297886
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-39.776408	-39.776408
250	$p_{0,13},$	$p_{0,17},$	1	-11.464253	-11.464253
Sum					-305.862144304529

ΔG = -39.98362163825635
ΔE = -0.1164967382608772
|E| = 6
|U| = 5

0.3.2 Solution 1

Overall Data

```
Objective value (non-integral): -0.116497
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  -3.000000  64
p_{0,15}      0  0   -10.625195  -3.000000  2
p_{0,1}       0  0   -10.610101  1.000000   1
p_{0,56}      0  1   -31.869260  -2.386935  67
p_{0,5}       0  0   -16.158998  -3.000000  2
```

Filtered Graph

p_{0,56}

p_{0,13}

f 1

H_2N   O

p_{0,15}

f 1

HO   NH

p_{0,1}

HO   N   NH

p_{0,5}

f 1

f 1

H_2O

g_2

f 1

f 2

f 3

N≡CH

g_0

f 3

File: `out/040_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	-14458.99666	1.0	-14455.670875	0
g_2	3	0	-13306.118349	1.0	-13302.792564	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,5}$	0	0	-42425.44262	-3.0	-42435.419975	2
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	64
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,56}$	0	1	-83672.731446	-2.386935	-83680.669878	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-94.196385	-94.196385
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-122.1006	-122.1006
36	$p_{0,1},$	$p_{0,15},$	1	-49.606057	-49.606057
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-38.212964	-38.212964
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-305.862144304529

$\Delta G = $ -39.830627473064716

$\Delta E = $ -0.1164967382608772

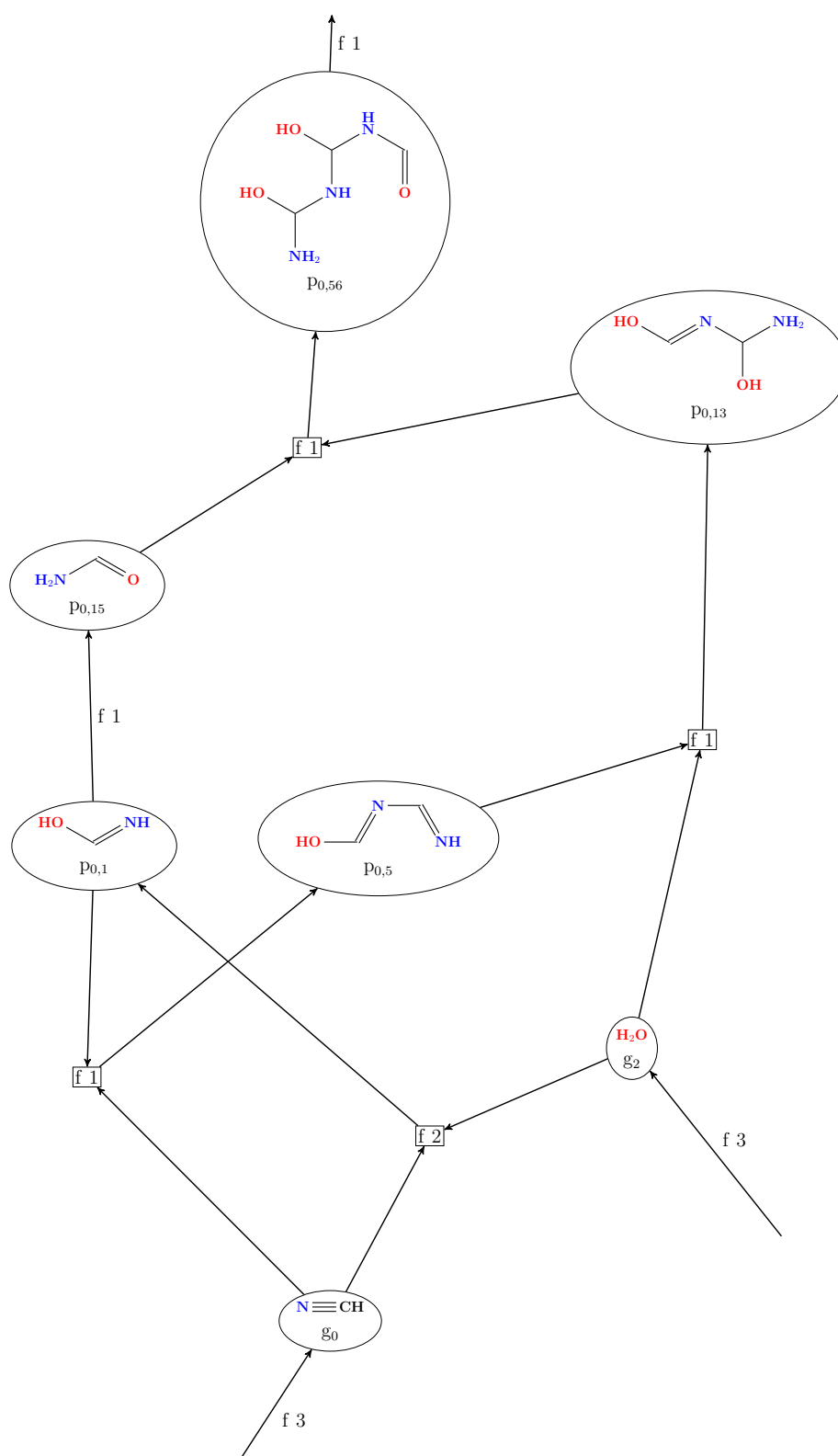$|E| = 6$

$|U| = 5$

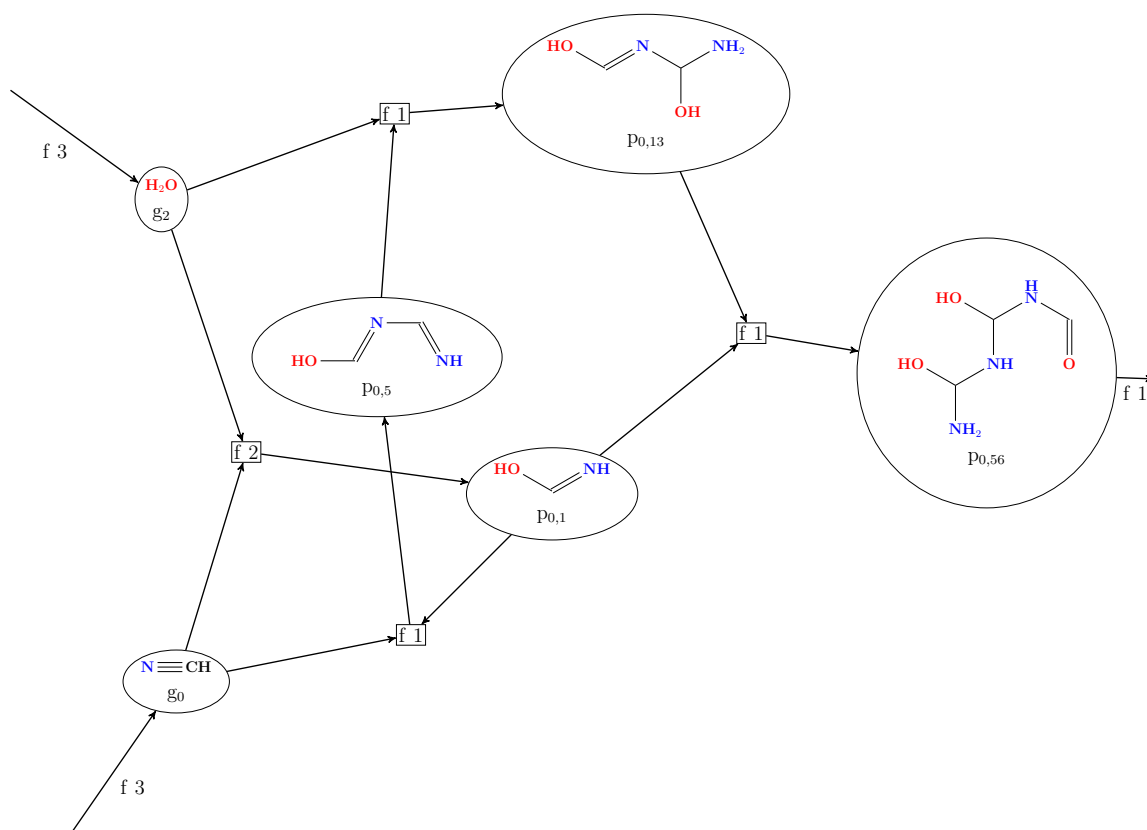## 0.3.3 Solution 2

Overall Data

```
Objective value (non-integral): -0.116497
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 -3.000000 3
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -3.000000 67
p_{0,5}      0  0   -16.158998 -3.000000 2
```

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	1.0	-27853.491269	1
$p_{0,5}$	0	0	-42425.44262	-3.0	-42435.419975	2
$p_{0,13}$	0	0	-55767.391129	-3.0	-55777.368484	3
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-74.186144	-74.186144
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-112.094327	-112.094327
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-28.320531	-28.320531
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-51.184947	-51.184947
Sum					-305.8621443045309

ΔG = -33.99720835807959
ΔE = -0.11649673826087792
|E| = 5
|U| = 4

0.3.4 Solution 3

Overall Data

```
Objective value (non-integral): -0.116497
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 -3.000000 33
p_{0,15}     0  0   -10.625174 0.983033  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 -3.000000 67
p_{0,5}      0  0   -16.158998 -3.000000 32
```

