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}

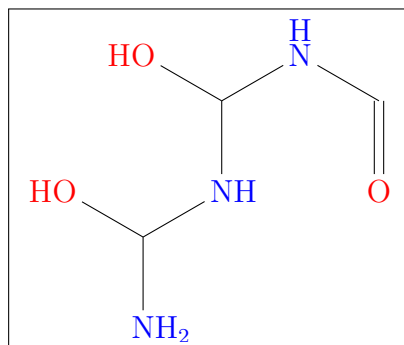File: out/009_g_2_10300000

$$H_2O$$

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): -0.100346
Vertex/Graph In Out G          logK      t_order
g_{0}        3  0   -5.507141  -3.000000 0
g_{2}        3  0   -5.068043  -3.000000 0
p_{0,13}     0  0   -21.240635 -3.000000 64
p_{0,15}     0  0   -10.625174 -6.000000 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 -6.000000 63
```

Filtered Graph
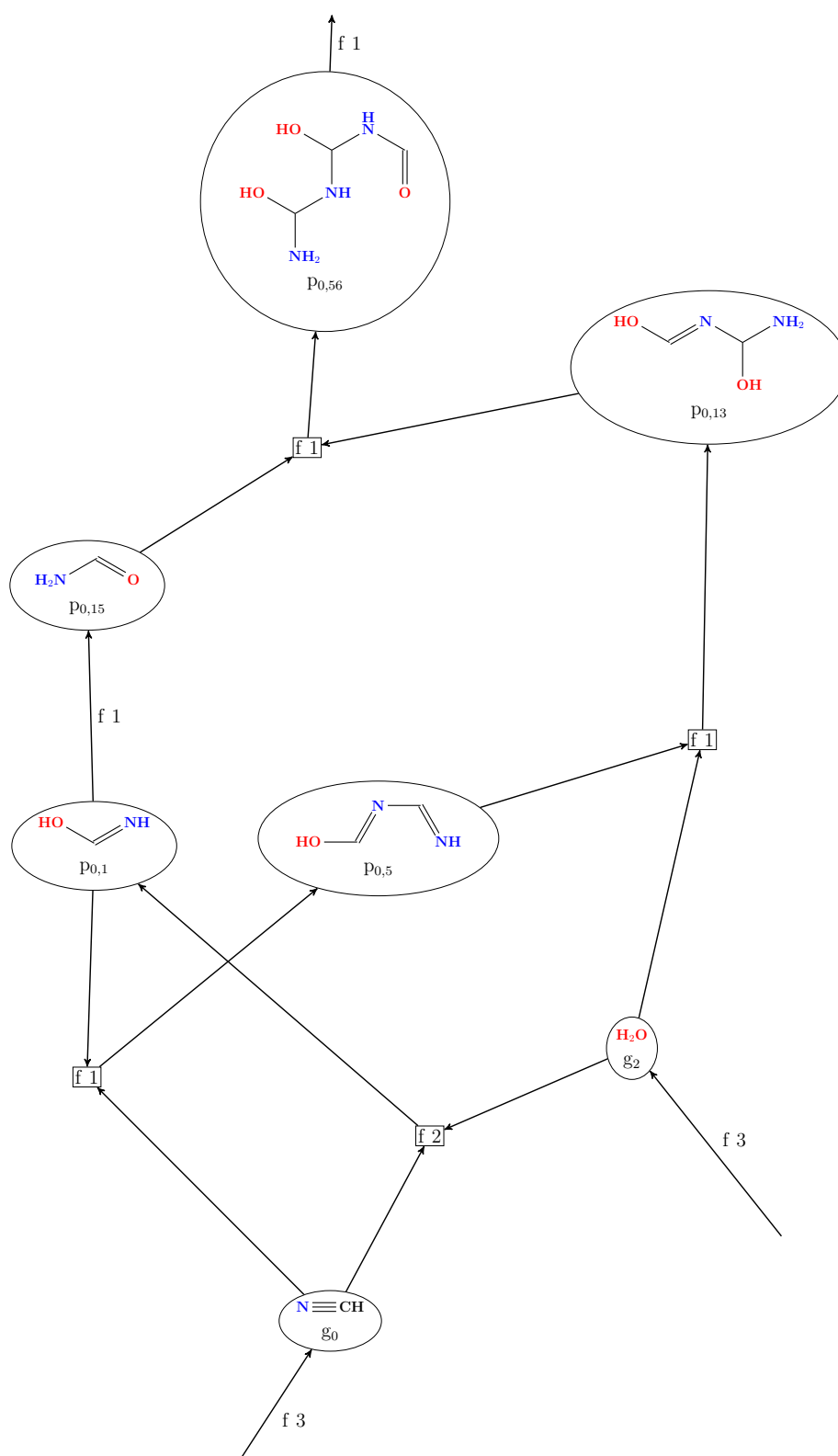
File: `out/029_dg_0_11100_f_0_0_filt`

Vertex	InFlow	OutFlow	$x_v^{\Delta G^0}$	x_v^K	$x_v^{\Delta G}$	t_v
g_0	3	0	-14458.99666	-3.0	-14468.974015	0
g_2	3	0	-13306.144961	-3.0	-13316.122316	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,5}$	0	0	-42425.44262	-6.0	-42445.397331	63
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	64
$p_{0,15}$	0	0	-27896.389963	-6.0	-27916.344673	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	-84.192417	-84.192417
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-109.628906	-109.628906
36	$p_{0,1},$	$p_{0,15},$	1	-47.055925	-47.055925
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-20.72598	-20.72598
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-1.746218	-1.746218
Sum					-263.4583849519488

ΔG = -34.75418585038536

ΔE = -0.10034599928725518

|E| = 6

|U| = 5

0.3.2   Solution 1
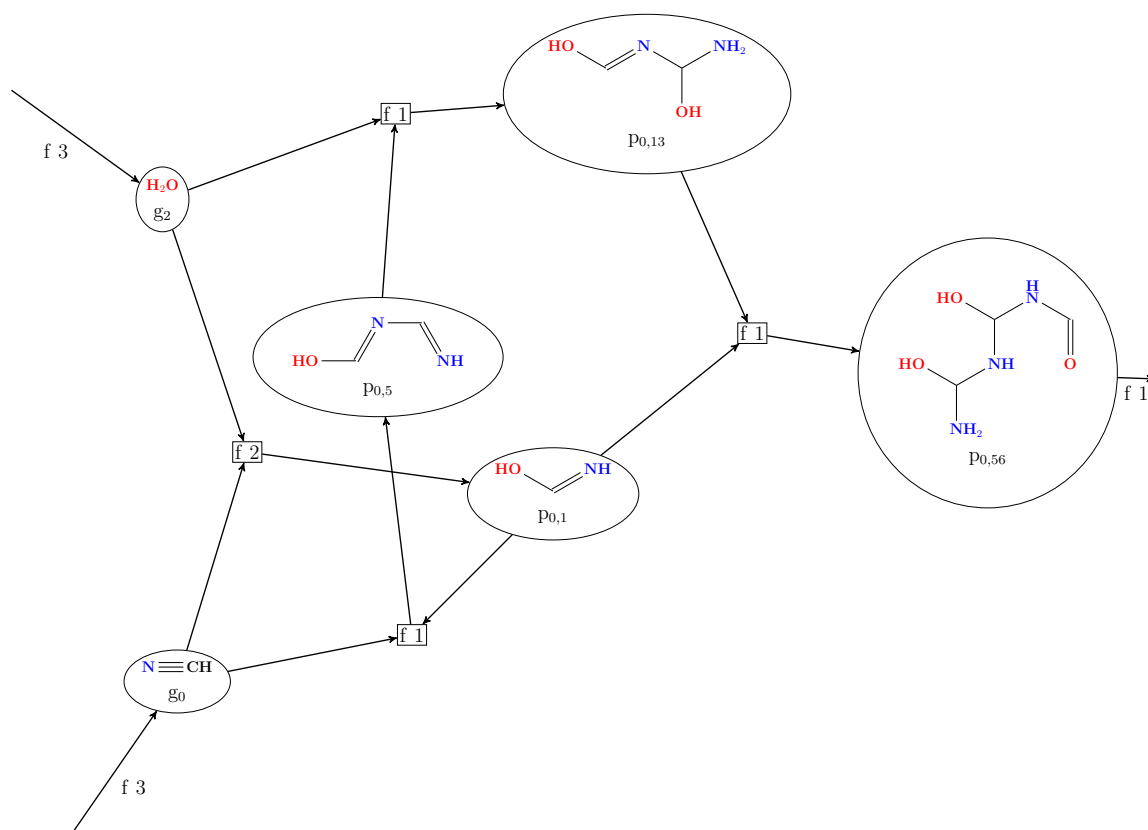
Overall Data

