Supporting Information for R. A. Alberty "Calculation of Thermodynamic Properties of Species of Biochemical Reactants Using the Inverse Legendre Transform"

The calculation of $\Delta_f G^\circ$ (298.15 K, $I=0$) and $\Delta_f H^\circ$ (298.15 K, $I=0$) for species of reactants in enzyme-catalyzed reactions involves six programs, four of which are published in this article. These programs produce small matrices with a row \{ $\Delta_f G^\circ$, $\Delta_f H^\circ$, $z_1$, $N_{H1}$ \} for each species. The first three programs produce \{ $\Delta_f G^\circ$, $\_1$, $z_1$, $N_{H1}$ \}, and the second three programs fill in the $\Delta_f H^\circ$ (298.15 K, $I=0$).

These calculations use calcGef2sp and calxdGf3sp that are in BasicBiochemicalData2. http://library.wolfram.com/in/Content/MathSource/797

Data on species required in these calculations have been taken from BasicBiochemical Data2 and subsequent publications.

The six programs, which are based on the concept of the inverse Legendre transform, are as follows:

```math
calcGef1sp[equat_, pHc_, ionstr_, z1_, nH1_] :=
Module[{energy, trGereactant, gef1}, (*This program uses $\Sigma \Delta f_{Gi}^{\circ}=-RT\ln K'$ to calculate the standard Gibbs energy of formation of the species of a reactant that does not have a pK in the range 4 to 10. The equation is of the form pyruvate+atp-x-adp==-8.31451*.29815*Log[K'], where K' is the apparent equilibrium constant at 298.15 K, pHc, and ionic strength is. The reactant has charge number z1 and hydrogen atom number nH1. The output is the species vector without the standard enthalpy of formation.*)
energy = Solve[equat, x] /. pH -> pHc /. is -> ionstr;
trGereactant = energy[[1,1,2]]; gef1 = trGereactant - nH1*8.31451*0.29815*Log[10]*pHc + (2.91482*(z1^2 - nH1)*ionstr^0.5)/(1 + 1.6*ionstr^0.5); {{gef1, _, z1, nH1}}

calcGef2sp[equat_, pHc_, ionstr_, z1_, nH1_, pK0_] :=
Module[{energy, trGereactant, pKe, trgefpHis, gef1, gef2}, (*This program uses $\Sigma \Delta f_{Gi}^{\circ}=-RT\ln K'$ to calculate the standard Gibbs energies of formation of the two species of a reactant for which the pK at zero ionic strength is pK0. The equation is of the form pyruvate+atp-x-adp==-8.31451*.29815*Log[K'], where K' is the apparent equilibrium constant at 298.15 K, pHc, and ionic strength is. The more basic form of the reactant has charge number z1 and hydrogen atom number nH1. The output is the species matrix without the standard enthalpies of formation.*)
energy = Solve[equat, x] /. pH -> pHc /. is -> ionstr;
trGereactant = energy[[1,1,2]]; pKe = pK0 + (0.510651*ionstr^0.5*2*z1)/(1 + 1.6*ionstr^0.5); trgefpHis = trGereactant + 8.31451*0.29815*Log[1 + 10^(pKe - pHc)];
gef1 = trgefpHis - nH1*8.31451*0.29815*Log[10]*pHc + (2.91482*(z1^2 - nH1)*ionstr^0.5)/(1 + 1.6*ionstr^0.5); gef2 = gef1 + 8.31451*0.29815*Log[10]^(-pK0)); {{gef1, _, z1, nH1}, {gef2, _, z1 + 1, nH1 + 1}}
```
calcGef3sp[equat_, pHc_, ionstr_, z1_, nH1_, pK10_, pK20_] := Module[{energy, trGereactant, pKe, trgefpHis, gef1, gef2, gef3, pK1e, pK2e}, (*This program uses $\sum \Delta f_{i}' = -RT\ln K$ to calculate the standard Gibbs energies of formation of the three species of a reactant for which the pKs at zero ionic strength is pK10 and pK20. The equation is of the form pyruvate+atp-x-adp==-8.31451*0.29815*Log[K'], where K' is the apparent equilibrium constant at 298.15 K, pHc, and ionic strength is. The more basic form of the reactant has charge number z1 and hydrogen atom number nH1. The output is the species matrix without the standard enthalpies of formation of the three species.*)