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	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	-3.0	-42435.419975	32
$p_{0,13}$	0	0	-55767.391129	-3.0	-55777.368484	33
$p_{0,15}$	0	0	-27896.389963	0.983033	-27893.120606	2
$p_{0,17}$	0	0	-55788.944315	1.0	-55785.61853	64
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	2	-94.140854	-94.140854
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-122.071682	-122.071682
36	$p_{0,1},$	$p_{0,15},$	1	-39.61523	-39.61523
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-38.297886	-38.297886
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	0.006113	0.006113
250	$p_{0,13},$	$p_{0,17},$	1	-11.575831	-11.575831
Sum					-305.86214430452713

ΔG = -39.98362190080631

ΔE = -0.11649673826087648

|E| = 7
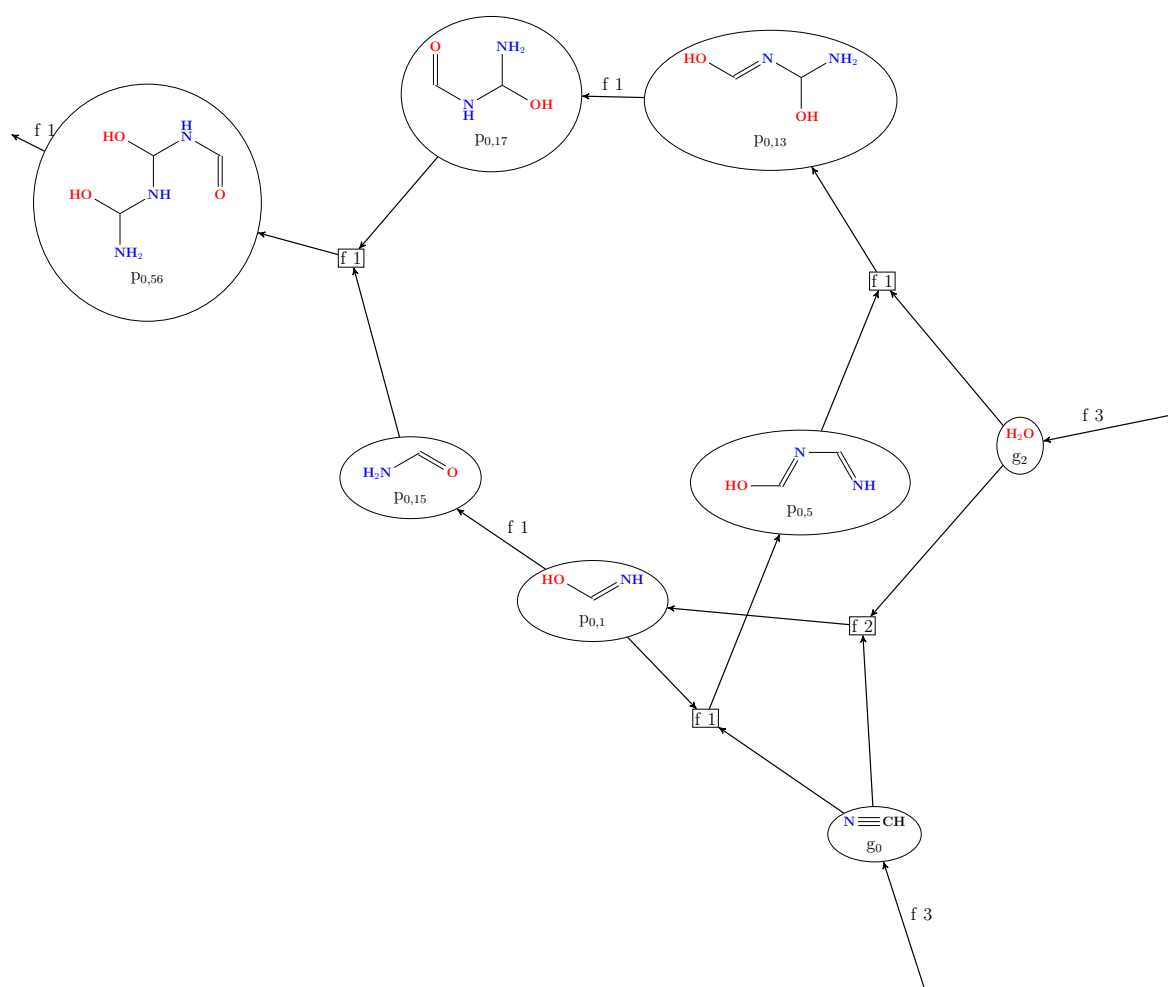
|U| = 6

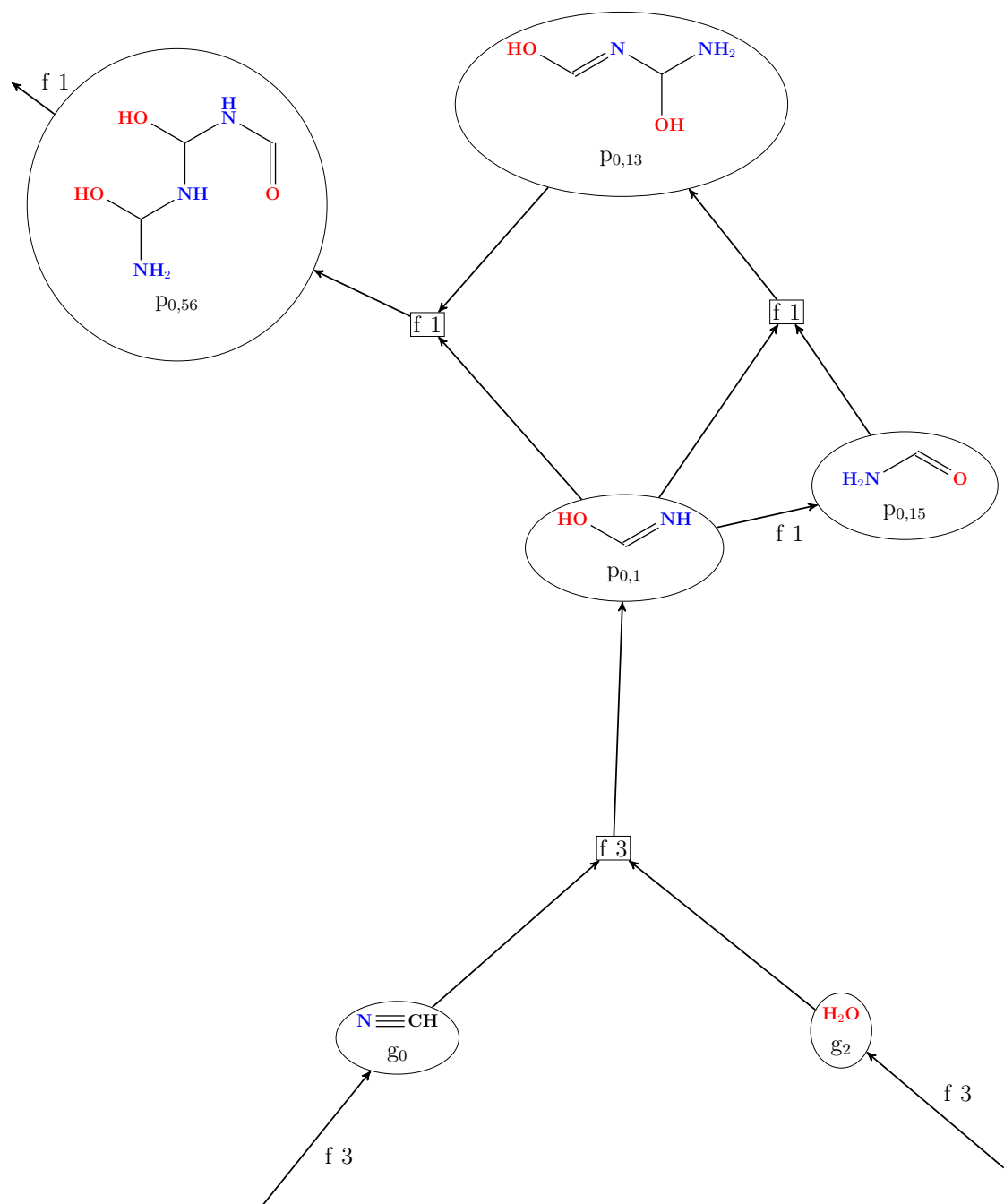### 0.3.5 Solution 4

Overall Data

```
Objective value (non-integral): -0.0806405
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 -0.333395 65
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   -31.869260 1.000000  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	-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	-0.333395	-55768.49993	65
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,56}$	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	-84.163499	-84.163499
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
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	-37.714307	-37.714307
Sum					-211.72147327186593

ΔG = -32.98273840178135
ΔE = -0.0806404503311221
|E| = 6
|U| = 4

0.3.6 Solution 5

Overall Data

```
Objective value (non-integral): -0.0806405
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 1.000000  64
p_{0,15}     0  0   -10.625195 -3.000000 62
p_{0,17}     0  0   -21.248887 1.000000  65
p_{0,1}      0  0   -10.610080 1.000000  1
p_{0,56}     0  1   -31.869324 -3.000000 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	-27856.761341	1.0	-27853.435556	1
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	64
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	62
$p_{0,17}$	0	0	-55788.944315	1.0	-55785.61853	65
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.13043	-74.13043
36	$p_{0,1},$	$p_{0,15},$	1	-49.66177	-49.66177
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-6.589481	-6.589481
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-39.66483	-39.66483
250	$p_{0,13},$	$p_{0,17},$	1	-21.664721	-21.664721
Sum					-211.72147327186403