```
Objective value (non-integral): -0.100346
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   -21.240678 -6.000000 34
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 33
```

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	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,5}$	0	0	-42425.44262	-6.0	-42445.397331	33
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	34
$p_{0,56}$	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	-69.197466	-69.197466
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-102.116972	-102.116972
123	$g_2, p_{0,5},$	$p_{0,13},$	1	-20.837515	-20.837515
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-41.207592	-41.207592
Sum					-263.4583849519478

ΔG = -30.255700976893987

ΔE = -0.100345999287254

|E| = 5

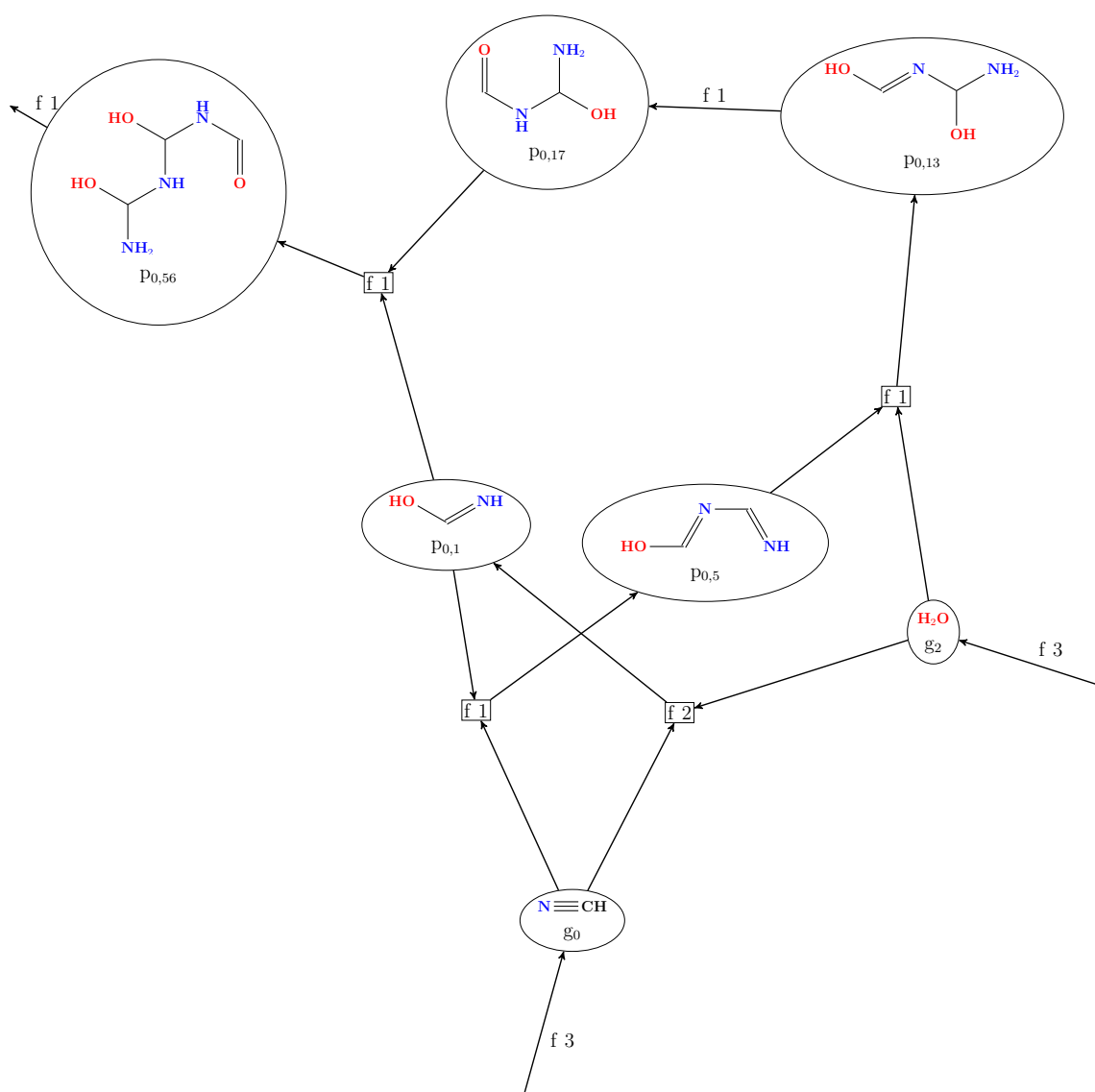|U| = 4

0.3.3 Solution 2

Overall Data

```
Objective value (non-integral): -0.100346
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   -21.240678 -3.000000  3
p_{0,17}     0  0   -21.248887 -6.000000  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/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	-13306.118349	-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	-55767.391129	-3.0	-55777.368484	3
$p_{0,17}$	0	0	-55788.944315	-6.0	-55808.899025	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	-84.190111	-84.190111
14	$g_0, p_{0,1},$	$p_{0,5},$	1	-109.599988	-109.599988
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	-19.654406	-19.654406
250	$p_{0,13},$	$p_{0,17},$	1	-29.036202	-29.036202
Sum					-263.45838495194414