energy = Solve[equat, x] /. pH -> pHc /. is -> ionstr;
trGereactant = energy[[1, 1, 2]];
pK1e = pK10 + (0.510651*ionstr^0.5*2*z1)/(1 + 1.6*ionstr^0.5);
pK2e = pK20 + (0.510651*ionstr^0.5*(2*z1 + 2))/(1 + 1.6*ionstr^0.5);
trgefpHis = trGereactant + 8.31451*0.29815*
Log[1 + 10^(-pK1e - pHc) + 10^(pK1e + pK2e - 2*pHc)];
gef1 = trgefpHis - nH1*8.31451*0.29815*Log[10]*pHc +
(2.91482*(z1^2 - nH1)*ionstr^0.5)/(1 + 1.6*ionstr^0.5);
gef2 = gef1 + 8.31451*0.29815*Log[10^(-pK10)];
gef3 = gef2 + 8.31451*0.29815*Log[10^(-pK20)];
{{gef1, _, z1, nH1}, {gef2, _, z1 + 1, nH1 + 1},
{gef3, _, z1 + 2, nH1 + 2}}]
calcHf1sp[equat_, spmat_, pHc_, ionstr_] := Module[{energy, trHreactant, enthf1, gef1, dHzero1, z1, nH1}, (*This program uses $\sum \Delta f_{i}' = -\Delta rH'$ (298.15 K) to calculate the standard enthalpy of formation (I=0) of the single species of a reactant for which the species matrix (spmat) contains $\Delta f_{i}'$ at zero ionic strength. The reaction equation (equat) is of the form x+nadredh-malateh-nadoxh==89.5, where 89.5 kJ mol^-1 is the heat of reaction and x is oxaloacetate. The species matrix (spmat) is that for oxaloacetate. The calorimetric experiment is at pHc and ionic strength ionstr. The reactant x has charge number z1 and hydrogen atom number nH1. The output is the complete species matrix for x. 11-21-04*)

{gef1, dHserol, z1, nH1} = Transpose[spmat];
energy = Solve[equat, x] /. pH -> pHc /. is -> ionstr;
trHreactant = energy[[1, 1, 2]];
enthf1 = trHreactant - 1.4775*(z1^2 - nH1)*ionstr^0.5 *(1 + 1.6*ionstr^0.5);
{Flatten[{{gef1, enthf1, z1, nH1}}]}]
calcHf2sp[equat_, spmat_, pHc_, ionstr_, dHdisszero_] := 
Module[{dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp, energy},
  trHreactant, stdtrGereactant, r1, r2, solution, dH1zero, dH2zero, dH1, dH2},
  (*This program uses ∑viΔfH°=ΔH°(298.15 K) to calculate the standard enthalpy
   of formation (I=0) of the two species of a reactant for which the species
   matrix (spmat) contains ΔfG° at zero ionic strength for the two species of the
   reactant. The reaction equation (equat) is of the form mannoseh+pih-x-h2oh
   1.7, where 1.7 kJ mol^-1 is the heat of reaction and x is mannnose6phosh. The
   species matrix (spmat) is that for mannnose6phos. The calorimetric experiment
   is at pH_i and ionic strength ionstr. The first step in the calculation
   is to use the information on the standard Gibbs energies of formation of
   the species of the reactant of interest to calculate the equilibrium mole
   fractions r1 (base form) and r2 (acidform) of the two species of the reactant
   of interest. The final output is the complete species matrix for x.*)
  {dGzero, dHzero, zi, nHi} = Transpose[spmat];
  pHterm = nHi*8.31451*0.29815*Log[10^(-pH) - pH - pHc];
  isterm = 2.91482*((zi^2) - nHi)*(is^0.5) (1 + 1.6*is^0.5). is -> ionstr;
  gpfnsp = dGzero - pHterm - isterm;
  stdtrGereactant =
    -8.31451*0.29815*Log[Apply[Plus, Exp[-1*gpfnsp (8.31451*0.29815)]]];
  r1 = Exp[(stdtrGereactant - gpfnsp[[1]]) (8.31451*0.29815)];
  r2 = Exp[(stdtrGereactant - gpfnsp[[2]]) (8.31451*0.29815)];
  (*Now calculate dH° (reactant) from ΔH°(298.15 K) for the reaction.*)
  energy = Solve[equat, x] . pH -> pHc . is -> ionstr;
  trHreactant = energy[[1, 1, 2]];
  (*dH1zero is given by the following equation. dH2zero is
   calculated from the equation for the enthalpy of dissociation.*)
  solution = Solve[trHreactant ==
    r1*(dH1zero + 1.4775*(zi[[1]]^2 - nHi[[1]]))*ionstr^0.5
    + r2*(dH1zero - dHdisszero + 1.4775*(zi[[2]]^2 - nHi[[2]])*
      ionstr^0.5 (1 + 1.6*ionstr^0.5), dH1zero];
  dH1 = solution[[1, 1, 2]];
  dH2 = dH1 - dHdisszero;
  Transpose[{dGzero, {dH1, dH2}, zi, nHi}]
calcpropsspecies12-20-04.nb