ΔG = -33.99720809552962

ΔE = -0.08064045033112138

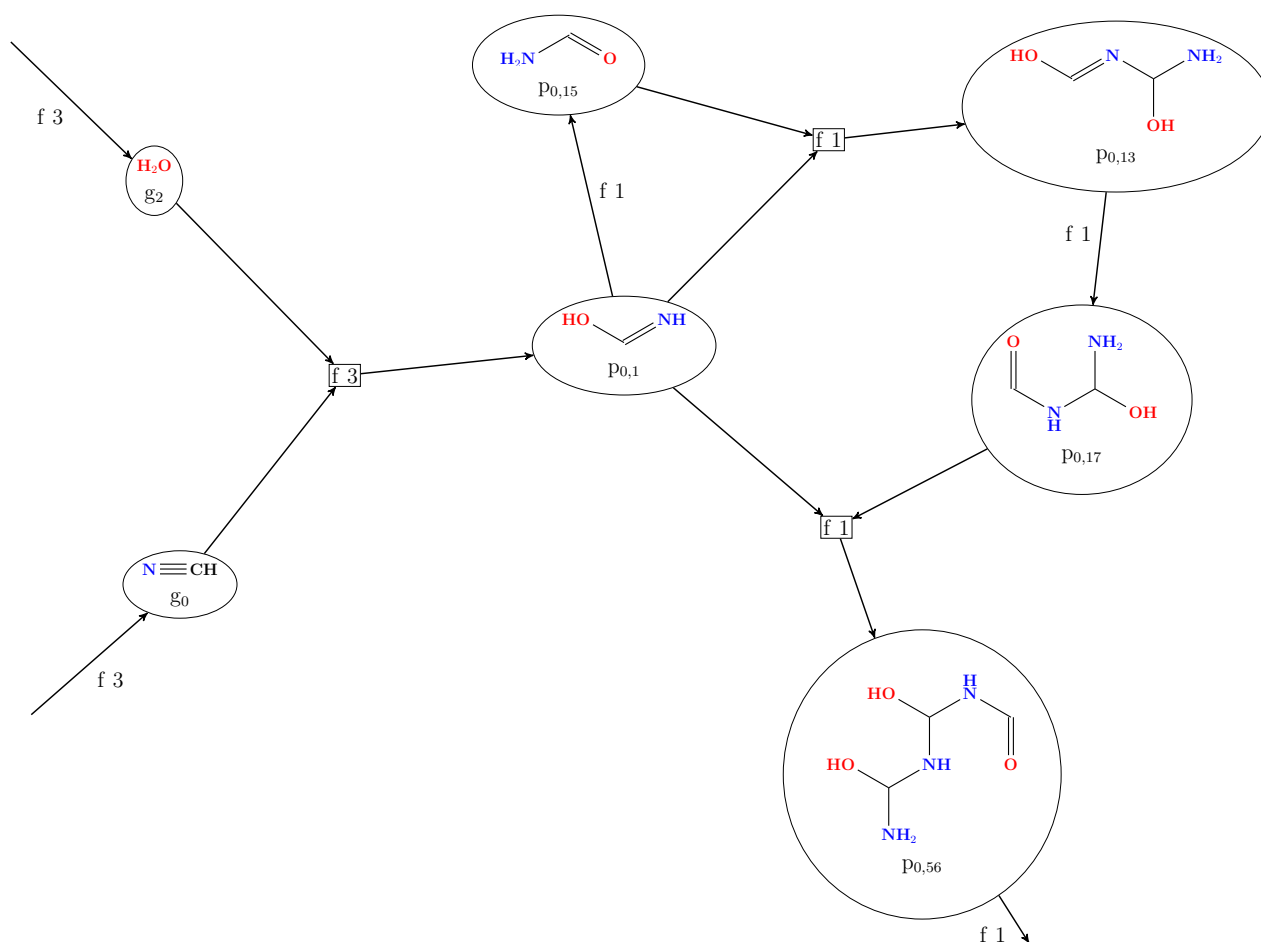$|E| = 7$
$|U| = 5$

0.3.7 Solution 6
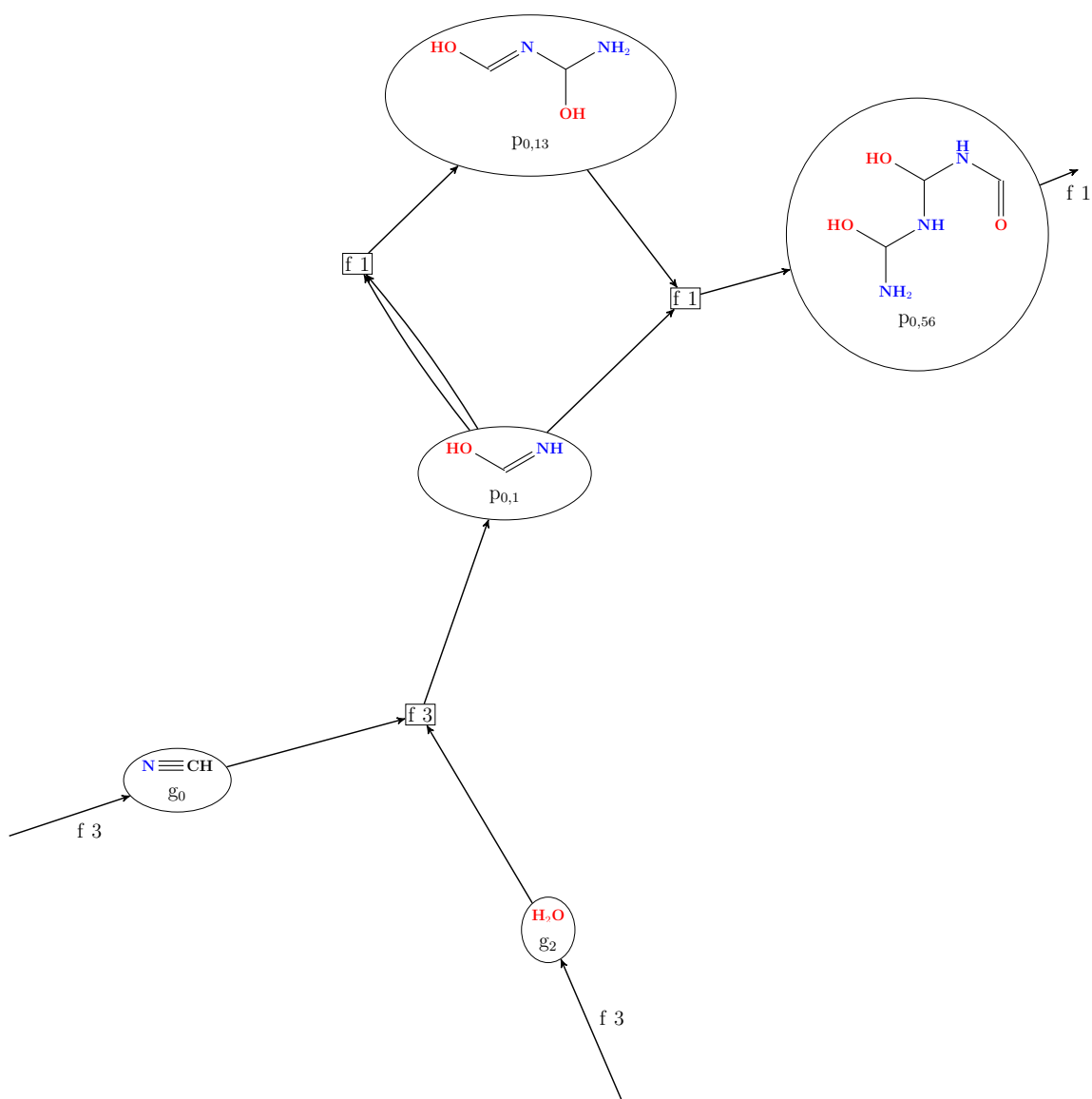
Overall Data

```
Objective value (non-integral): -0.0806405
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 1.000000  45
p_{0,1}     0   0  -10.610080 1.000000  21
p_{0,56}    0   1  -31.869324 -3.000000 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	1.0	-27853.435556	21
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	45
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.13043	-74.13043
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.251251	-56.251251
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-61.329551	-61.329551
Sum					-211.72147327186403

ΔG = -33.99720862062955

ΔE = -0.08064045033112138

|E| = 5

|U| = 3
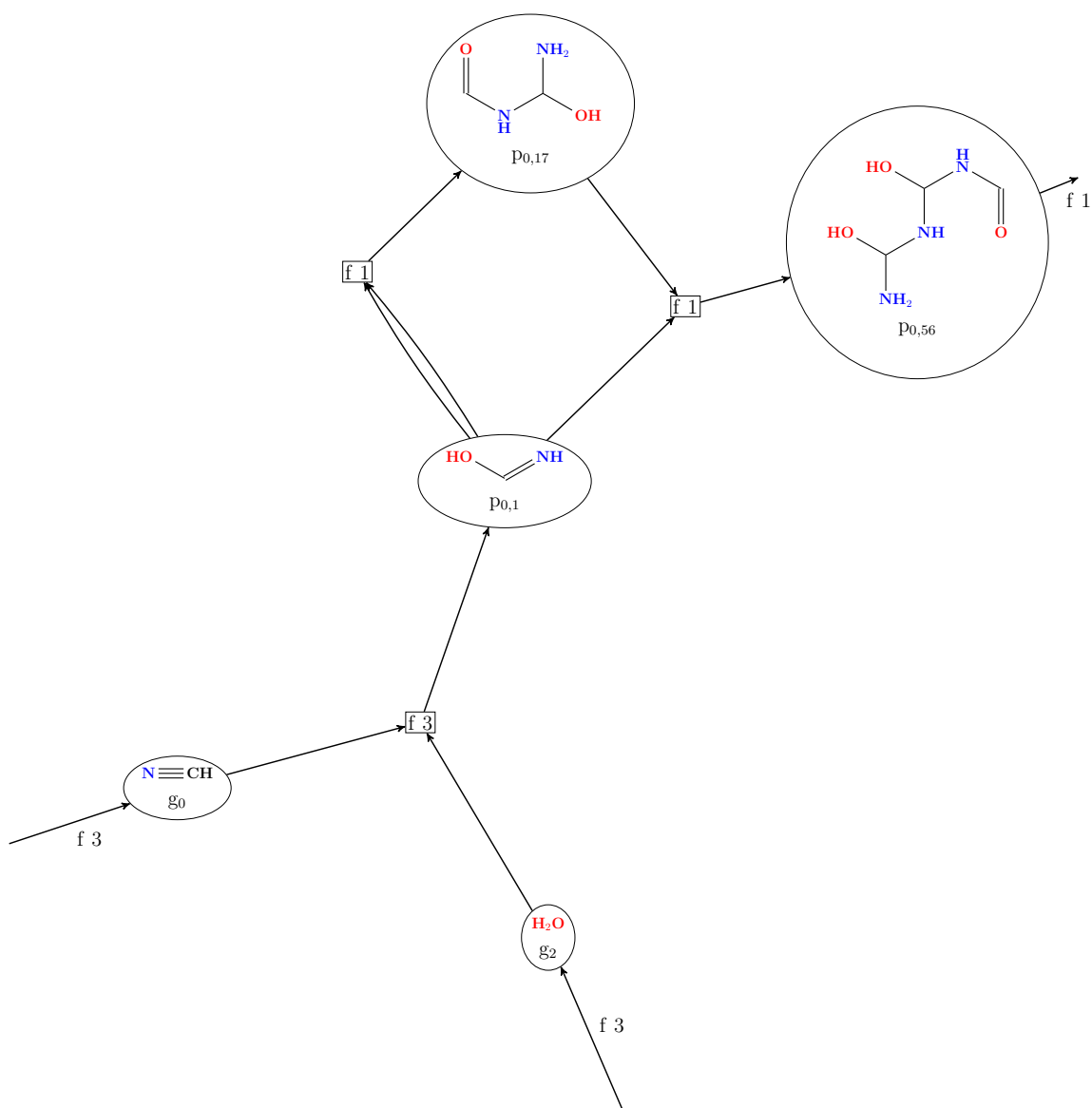
0.3.8 Solution 7

Overall Data