ΔG = -34.7534937686804

ΔE = -0.1003459992872534

|E| = 6

|U| = 5

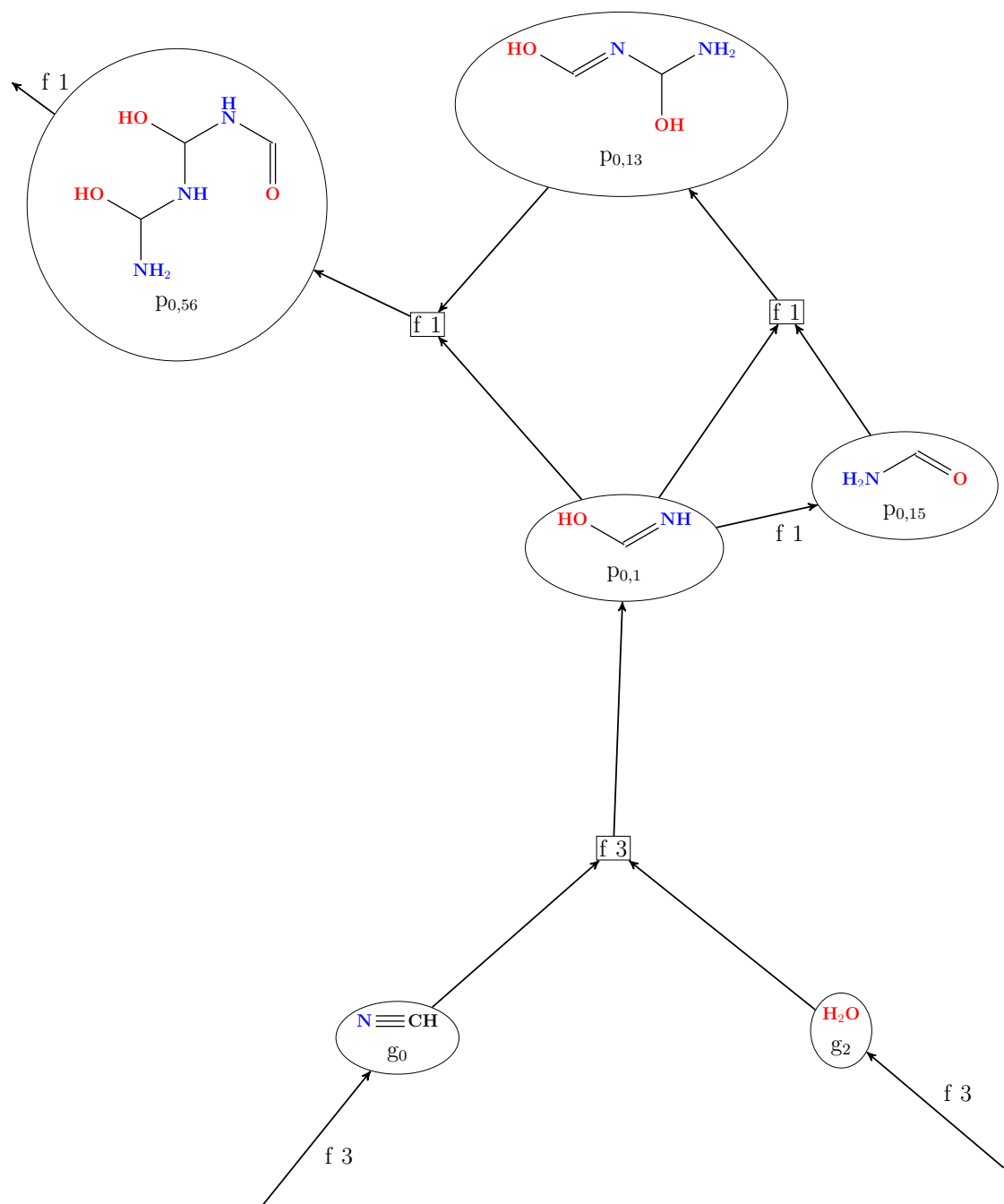## 0.3.4 Solution 3

Overall Data

```
Objective value (non-integral): -0.0682899
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   -21.240678 -6.000000 65
p_{0,15}     0  0   -10.625174 -6.000000 33
p_{0,1}      0  0   -10.610101 -5.688972 1
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	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.817054	-5.688972	-27875.737354	1
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	65
$p_{0,15}$	0	0	-27896.389963	-6.0	-27916.344673	33
$p_{0,56}$	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	-75.904675	-75.904675
36	$p_{0,1},$	$p_{0,15},$	1	-40.348717	-40.348717
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	-26.850022	-26.850022
Sum					-179.29506906107235

$\Delta G = -29.490664250894866$

$\Delta E = -0.0682898852336476$

$|E| = 6$

$|U| = 4$
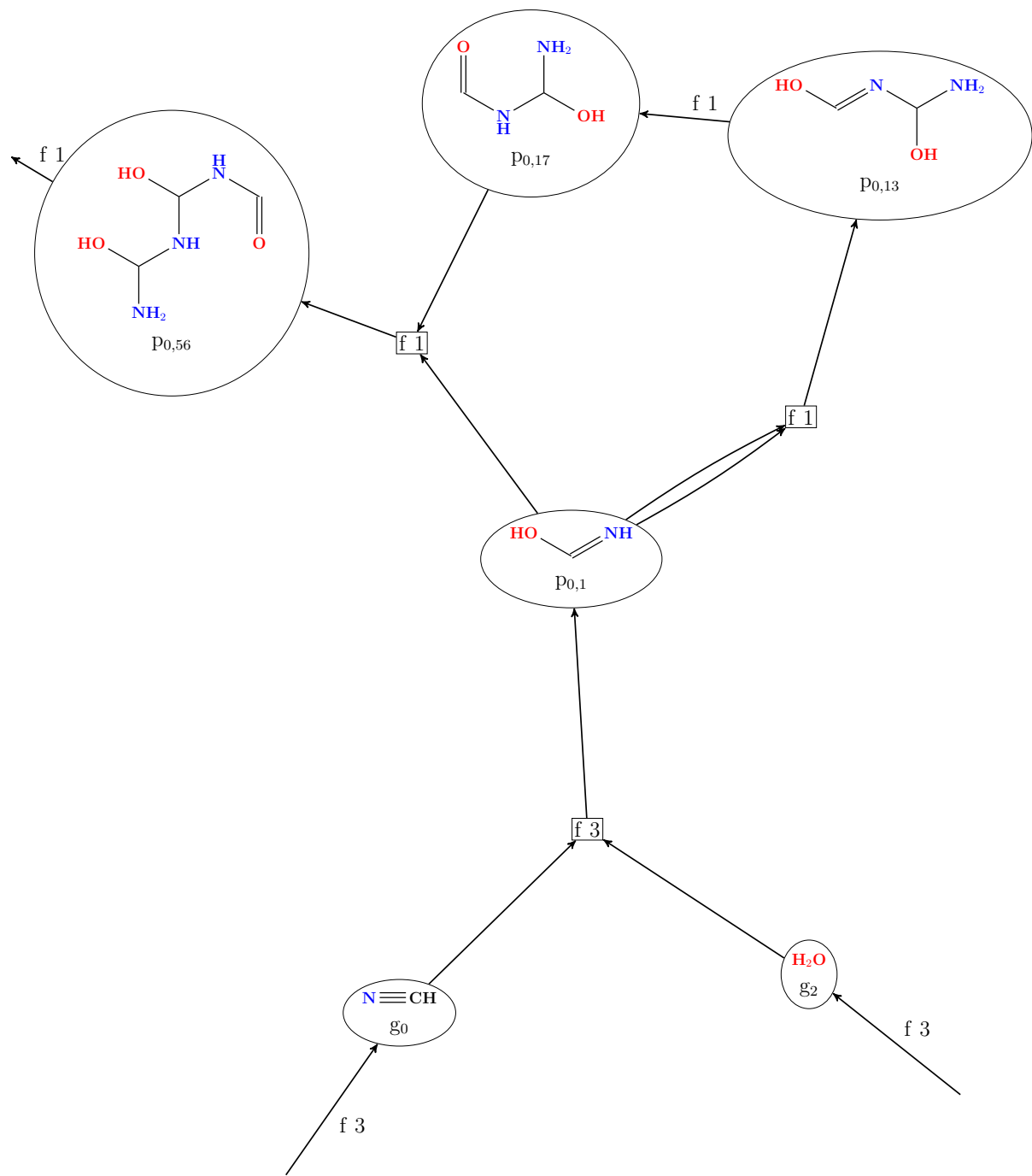
0.3.5 Solution 4

Overall Data