The following six

gfns = pDzero, is term, pHterm = dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp, energy, trHreactant,

Module[(dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp, energy, trHreactant, stdtrGereactant, r1, r2, r3, solution, dH1zero, dH2zero, dH3zero, dH1expt, dH2expt, dH3expt, dH1, dH2, dH3), (*This program uses \( \sum_i \Delta H_i = \Delta H^\circ \) (298.15 K) to calculate the standard enthalpy of formation (I=0) of the

three species of a reactant for which the species matrix (spmat) contains \( \Delta fG^\circ \) at zero ionic strength for the three species of the reactant. The

reaction equation (equat) is of the form adpH-x-fructose6phos-atpm -84.2, where 84.2 kJ mol^-1 is the heat of reaction and x is fructose6phos. The

species matrix (spmat) is that for fructose6phos. The calorimetric experiment is at pH and ionic strength ionstr. The first step in the calculation is to

use the information on the standard Gibbs energies of formation of the species of the reactant of interest to calculate the equilibrium mole

fractions r1 (base form) and r2 (acidiform) of the two species of the reactant of interest. The final output is the complete species matrix for x.*)

{dGzero, dHzero, zi, nHi} = Transpose[spmat];

pHterm = nHi * 8.31451 * .29815 * Log[10^-pH] . pH -> pHc;

isterm = 2.91482 * ((zi^2) - nHi) * (is^-.5) (1 + 1.6 * is^-.5) . is -> ionstr;

gfns = dGzero - pHterm - isterm;

Module[(dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp, energy, trHreactant, stdtrGereactant, r1, r2, r3, solution, dH1zero, dH2zero, dH3zero, dH1expt, dH2expt, dH3expt, dH1, dH2, dH3), (*This program uses \( \sum_i \Delta H_i = \Delta H^\circ \) (298.15 K) to calculate the standard enthalpy of formation (I=0) of the

three species of a reactant for which the species matrix (spmat) contains \( \Delta fG^\circ \) at zero ionic strength for the three species of the reactant. The

reaction equation (equat) is of the form adpH-x-fructose6phos-atpm -84.2, where 84.2 kJ mol^-1 is the heat of reaction and x is fructose6phos. The calorimetric experiment is at pH and ionic strength ionstr. The first step in the calculation is to

use the information on the standard Gibbs energies of formation of the species of the reactant of interest to calculate the equilibrium mole

fractions r1 (base form) and r2 (acidiform) of the two species of the reactant of interest. The final output is the complete species matrix for x.*)