```
Objective value (non-integral): -0.0806405
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -3.000000  0
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 -3.000000  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	1.0	-14455.699793	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	21
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	45
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.107786	-84.107786
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-77.804394	-77.804394
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-39.776408	-39.776408
Sum					-211.72147327186403

$\Delta G = -36.99041499816797$

$\Delta E = -0.08064045033112138$

|E| = 5
|U| = 3

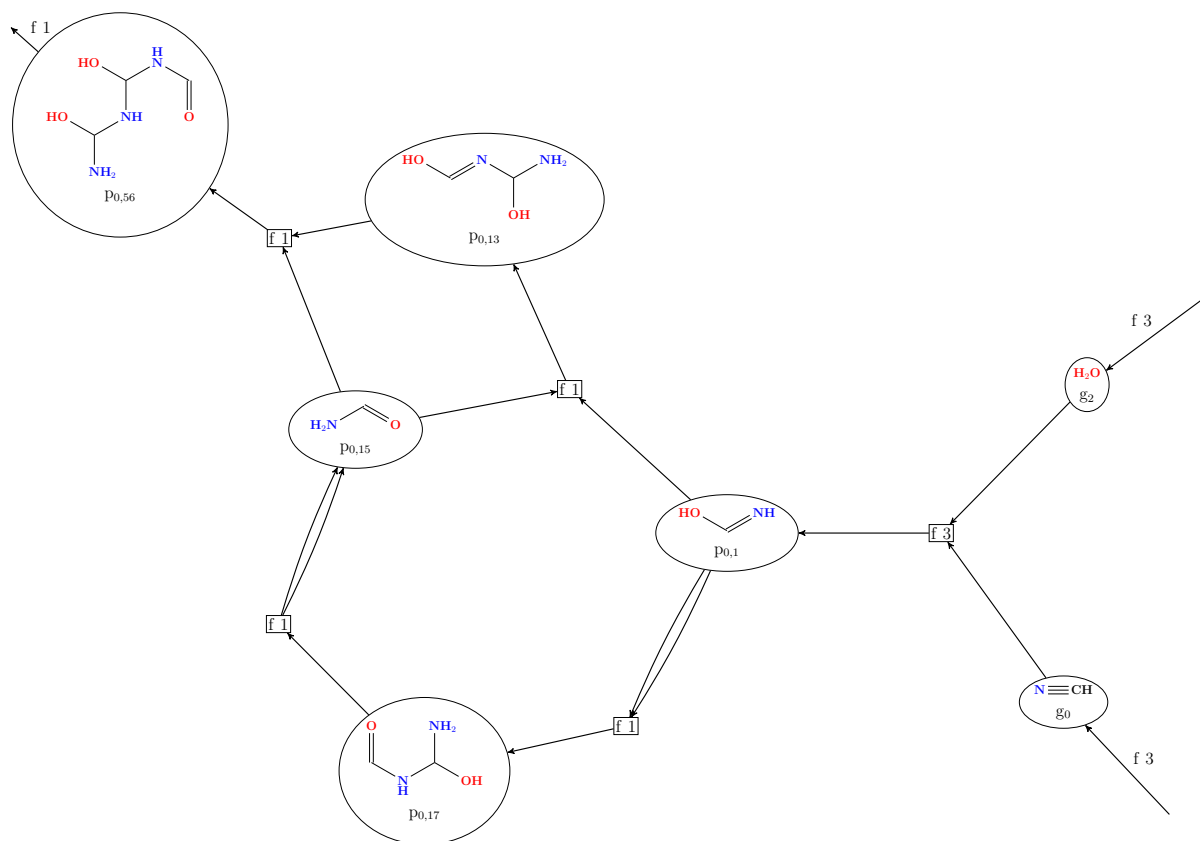## 0.3.9 Solution 8

Overall Data

```
Objective value (non-integral): -0.0806405
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 1.000000   40
p_{0,15}     0   0   -10.625174 1.000000   26
p_{0,17}     0   0   -21.248844 0.415090   3
p_{0,1}      0   0   -10.610101 1.000000   1
p_{0,56}     0   1   -31.869324 -3.000000  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	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	-55767.279594	1.0	-55763.953809	40
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	26
$p_{0,17}$	0	0	-55788.832737	0.41509	-55787.452236	3
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-94.140854	-94.140854
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-79.15193	-79.15193
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-21.700929	-21.700929
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-16.566916	-16.566916
237	$p_{0,17},$	$p_{0,15}, p_{0,15},$	1	0.006113	0.006113
Sum					-211.72147327186318

ΔG = -39.983621375706385

ΔE = -0.08064045033112105

|E| = 7

|U| = 5

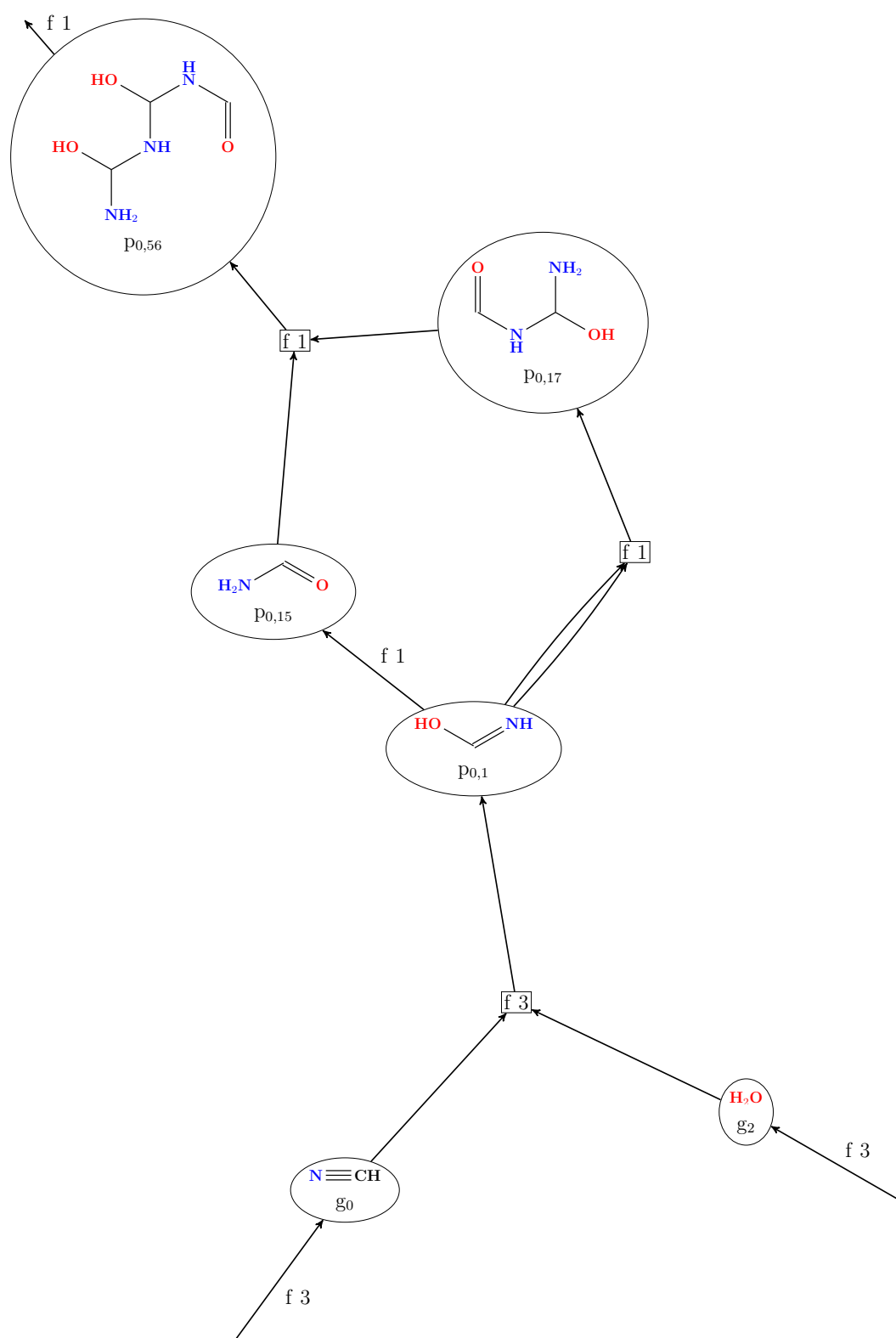## 0.3.10 Solution 9

Overall Data