```
Objective value (non-integral): -0.0682899
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_{0,17}     0  0   -21.248844 -3.000000 65
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
$p_{0,17}$	0	0	-55788.832737	-3.0	-55798.810092	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	$g_0, g_2,$	$p_{0,1},$	3	-69.168365	-69.168365
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-46.273896	-46.273896
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-27.304714	-27.304714
250	$p_{0,13},$	$p_{0,17},$	1	-21.553143	-21.553143
Sum					-179.29506906107076

ΔG = -30.263683808547825
ΔE = -0.068289885233647
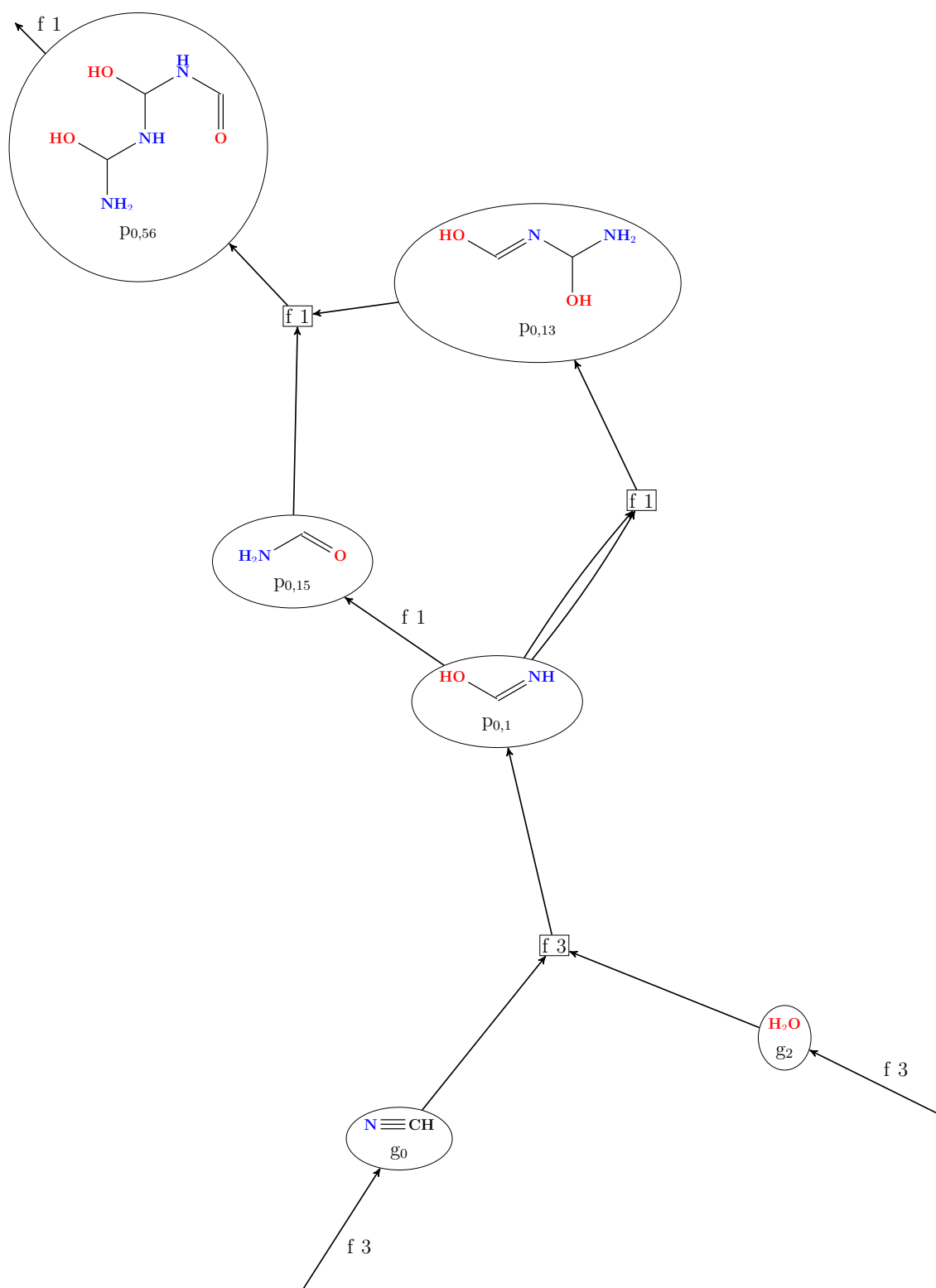|E| = 6
|U| = 4

0.3.6 Solution 5

Overall Data

```
Objective value (non-integral): -0.0682899
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 -3.635441 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 -3.000000 67
```

f 1

HO
H
N
HO
NH
NH₂
O

p₀,₅₆

HO
N
NH₂
OH

p₀,₁₃

f 1

f 1

H₂N
O

p₀,₁₅

f 1

f 1

HO
NH

p₀,₁

f 3

H₂O
g₂

f 3

N≡CH
g₀

f 3

File: `out/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	-6.0	-14478.980288	0
g_2	3	0	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.817054	-3.0	-27866.79441	1
$p_{0,13}$	0	0	-55767.391129	-3.635441	-55779.481823	3
$p_{0,15}$	0	0	-27896.445756	-3.0	-27906.423111	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	-69.224079	-69.224079
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-47.859008	-47.859008
36	$p_{0,1},$	$p_{0,15},$	1	-39.628701	-39.628701
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	0.006113	0.006113
Sum					-179.2950690610697