{dGzero, dHzero, zi, nHi} = Transpose[spmat];

pHterm = nHi * 8.31451 * .29815 * Log[10^-pH] . pH -> pHc;

isterm = 2.91482 * ((zi^2) - nHi) * (is^-.5) (1 + 1.6 * is^-.5) . is -> ionstr;

gfns = dGzero - pHterm - isterm;

trHreactant = energy[[1, 1, 2]];(*The standard transformed enthalpies of formation of the three

species are given by the following six equations. dH1zero, dH2zero, and dH3zero are also related by the equations for the enthalpy of dissociation.*)

solution = Solve[{dH1expt == dH1zero + 1.4775 * (z[i][[1]]^2 - nHi[[1]]) * ionstr^0.5 (1 + 1.6 * ionstr^0.5),

dH2expt == dH2zero + 1.4775 * (z[i][[2]]^2 - nHi[[2]]) * ionstr^0.5 (1 + 1.6 * ionstr^0.5),

dH3expt == dH3zero + 1.4775 * (z[i][[3]]^2 - nHi[[3]]) * ionstr^0.5 (1 + 1.6 * ionstr^0.5),

tHreactant == r1 * dH1expt + r2 * dH2expt + r3 * dH3expt,

dH1zero + dH2zero - dH3zero, dH1zero - dH3zero, dH2zero - dH3zero,}

{dH1zero, dH2zero, dH3zero, dH1expt, dH2expt, dH3expt}];

{dH1zero, dH2zero, dH3zero, dH1expt, dH2expt, dH3expt} = Transpose[{{dGzero, dHzero, zi, nHi}}];

dH3zero = Transpose[solution[[1, 1, 2]], solution[[1, 2, 2]]],

The following six programs are used in checking the calculations

calcdGmat[speciesmat_] :=

Module[(dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp), (*This program produces the function of pH and ionic strength (is) that gives the standard transformed Gibbs energy of formation of a reactant (sum of species) at 298.15 K. The input speciesmat is a matrix that gives the standard Gibbs energy of formation, the standard enthalpy of formation, the electric charge, and the number of hydrogen atoms in each species. There is a row in the matrix for each species of the reactant. gpfnsp is a list of the functions for the species. Energies are expressed in kJ mol^-1.*)

{dGzero, dHzero, zi, nHi} = Transpose[speciesmat];

pHterm = nHi * 8.31451 * .29815 * Log[10^-pH];

isterm = 2.91482 * ((zi^2) - nHi) * (is^-.5) (1 + 1.6 * is^-.5);

gfnsp = dGzero - pHterm - isterm;


The following six programs are used in checking the calculations

calcdGmat[speciesmat_] :=

Module[(dGzero, dHzero, zi, nHi, pHterm, isterm, gpfnsp), (*This program produces the function of pH and ionic strength (is) that gives the standard transformed Gibbs energy of formation of a reactant (sum of species) at 298.15 K. The input speciesmat is a matrix that gives the standard Gibbs energy of formation, the standard enthalpy of formation, the electric charge, and the number of hydrogen atoms in each species. There is a row in the matrix for each species of the reactant. gpfnsp is a list of the functions for the species. Energies are expressed in kJ mol^-1.*)

{dGzero, dHzero, zi, nHi} = Transpose[speciesmat];

pHterm = nHi * 8.31451 * .29815 * Log[10^-pH];

isterm = 2.91482 * ((zi^2) - nHi) * (is^-.5) (1 + 1.6 * is^-.5);

gfnsp = dGzero - pHterm - isterm;