```
Objective value (non-integral): -0.0806405
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_{0,15}     0  0   -10.625174 0.983033  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 -3.000000 67
```

Filtered Graph

f 1

HO

H
N

HO NH

O

NH₂

p₀,₅₆

f 1

O NH₂

N
H OH

p₀,₁₇

f 1

H₂N O

p₀,₁₅

f 1

HO NH

p₀,₁

f 3

N≡CH

g₀

H₂O

g₂

f 3

f 3

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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,15}$	0	0	-27896.389963	0.983033	-27893.120606	2
$p_{0,17}$	0	0	-55788.944315	1.0	-55785.61853	3
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.186144	-74.186144
36	$p_{0,1},$	$p_{0,15},$	1	-39.61523	-39.61523
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-77.804545	-77.804545
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-211.72147327186215

ΔG = -33.99720862062955

ΔE = -0.08064045033112066

|E| = 6

|U| = 4

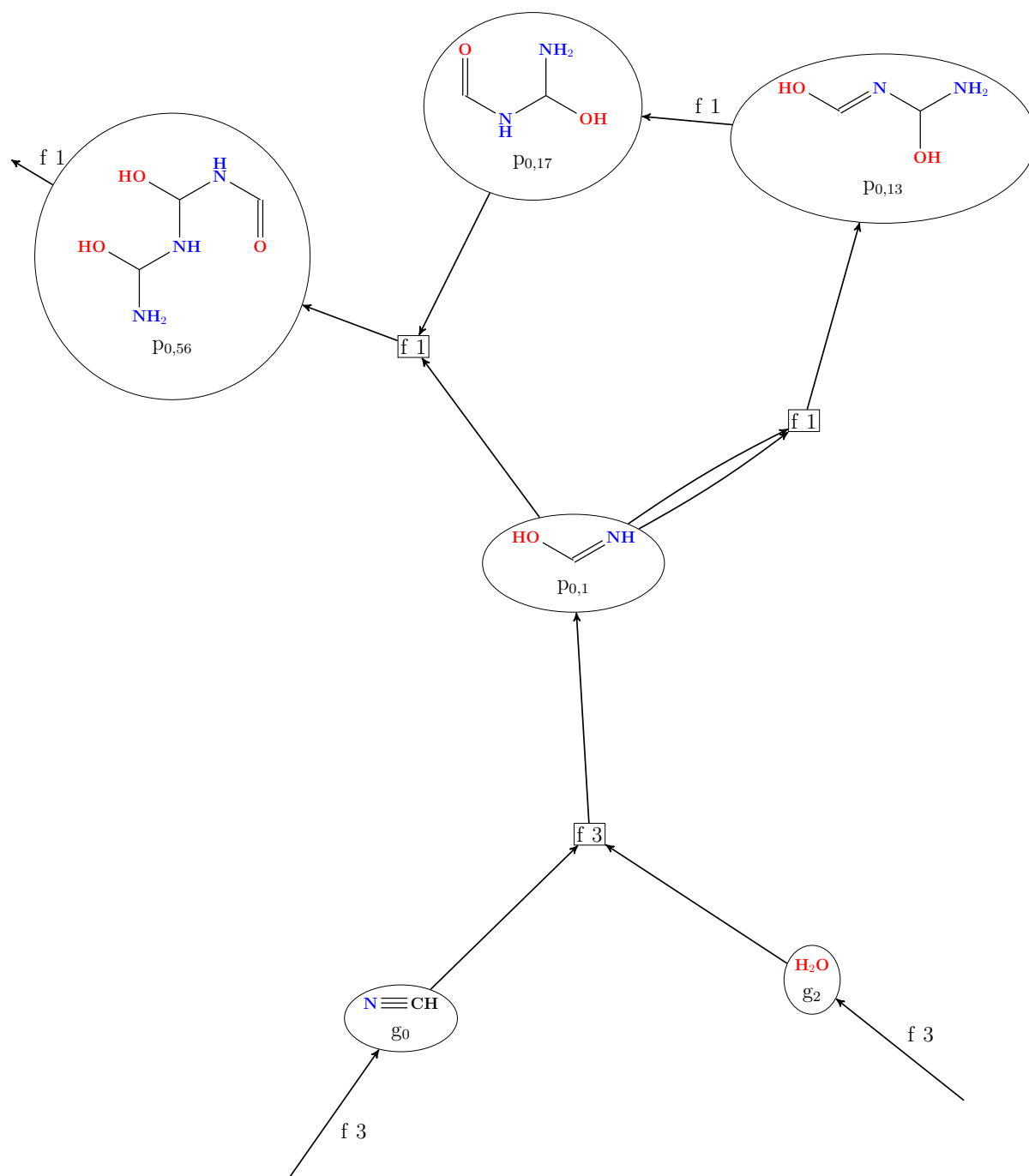## 0.3.11   Solution 10

Overall Data

```
Objective value (non-integral): -0.0806405
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 1.000000  64
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 -3.000000 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	-27856.761341	1.0	-27853.435556	1
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	64
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	65
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-94.085141	-94.085141
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.251251	-56.251251
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-39.776408	-39.776408
250	$p_{0,13},$	$p_{0,17},$	1	-21.553143	-21.553143
Sum					-211.72147327186215