ΔG = -29.515383067450603
ΔE = -0.0682898852336466
|E| = 6
|U| = 4

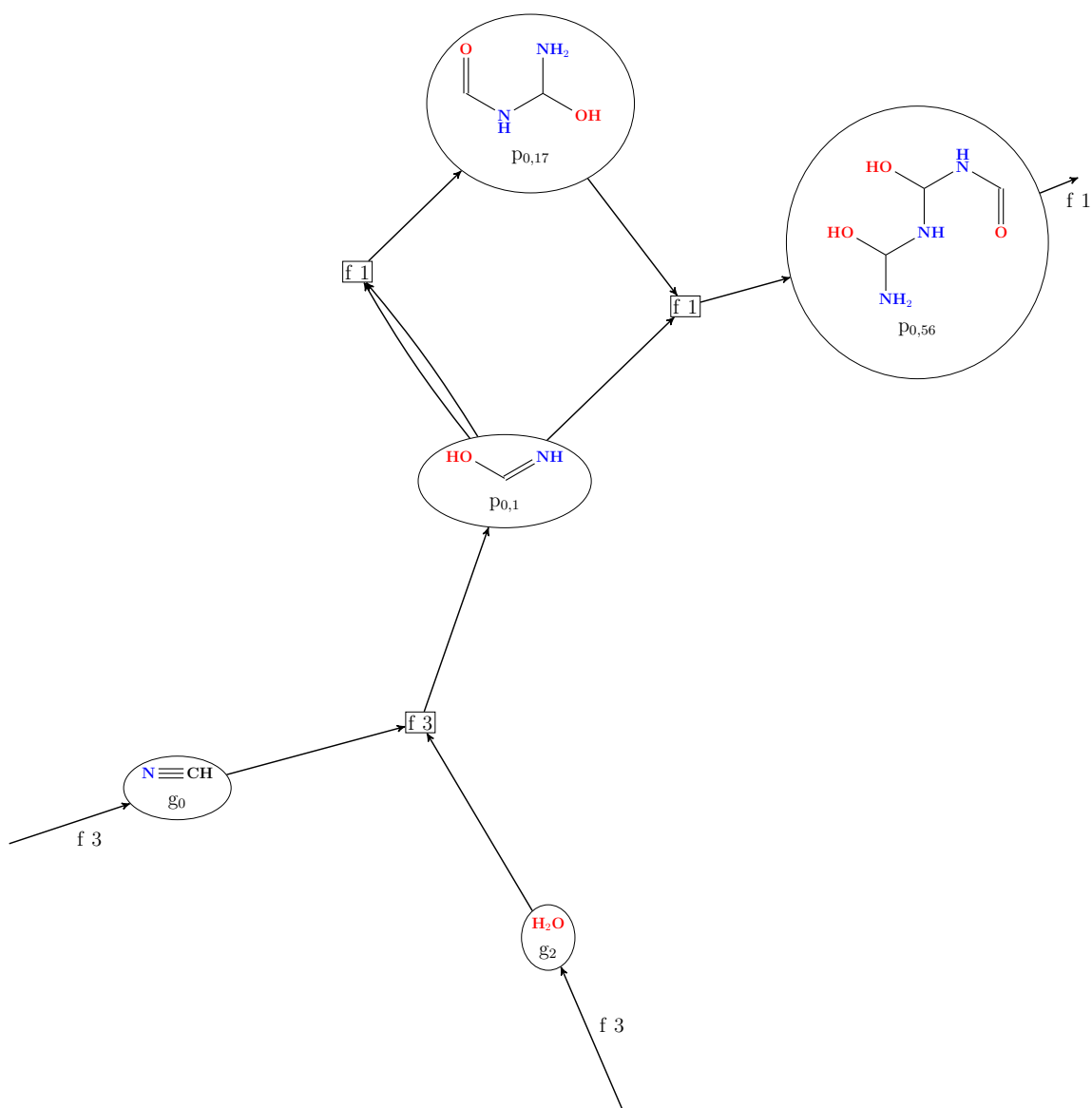### 0.3.7 Solution 6

Overall Data

```
Objective value (non-integral): -0.0682899
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_{0,17}     0  0   -21.248844 -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/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	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	1
$p_{0,17}$	0	0	-55788.832737	-3.0	-55798.810092	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	-76.624769	-76.624769
40	$p_{0,1}, p_{0,1},$	$p_{0,17},$	1	-67.827039	-67.827039
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-27.304714	-27.304714
Sum					-179.2950690610687

$\Delta G = $ -32.50060556313533

$\Delta E = $ -0.06828988523364621

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

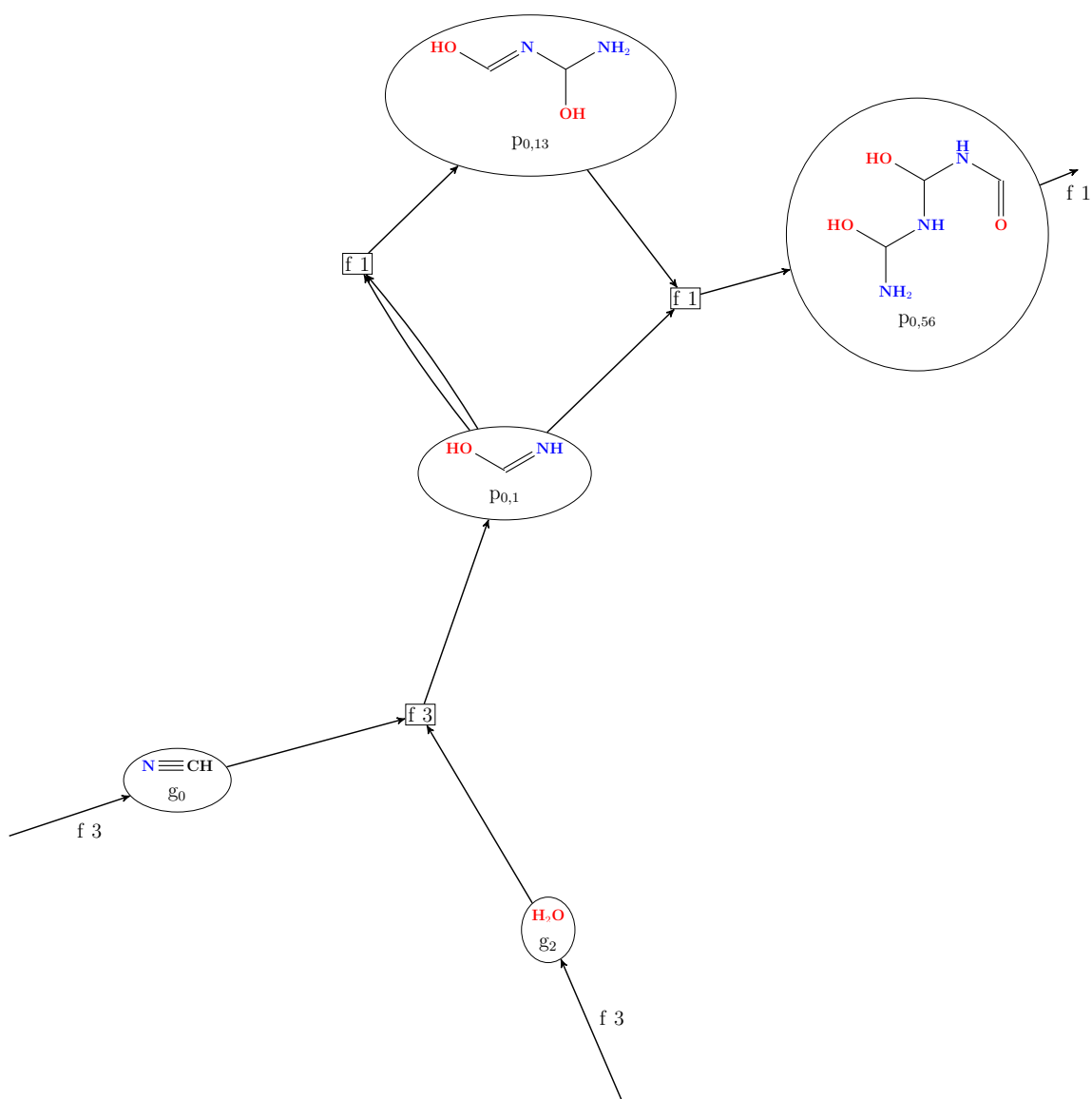### 0.3.8 Solution 7

Overall Data