calcHMat[speciesmat_] := Module[{dGzero, dHzero, zi, nH, dhfnsp, pHterm, isenth, dgfnsp, dGreactant, ri},
(*This program produces the function of ionic strength (is) that gives the standard transformed enthalpy of formation of a reactant (sum of species) at 298.15 K. The input is a matrix that gives the standard Gibbs energy of formation, the standard enthalpy of formation, the electric charge, and the number of hydrogen atoms in the species in the reactant. There is a row in the matrix for each species of the reactant. dhfnsp is a list of the functions for the species. Energies are expressed in kJ mol^-1.*)
{dGzero, dHzero, zi, nH} = Transpose[speciesmat];
isenth = 1.4775* ((zi^2) - nH) *(is^0.5) (1 + 1.6 *is^0.5);
dhfnsp = dHzero + isenth;
(*Now calculate the functions for the standard Gibbs energies of formation of the species.*)
dGzero = speciesmat[[All, 1]]; pHterm = nH*8.31451* .29815* Log[10^-pH];
gpfnsp = dGzero - pHterm - isenth*2.91482 1.44775;
(*Now calculate the standard transformed Gibbs energy of formation for the reactant.*)
(*Now calculate the equilibrium mole fractions of the species in the reactant and the mole fraction-weighted average of the functions for the standard transformed enthalpies of the species.*)
ri = Exp[(dGreactant - gpfnsp) (8.31451*.29815)];
ri.dhfnsp]
calcKprime[eq_, pHlist_, islist_] := Module[{energy, dG}, (*Calculates the apparent equilibrium constant at specified pHs and ionic strengths for a biochemical reaction typed in the form atp+h2o+de adp+pi. The names of reactants call the appropriate functions of pH and ionic strength. pHlist and islist can be lists.*)
energy = Solve[eq, de];
dG = energy[[1,1,2]] /. pH -> pHlist /. is -> islist; E^(-dG/(8.31451*0.29815))]
calcpK[speciesmat_, no_, is_] := Module[{lnkzero, sigmanuzsq, lnK}, (*Calculates pKs for a weak acid at 298.15 K at specified ionic strengths (is) when the number no of the pK is specified. pKs are numbered 1, 2, 3,... from the highest pK to the lowest pK, but the highest pK for a weak acid may be omitted if it is outside of the range 5 to 9. For h3PO4,
pK1=calcpK[species, pK1=0, 1.0] = 7.22.*)
lnkzero = (speciesmat[[no + 1,1]] - speciesmat[[no,1]])/(8.31451*0.29815);
sigmanuzsq = speciesmat[[no,3]]^2 - speciesmat[[no + 1,3]]^2 + 1;
lnK = lnkzero + (1.17582*is^0.5*sigmanuzsq)/ (1 + 1.6 *is^0.5); N[(-lnK/Log[10])]]
calctrGorHrx[eq_, pHlist_, islist_] := Module[{energy}, (*Calculates the standard transformed Gibbs energy of reaction in kJ mol^-1 at specified pHs and ionic strengths for a biochemical reaction typed in the form atp+h2o+de adp+pi. The names of reactants call the appropriate functions of pH and ionic strength. This program can also be used to calculate the standard transformed enthalpy of reaction by using atp+h2o+de adp+pi. pHlist and islist can be lists.*)
energy = Solve[eq, de]; energy[[1, 1, 2] . pH-> pHlist . is-> islist]
calcGHSdiss[speciesmat_, no_, is_] :=
Module[{lnkzero, sigmanuszsq, lnK, dGI, dHzero, dHI, dSI},
  (*Calculates (dGI,dHI,dSI) for a weak acid at 298.15 K at specified ionic  
   strengths (is) when the number no of the pk is specified. pks are numbered 1,2,  
   3,... from the highest pk to the lowest pk,but the highest pk for a weak acid  
   may be omitted if it is outside of the range 5 to 9. The Gibbs energy and enthalpy  
   are given in kJ mol^-1, and the entropy is given in J K^-1 mol^-1. For H3PO4,  
   pK1=calcGHSdiss[pisp,1,{0}]={{41.2},{3.6},{-126.111}}.  
   lnkzero = (speciesmat[[no+1,1]] - speciesmat[[no,1]]) (8.31451*0.29815);  
   sigmanuszsq = speciesmat[[no,3]]^2 - speciesmat[[no+1,3]]^2 + 1;  
   lnK = lnkzero + (1.17582*is^0.5*sigmanuszsq) (1 + 1.6*is^0.5);  
   (*Calculate the Gibbs energy of dissociation.*)  
   dGI = -8.31451* .29815*lnK;  
   (*Calculate the enthalpy of dissociation.*)  
   dHzero = speciesmat[[no,2]] - speciesmat[[no+1,2]];  
   sigmanuszsq = speciesmat[[no,3]]^2 - speciesmat[[no+1,3]]^2 + 1;  
   dHI = dHzero - (1.4775*is^0.5*sigmanuszsq) (1 + 1.6*is^0.5);  
   (*Calculate the entropy of dissociation.*)  
   dSI = (dHI - dGI) .29815;  
   {dGI, dHI, dSI}]  
]