$\Delta G = -39.98362163825635$

$\Delta E = -0.08064045033112066$

$|\text{E}| = 6$
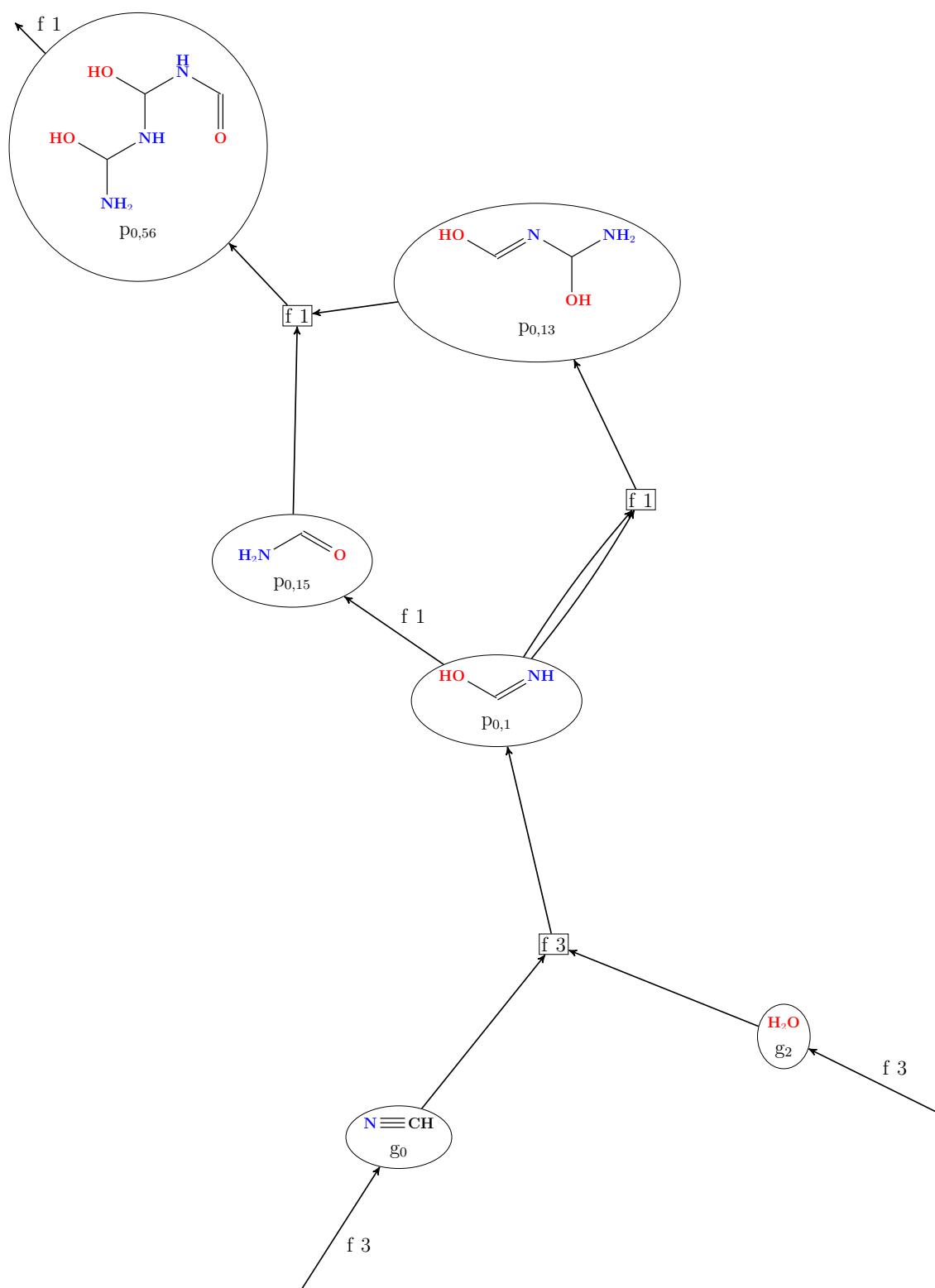
$|\text{U}| = 4$

0.3.12   Solution 11

Overall Data

```
Objective value (non-integral): -0.0806405
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 -3.000000 3
p_{0,15}     0  0   -10.625195 -3.000000 2
p_{0,1}      0  0   -10.610101 1.000000  1
p_{0,56}     0  1   -31.869324 -2.364559 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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,13}$	0	0	-55767.391129	-3.0	-55777.368484	3
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,56}$	0	1	-83672.898792	-2.364559	-83680.762809	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.186144	-74.186144
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-66.228714	-66.228714
36	$p_{0,1},$	$p_{0,15},$	1	-49.606057	-49.606057
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-211.72147327186215

ΔG = -33.83870799504404
ΔE = -0.08064045033112066
|E| = 6
|U| = 4

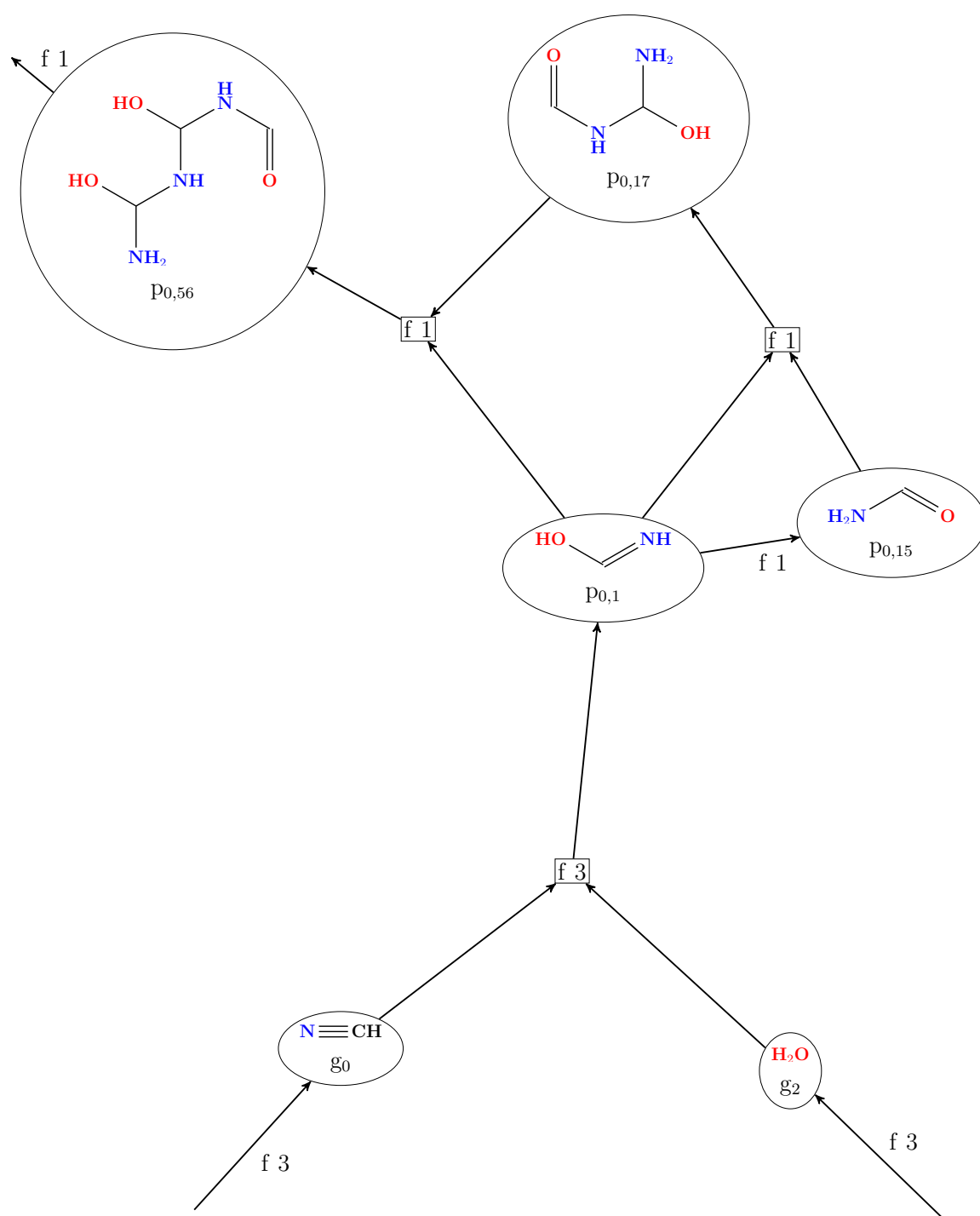## 0.3.13 Solution 12

Overall Data

```
Objective value (non-integral): -0.0806405
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_{0,15}       0  0   -10.625195 -3.000000 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 -3.000000 67
```

Filtered Graph

File: `out/139_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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	1
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	2
$p_{0,17}$	0	0	-55788.832737	1.0	-55785.506952	4
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.13043	-74.13043
36	$p_{0,1},$	$p_{0,15},$	1	-49.66177	-49.66177
183	$p_{0,1}, p_{0,15},$	$p_{0,17},$	1	-28.142624	-28.142624
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-39.776408	-39.776408
Sum					-211.72147327186215

ΔG = -33.99720835807959
ΔE = -0.08064045033112066
$|E| = 6$
$|U| = 4$

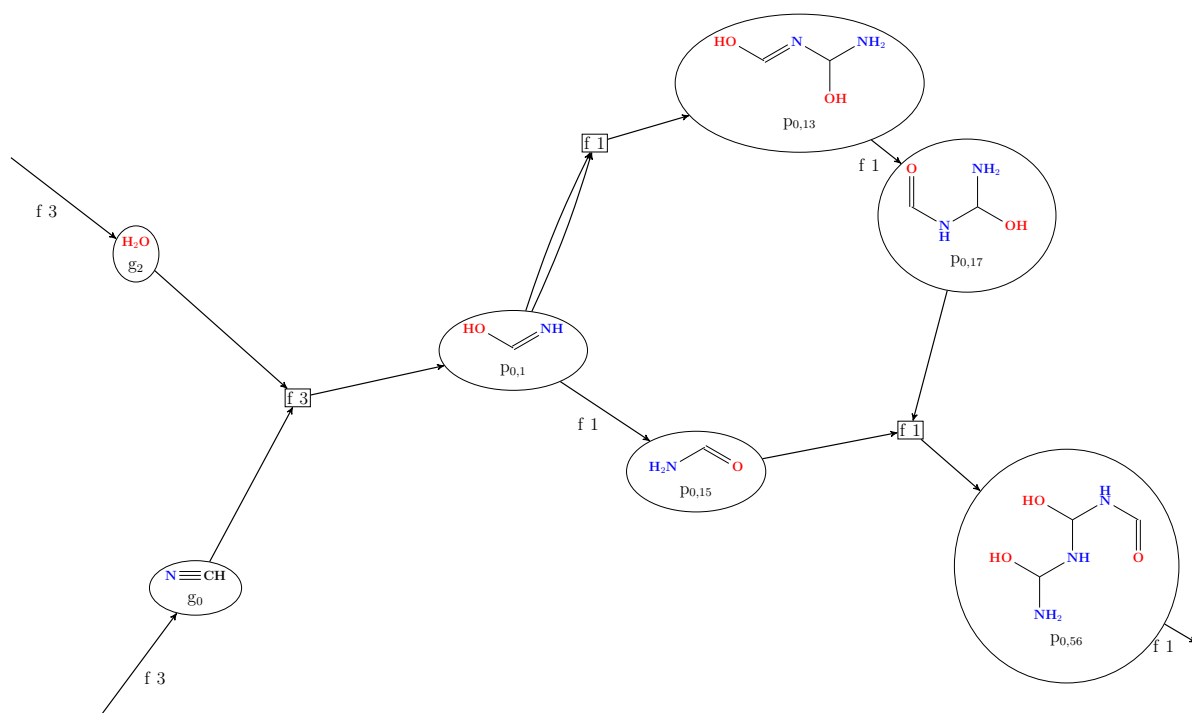## 0.3.14   Solution 13

Overall Data