```
Objective value (non-integral): -0.0682899
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 45
p_{0,1}     0  0   -10.610080 -3.000000 21
p_{0,56}    0  1   -31.869324 -6.000000 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	-13306.118349	-6.0	-13326.073059	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	21
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	45
$p_{0,56}$	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	-69.168365	-69.168365
30	$p_{0,1}, p_{0,1},$	$p_{0,13},$	1	-46.273896	-46.273896
263	$p_{0,1}, p_{0,13},$	$p_{0,56},$	1	-48.857857	-48.857857
Sum					-179.2950690610687

ΔG = -30.263683808547825

ΔE = -0.06828988523364621

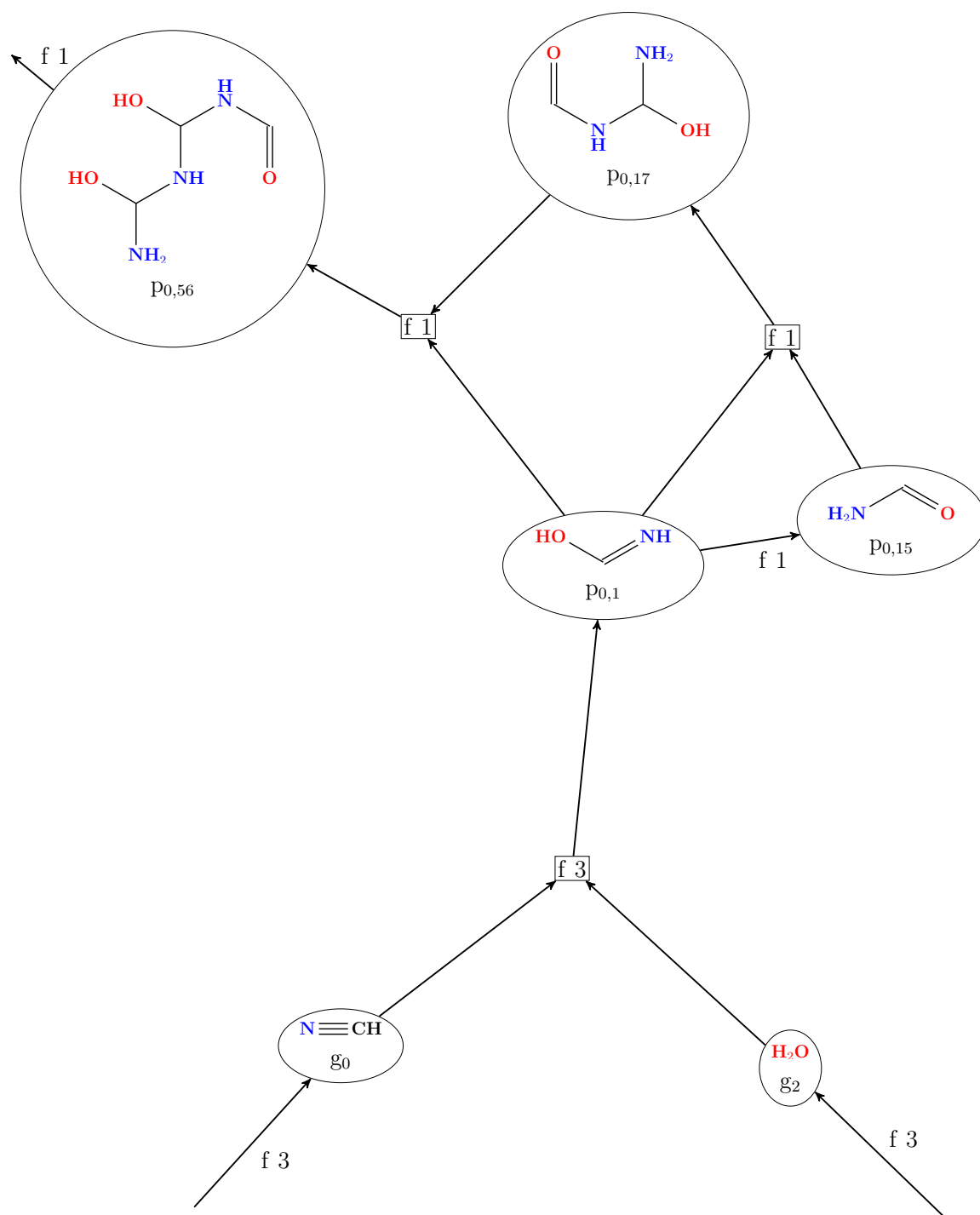$|E| = 5$

$|U| = 3$

0.3.9   Solution 8

Overall Data

```
Objective value (non-integral): -0.0682899
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_{0,15}     0  0   -10.625195 -6.000000 22
p_{0,17}     0  0   -21.248844 -3.000000 44
p_{0,1}      0  0   -10.610080 -3.000000 21
p_{0,56}     0  1   -31.869324 -6.000000 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	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	21
$p_{0,15}$	0	0	-27896.445756	-6.0	-27916.400466	22
$p_{0,17}$	0	0	-55788.832737	-3.0	-55798.810092	44
$p_{0,56}$	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	-69.141753	-69.141753
36	$p_{0,1},$	$p_{0,15},$	1	-47.167431	-47.167431
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	-27.304714	-27.304714
