

(a)

```
> info('LYSC_CHICK')
protein: found LYSC_CHICK (C613H959N1930185S10, 129 residues).
info: 3021 refers to LYSC_CHICK, C613H959N1930185S10 aq (BBA+03).
> info(3021)
      name abbrv      formula state source1 source2 date      G      H
3021 LYSC_CHICK <NA> C613H959N1930185S10 aq BBA+03 <NA> <NA> -4206050 -10369700
      S      Cp      V      a1      a2      a3      a4      c1      c2      omega Z
3021 4175.86 6415.553 10420.89 251.258 34588 450.87 -4095000 7768.7 -7015000 -794000 0
```

(b)

```
> subcrt('LYSC_CHICK')
subcrt: 1 species at 15 values of T and P (wet).
$species
      name      formula state ispecies
3021 LYSC_CHICK C613H959N1930185S10 aq 3021
$out
$out$LYSC_CHICK
      T      P      rho      logK      G      H      S      V      Cp
1 0.01 1.000000 0.9998289 3286.749 -4108100 -10510350 3684.406 10049.21 4409.319
2 25.00 1.000000 0.9970614 3083.063 -4206050 -10369700 4175.860 10420.95 6415.518
3 50.00 1.000000 0.9880295 2919.759 -4317263 -10199867 4722.506 10600.23 7073.981
4 75.00 1.000000 0.9748643 2788.465 -4442106 -10018826 5261.992 10708.15 7376.581
5 100.00 1.013220 0.9583926 2682.511 -4580176 -9832092 5779.892 10782.93 7548.444
6 125.00 2.320144 0.9390726 2596.618 -4730554 -9641537 6273.262 10840.94 7665.198
7 150.00 4.757169 0.9170577 2526.937 -4892670 -9448098 6742.892 10891.15 7760.881
8 175.00 8.918049 0.8923427 2470.400 -5065799 -9251881 7190.897 10940.05 7856.945
9 200.00 15.536499 0.8647434 2424.600 -5249238 -9052464 7620.111 10994.29 7974.628
10 225.00 25.478603 0.8338733 2387.629 -5442322 -8848798 8034.140 11063.40 8146.453
11 250.00 39.736493 0.7990719 2357.970 -5644451 -8638774 8438.039 11165.02 8439.891
12 275.00 59.431251 0.7592362 2334.423 -5855127 -8417956 8840.380 11338.89 9030.924
13 300.00 85.837843 0.7124075 2316.077 -6074053 -8175407 9259.928 11694.88 10513.444
14 325.00 120.457572 0.6545772 2302.355 -6301438 -7875355 9754.686 12644.61 15882.325
15 350.00 165.211289 0.5746875 2293.455 -6539432 -7308661 10654.664 17027.35 60917.017
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(c)

```
> basis('CHNOS')
      C H N O S ispecies logact state
CO2 0 0 0 2 0 69 -3 aq
H2O 0 2 0 1 0 1 0 liq
NH3 0 3 1 0 0 68 -4 aq
H2S 0 2 0 0 1 70 -7 aq
O2 0 0 0 2 0 2469 -80 gas
> subcrt(c('CSG_METVO', 'CSG_METJA'), c(-1/553, 1/530), T=c(25, 50, 100))
protein: found CSG_METVO (C2575H4097N6450884S11, 553 residues).
protein: found CSG_METJA (C2555H4032N6400865S14, 530 residues).
subcrt: 2 species at 3 values of T and P (wet).
subcrt: reaction is not balanced; it is missing this composition:
      C      H      N      O      S
-0.1643352 -0.1988672 -0.04118189 -0.03352213 -0.006523593
subcrt: adding missing composition from basis definition and restarting...
subcrt: 7 species at 3 values of T and P (wet).
$reaction
      coeff      name      formula state ispecies
3022 -0.001808318 CSG_METVO C2575H4097N6450884S11 aq 3022
3023 0.001886792 CSG_METJA C2555H4032N6400865S14 aq 3023
69 -0.164335187 CO2 CO2 aq 69
1 -0.031137193 water H2O liq 1
68 -0.041181890 NH3 NH3 aq 68
70 -0.006523593 H2S H2S aq 70
2469 0.163142721 oxygen O2 gas 2469
$out
      T      P      logK      G      H      S      V      Cp
1 25 1.000000 -12.09114 16495.26 17332.75 2.824065 -4.911481 -7.379423
2 50 1.000000 -11.11283 16431.84 17160.39 2.268477 -5.114446 -6.544202
3 100 1.013222 -9.57098 16341.70 16848.21 1.369472 -5.355989 -6.080541
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