```
Objective value (non-integral): -0.0806405
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 1.000000   43
p_{0,15}      0  0  -10.625174 1.000000   22
p_{0,17}      0  0  -21.248844 1.000000   44
p_{0,1}       0  0  -10.610101 1.000000   21
p_{0,56}      0  1  -31.869324 -3.000000  67
```

Filtered Graph

File: `out/148_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	1.0	-27853.491269	21
$p_{0,13}$	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	-55788.832737	1.0	-55785.506952	44
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-94.140854	-94.140854
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-56.139824	-56.139824
36	$p_{0,1},$	$p_{0,15},$	1	-39.572909	-39.572909
181	$p_{0,15}, p_{0,17},$	$p_{0,56},$	1	-0.147786	-0.147786
250	$p_{0,13},$	$p_{0,17},$	1	-21.553143	-21.553143
Sum					-211.72147327186025

ΔG = -39.983621113156424
ΔE = -0.08064045033111994
$|\mathrm{E}|$ = 7
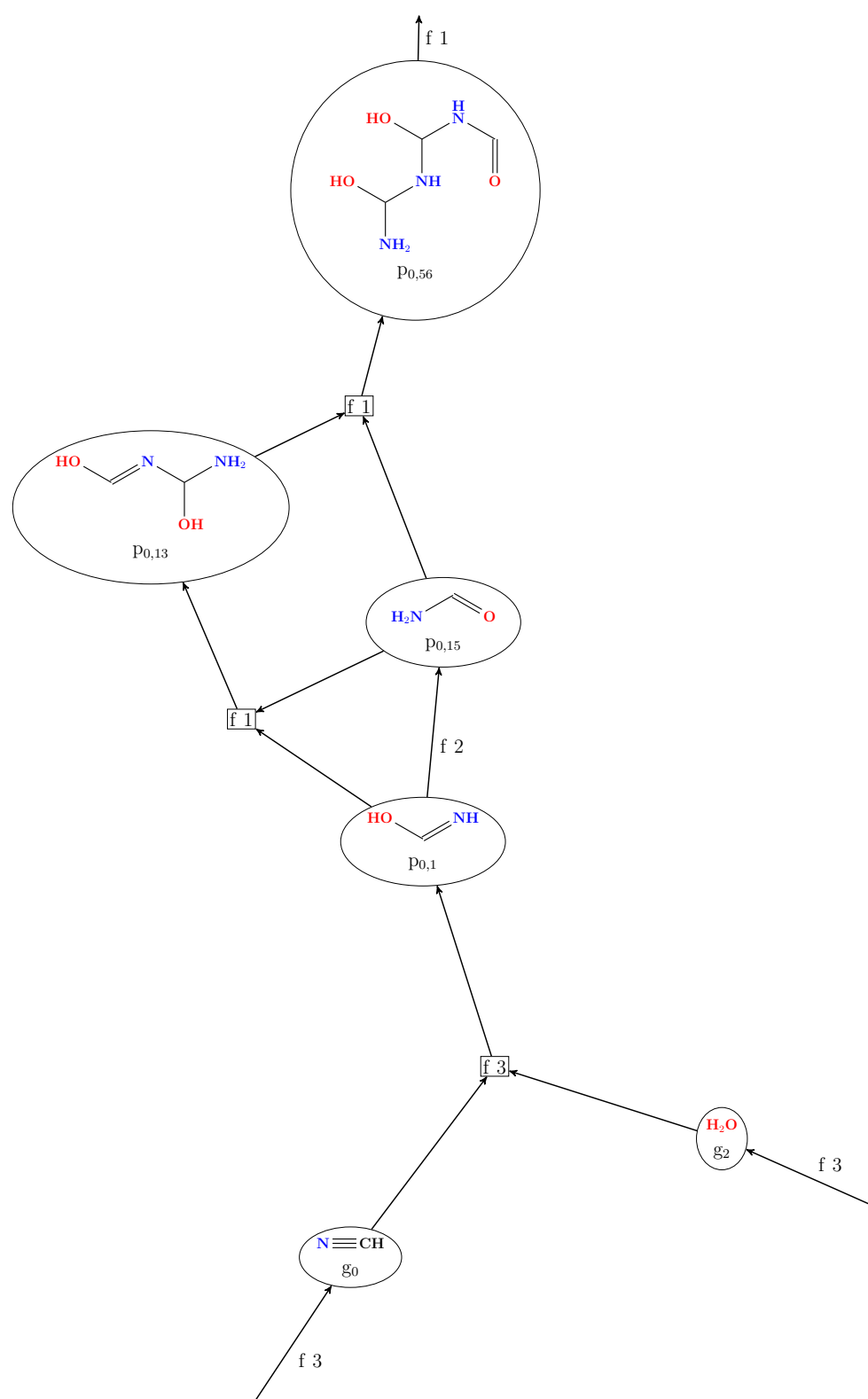$|\mathrm{U}|$ = 5

0.3.15   Solution 14

Overall Data

Objective value (non-integral): -0.0655467

```
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 -3.000000 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 -3.000000 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	-27856.761341	1.0	-27853.435556	1
$p_{0,13}$	0	0	-55767.391129	-3.0	-55777.368484	64
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	2
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-94.085141	-94.085141
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-11.612039	-11.612039
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-26.711519	-26.711519
Sum					-172.0928511680708

ΔG = -39.98362190080631
ΔE = -0.06554670531288098
|E| = 7
|U| = 4
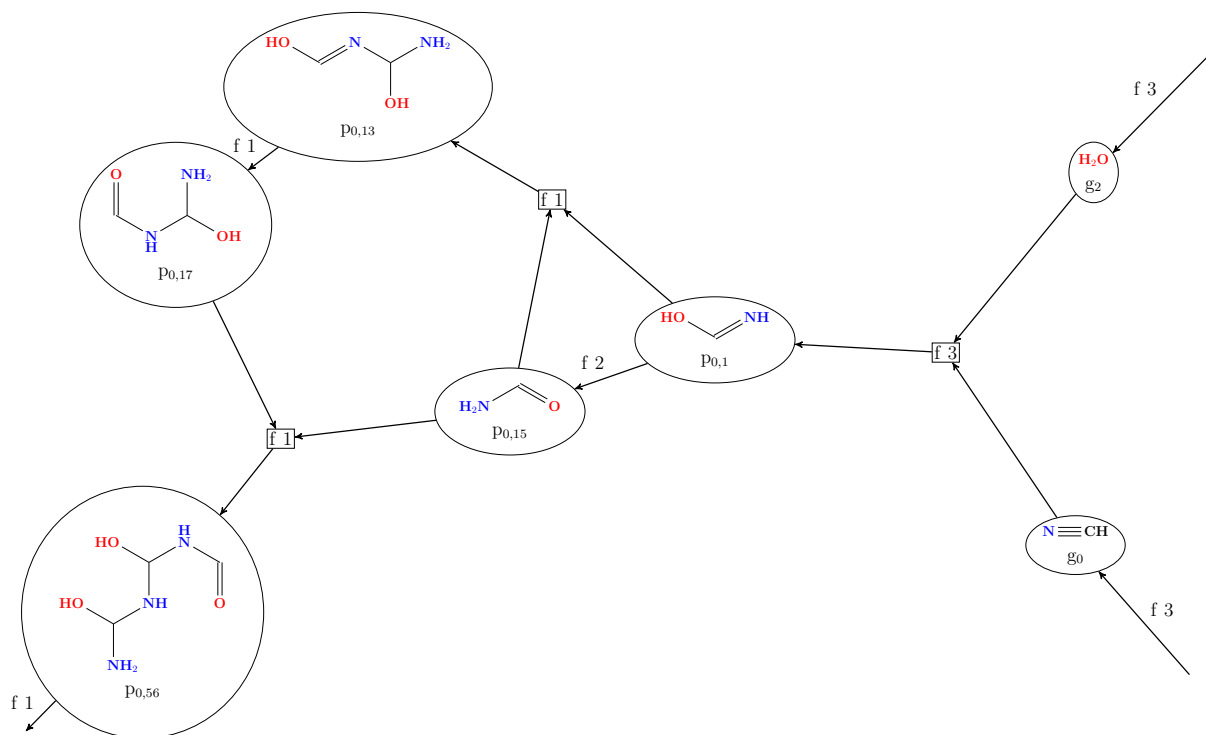
0.3.16 Solution 15

Overall Data

```
Objective value (non-integral): -0.0655467
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 1.000000  4
p_{0,15}      0  0   -10.625174 1.000000  2
p_{0,17}      0  0   -21.248887 0.985484  64
p_{0,1}       0  0   -10.610101 1.000000  1
p_{0,56}      0  1   -31.869324 -3.000000 67
```

Filtered Graph

File: `out/166_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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	1.0	-27853.491269	1
$p_{0,13}$	0	0	-55767.279594	1.0	-55763.953809	4
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	2
$p_{0,17}$	0	0	-55788.944315	0.985484	-55785.666807	64
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-74.186144	-74.186144
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	-16.566916	-16.566916
250	$p_{0,13},$	$p_{0,17},$	1	-21.700929	-21.700929
Sum					-172.09285116806893