The use of the six programs for calculating species properties is illustrated by using each one once. The literature data on the six reactions is summarized in the form (reaction, pH, is,K',ref,pages number in Goldgerg and Tewari,z,nH) as follows:

```
ec2x1x2x1 = "glycine+acetaldehyde+de=threonine,7.6,.002,56,57KAR,p 552, z=0,nH=9";
ec3x1x3x1B = "mannose6phos+h2o+de mannose+pi,8.5,.1,39,49MEY GRE,p 1046,z=-2,nH=11,pK0=6.44";
ec2x7x6x1 = "atp+ribose5phos+de amp+prpp,7.4,.25,64.5,92KIM KIN,p 600,z=-5,nH=8";
ec4x2x1x20 = "indole+serineL+de=tryptophaneL+ h2o,7.5,.20,81.2,85WIE HIN,p 1687,z=-5,nH=8,pK0=7.18,6.69";
ec2x7x1x40 = "atp+pyruvate+de adp+pep,8.5,.1,-31.9,82RED, p 580,dissH=-1.8";
ec2x7x1x11 = "atp+fructose6phos+de adp+ fructose6phos,7.0,.1,-84.2,75BOH SCH, p 678,dissH=-1.8,-1.8";
```

Summary Table of Literature Data

```
TableForm[{{ec2x1x2x1, ec3x1x3x1B, ec2x7x6x1, ec4x2x1x20, ec2x7x1x40, ec2x7x1x11},
  TableHeadings -> {{"ec2x1x2x1", "ec3x1x3x1B", "ec2x7x6x1"}, "ec4x2x1x20", "ec2x7x1x40", "ec2x7x1x11"}, None}]
```

d2 = TableHeadings; e = ec2x1x2x1, ec3x1x3x1B, ec2x7x6x1, ec4x2x1x20, ec2x7x1x40, ec2x7x1x11;