Sum					-179.2950690610697

ΔG = -30.255700189244095
ΔE = -0.0682898852336466
|E| = 6
|U| = 4
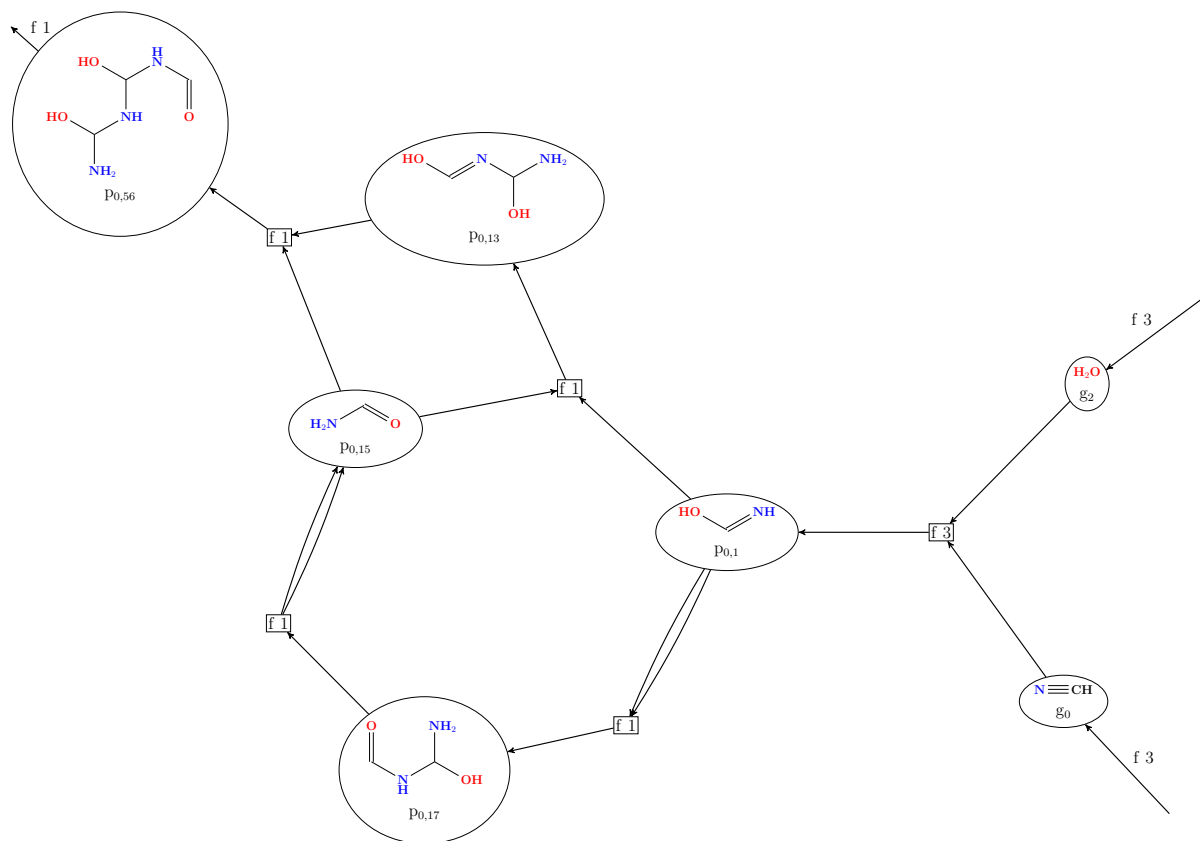
0.3.10 Solution 9

Overall Data

```
Objective value (non-integral): -0.0682899
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 -4.984418 39
p_{0,15}     0  0   -10.625174 -4.673390 27
p_{0,17}     0  0   -21.248887 -6.000000 26
p_{0,1}      0  0   -10.610101 -6.000000 11
p_{0,56}     0  1   -31.869324 -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	-3.0	-14469.002933	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.817054	-6.0	-27876.771765	11
$p_{0,13}$	0	0	-55767.391129	-4.984418	-55783.968232	39
$p_{0,15}$	0	0	-27896.389963	-4.67339	-27911.932655	27
$p_{0,17}$	0	0	-55788.944315	-6.0	-55808.899025	26
$p_{0,56}$	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	-84.163499	-84.163499
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	-12.183616	-12.183616
Sum					-179.29506906106667

ΔG = -32.50060530058536

ΔE = -0.06828988523364543

|E| = 7

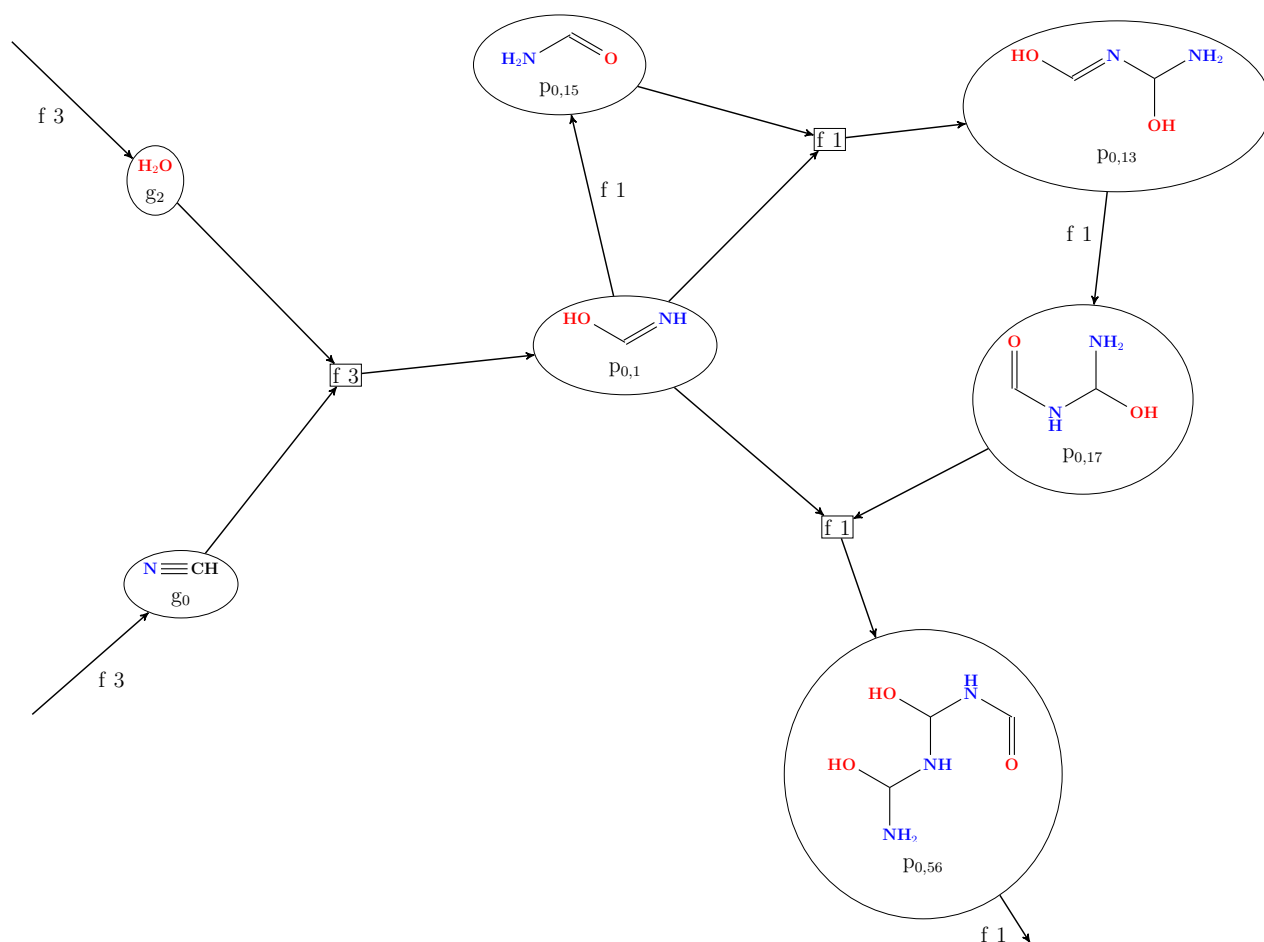|U| = 5

0.3.11 Solution 10

Overall Data

```
Objective value (non-integral): -0.0682899
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 -3.000000  4
p_{0,15}      0  0   -10.625174 -5.666593  2
p_{0,17}      0  0   -21.248887 -3.000000  65
p_{0,1}       0  0   -10.610080 -3.000000  1
p_{0,56}      0  1   -31.869324 -6.000000  67
```