ΔG = -33.99720783297966

ΔE = -0.06554670531288026

|E| = 8

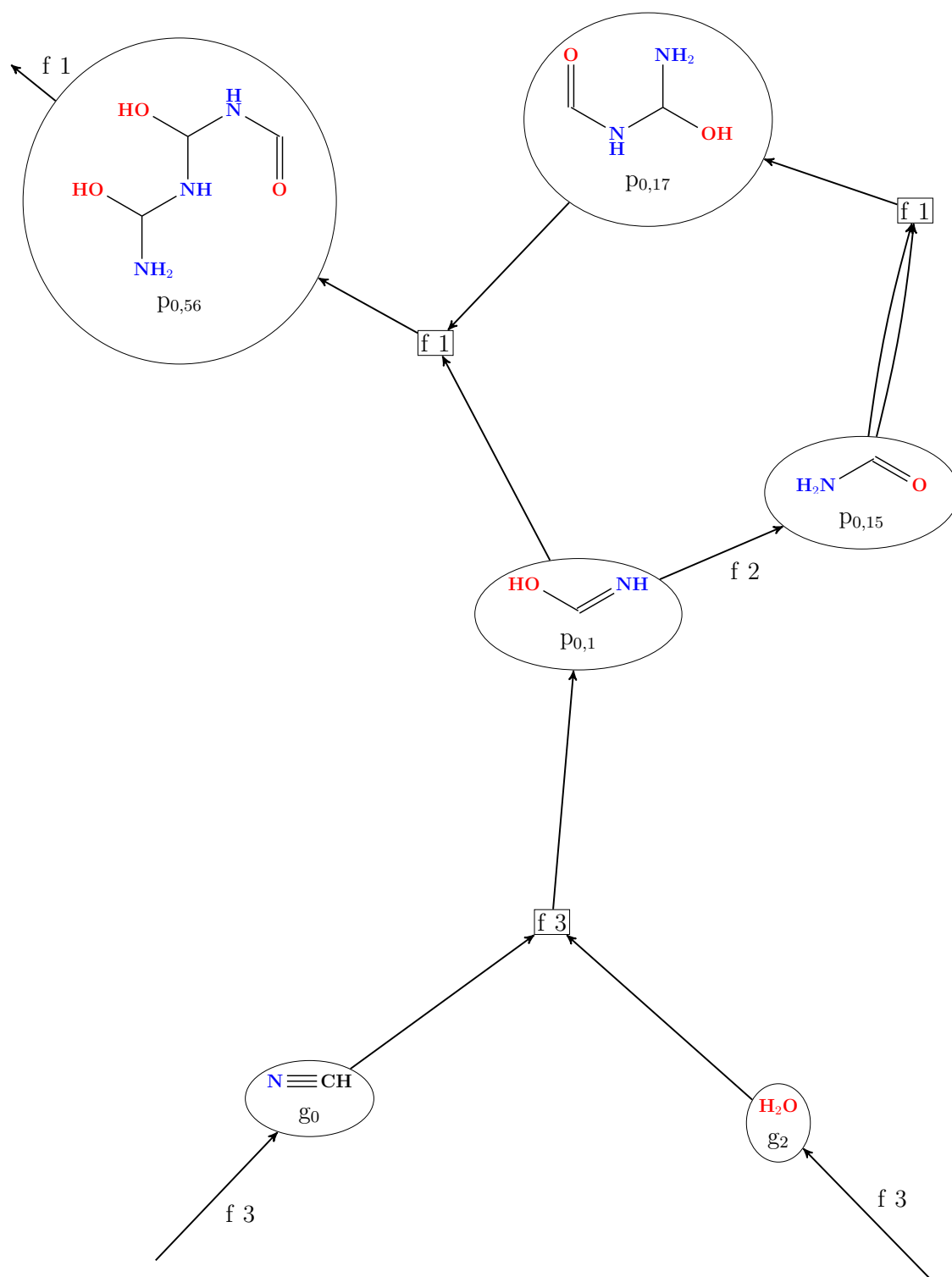|U| = 5

0.3.17 Solution 16

Overall Data

```
Objective value (non-integral): -0.0655467
Vertex/Graph In Out G          logK       t_order
g_{0}        3  0   -5.507152  1.000000   0
g_{2}        3  0   -5.068043  -3.000000 20
p_{0,15}     0  0   -10.625174 1.000000  22
p_{0,17}     0  0   -21.248844 0.417541  45
p_{0,1}      0  0   -10.610080 1.000000  21
p_{0,56}     0  1   -31.869324 -3.000000 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	-3.0	-13316.122316	20
$p_{0,1}$	0	0	-27856.761341	1.0	-27853.435556	21
$p_{0,15}$	0	0	-27896.389963	1.0	-27893.064178	22
$p_{0,17}$	0	0	-55788.832737	0.417541	-55787.444085	45
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-84.107786	-84.107786
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	-38.323558	-38.323558
Sum					-172.09285116806893

ΔG = -36.99041526071793
ΔE = -0.06554670531288026
$|E| = 7$
$|U| = 4$

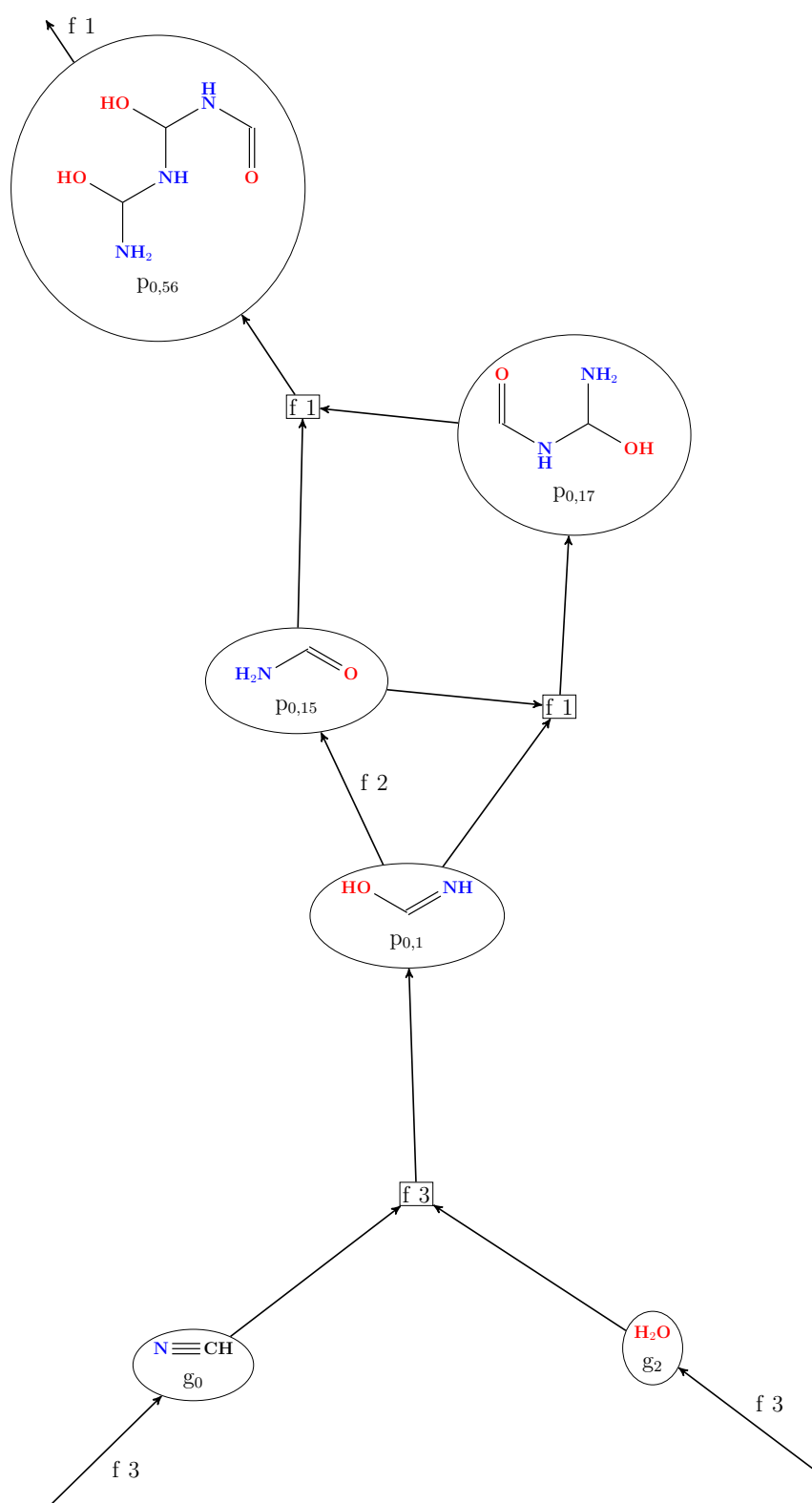## 0.3.18 Solution 17

Overall Data

```
Objective value (non-integral): -0.0655467
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  32
p_{0,17}      0  0   -21.248882 1.000000  34
p_{0,1}       0  0   -10.610101 1.000000  1
p_{0,56}      0  1   -31.869324 -3.000000 67
```

Filtered Graph

f 1

HO

H
N

HO

NH

O

NH₂

$p_{0,56}$

f 1

O

NH₂

N
H

OH

$p_{0,17}$

H₂N

O

$p_{0,15}$

f 1

f 2

HO

NH

$p_{0,1}$

f 3

N≡CH

g_0

H₂O

g_2

f 3

f 3

File: `out/184_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
$p_{0,15}$	0	0	-27896.445756	1.0	-27893.119971	32
$p_{0,17}$	0	0	-55788.930843	1.0	-55785.605058	34
$p_{0,56}$	0	1	-83672.898792	-3.0	-83682.876147	67

Hyperedge	Source	Target	Flow	$x_e^{\Delta G}$	$\overline{x}_e^{\Delta G}$
6	$g_0, g_2,$	$p_{0,1},$	3	-94.140854	-94.140854
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	-38.162372	-38.162372
Sum					-172.09285116806703

ΔG = -39.98362163825635

ΔE = -0.06554670531287954

|E| = 7

|U| = 4