Filtered Graph

File: `out/121_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	-6.0	-14478.980288	0
g_2	3	0	-13306.144961	-6.0	-13326.099672	0
$p_{0,1}$	0	0	-27856.761341	-3.0	-27866.738696	1
$p_{0,13}$	0	0	-55767.279594	-3.0	-55777.256949	4
$p_{0,15}$	0	0	-27896.389963	-5.666593	-27915.235834	2
$p_{0,17}$	0	0	-55788.944315	-3.0	-55798.92167	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	$g_0, g_2,$	$p_{0,1},$	3	-69.141753	-69.141753
36	$p_{0,1},$	$p_{0,15},$	1	-46.280009	-46.280009
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	0.006113	0.006113
196	$p_{0,1}, p_{0,17},$	$p_{0,56},$	1	-27.193136	-27.193136
250	$p_{0,13},$	$p_{0,17},$	1	-21.664721	-21.664721
Sum					-179.29506906106408

ΔG = -30.255700189244095
ΔE = -0.06828988523364445
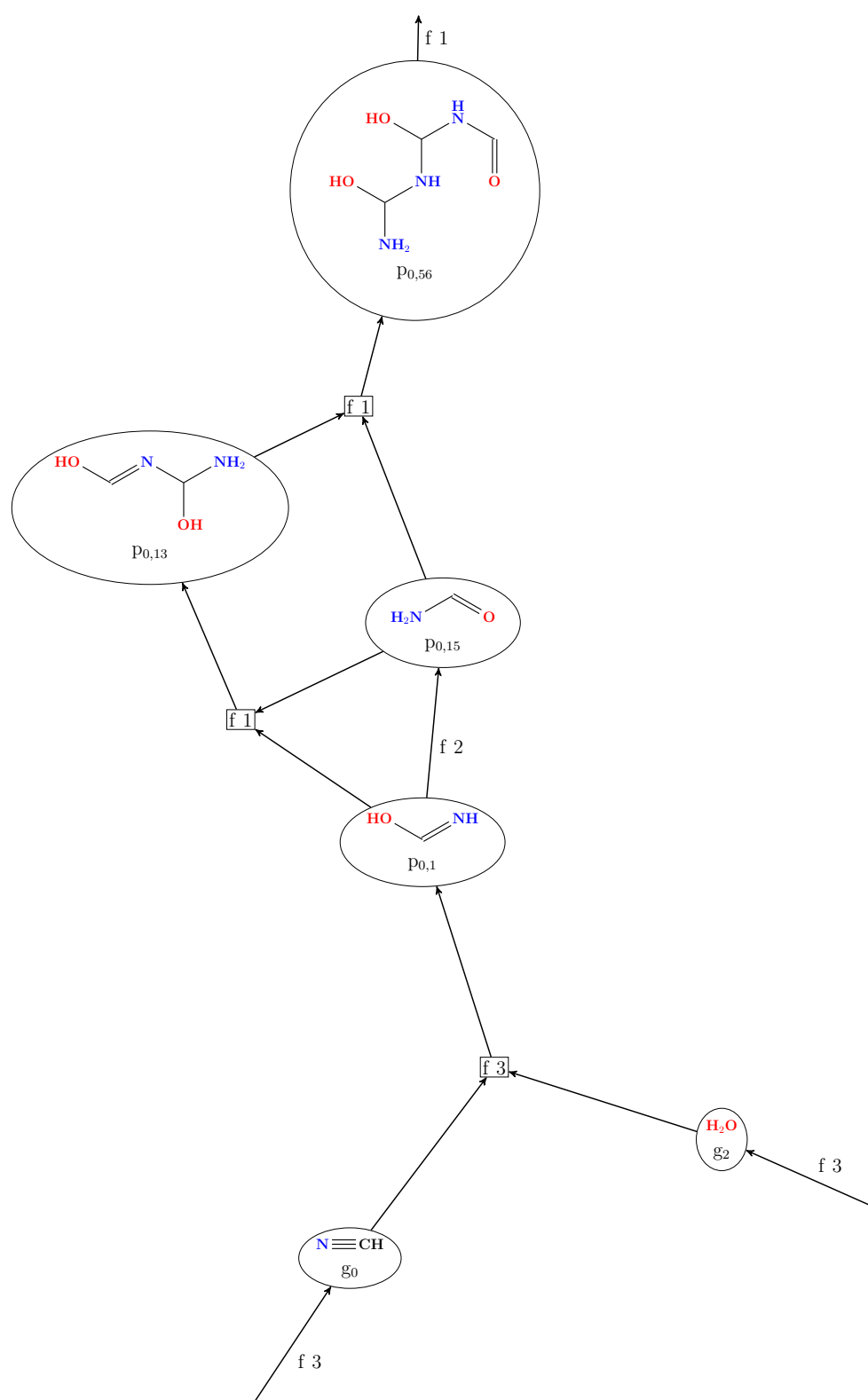|E| = 7
|U| = 5

0.3.12   Solution 11

Overall Data

```
Objective value (non-integral): -0.0531961
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 44
p_{0,15}     0  0   -10.625174 -3.000000 22
p_{0,1}      0  0   -10.610080 -3.000000 21
p_{0,56}     0  1   -31.869324 -6.000000 67
```

Filtered Graph

f 1

HO   N H

HO   NH   O

NH₂

$p_{0,56}$

HO   N NH₂

OH

$p_{0,13}$

f 1

H₂N O

$p_{0,15}$

f 1

f 2

HO   NH

$p_{0,1}$

f 3

H₂O

g_2

f 3

N≡CH

g_0

f 3

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	-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	21
$p_{0,13}$	0	0	-55767.391129	-6.0	-55787.345839	44
$p_{0,15}$	0	0	-27896.389963	-3.0	-27906.367318	22
$p_{0,56}$	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	-84.107786	-84.107786
36	$p_{0,1},$	$p_{0,15},$	2	-39.628622	-39.628622
169	$p_{0,13}, p_{0,15},$	$p_{0,56},$	1	-1.634684	-1.634684
192	$p_{0,1}, p_{0,15},$	$p_{0,13},$	1	-14.239825	-14.239825
Sum					-139.66644695727257

ΔG = -34.74551014937667

ΔE = -0.053196140215404704

|E| = 7

|U| = 4