d2 = TableForm[{{d2[[1]], d2[[2]], d2[[3]], d2[[4]], d2[[5]], d2[[6]]}, d2[[7]]},
  TableHeadings -> {{"ec2x1x2x1", "ec3x1x3x1B", "ec2x7x6x1"}, "ec4x2x1x20", "ec2x7x1x40", "ec2x7x1x11"}, None}]
```

The following species data from BasicBiochemicalData2 and subsequent publications is needed.
acetaldehyde = \text{acetaldehyde}\); 
acetaldehyde = \text{calcGmat}[\text{acetaldehyde}] = \{-1040.45, -1635.37, -2, 12\}, \{-1078.86, -1629.97, -1, 13\}, \{-1101.63, -1648.07, 0, 14\} 
amp = \text{calcGmat}[\text{amp}] = \{-1906.13, -2626.54, -3, 12\}, \{-1947.1, -2620.94, -2, 13\}, \{-1971.98, -2638.54, -1, 14\} 
adp = \text{calcGmat}[\text{adp}] = \{-2768.1, -3619.21, -4, 12\}, \{-2811.48, -3612.91, -3, 13\}, \{-2838.18, -3627.91, -2, 14\} 
amp = \text{calcGmat}[\text{amp}] 
adp = \text{calcGmat}[\text{adp}] 
atp = \text{calcGmat}[\text{atp}] 
atph = \text{calcGmat}[\text{atph}] 
fructose6phosph = \text{calcGmat}[\text{fructose6phosph}] 
fructose16phosph = \text{calcGmat}[\text{fructose16phosph}] 
glycine = \text{calcGmat}[\text{glycine}] 
h_{20} = \text{calcGmat}[\text{h}_{20}] 
h_{2oh} = \text{calcGmat}[\text{h}_{2oh}] 
indole = \text{calcGmat}[\text{indole}] 
mannose = \text{calcGmat}[\text{mannose}] 
pep = \text{calcGmat}[\text{pep}] 
psp = \text{calcGmat}[\text{psp}] 
pi = \text{calcGmat}[\text{pi}] 
pyruvate = \text{calcGmat}[\text{pyruvate}] 
ribose5phosph = \text{calcGmat}[\text{ribose5phosph}] 
serineL = \text{calcGmat}[\text{serineL}] 
tryptophaneL = \text{calcGmat}[\text{tryptophaneL}] 
tryptophaneLh = \text{calcGmat}[\text{tryptophaneLh}]

EC 2.1.2.1 Calculate $\Delta_f G^\circ$ (298.15 K, $I=0$) for one species of threonine

\text{threonine} = \text{calcGmat}[\text{threonine}];
\text{calcckprime}[\text{glycine} + \text{acetaldehyde} + \text{de} == \text{threonine}, 7.6, .002]
56.

**EC 3.1.3.1B** Calculate $\Delta_f G^\circ$ (298.15 K, $I=0$) for two species of mannose6phos

\[
\text{mannose6phoss} = \text{calcGef2sp}[\text{mannose} + \text{pi} - \text{x} - \text{h2o} - 8.31451 \times 29815 \times \text{Log[39]}, 8.5, 1, 2, 11]
\]

\[
\{\{-1759.87, _, -2, 11\}, \{-1796.63, _, -1, 12\}\}
\]

\[
\text{mannose6phos} = \text{calcdGmat}[\text{mannose6phos}]\;
\text{calcckprime}[\text{mannose6phos} + \text{h2o} + \text{de} \text{ mannose} + \text{pi}, 8.5, 1]\
39.
\text{calcpK}[\text{mannose6phos}, 1, 0]
6.44

**EC 2.7.6.1** Calculate $\Delta_f G^\circ$ (298.15 K, $I=0$) for three species of prpp (5-phospho-D-ribose 1-diphosphate)

\[
\text{prppsp} = \text{calcGef3sp}[\text{x} + \text{amp} - \text{atp} - \text{ribose5phos} - 8.31451 \times 29815 \times \text{Log[64.5]}, 7.3, .25, -5, 8, 7.18, 6]
\]

\[
\{\{-3284.25, _, -5, 8\}, \{-3325.23, _, -4, 9\}, \{-3363.42, _, -3, 10\}\}
\]

\[
\text{prpp} = \text{calcdGmat}[\text{prpp}]\;
\text{calcckprime}[\text{atp} + \text{ribose5phos} + \text{de} \text{ amp + prpp}, 7.3, .25]
64.5
\]

As a further check, we can calculate the two pKs at zero ionic strength.

\[
\text{calcpK[prppsp, 1, 0]}
7.18
\]

\[
\text{calcpK[prppsp, 2, 0]}
6.69
\]

**EC 4.2.1.20** Calculate $\Delta_f H^\circ$ (298.15 K, $I=0$) for one species of serineL

\[
\text{serineLsp} = \text{calcHf1sp}[\text{tryptophaneLh} + \text{h2oh} - \text{indoleh} - \text{x} 81.2, \text{serineLsp}, 7.4, .2]
\]

\[
\{\{-510.87, -869.73, 0, 7\}\}
\]

\[
\text{serineLh} = \text{calcdHmat}[\text{serineLsp}]\;
\text{calcctrGorHrx[indoleh + serineLh + de == tryptophaneLh + h2oh, 7.4, .20]}
81.2
\]

**EC 2.7.1.40** Calculate $\Delta_f H^\circ$ (298.15 K, $I=0$) for two species of pep (phosphoenolpyruvate)
pepsp = calcHf2sp[adph + x - atph - pyruvateh - 31.9, pepsp, 8.4, .1, -1.8]

{[-1263.65, -1621.38, -3, 2], [-1303.61, -1619.58, -2, 3]}

peph = calcDHmat[pepsp];

calctrGorHrx[atph + pyruvateh + de adph + peph, 8.4, .1]

-31.9

calcpK[pepsp, 1, 0]

7.00065

**EC 2.7.1.11 Calculate $\Delta_f H^\circ (298.15 \text{ K}, I=0)$ for three species of fructose16phos**

fructose16phosspsp =

calcHf3sp[adph + x - atph - fructose6phosh - 84.2, fructose16phossp, 6.9, .10, -1.8, -1.8]

{[-2601.4, -3343.25, -4, 10], [-2639.36, -3341.45, -3, 11], [-2673.89, -3339.65, -2, 12]}

fructose16phosh = calcDHmat[fructose16phossp];

calctrGorHrx[atph + fructose6phosh + de adph + fructose16phosh, 6.9, .1]

-84.1981

calcpK[fructose16phossp, 1, 0]

6.65027

calcpK[fructose16phossp, 2, 0]

6.04936

As a final check, we can calculate $\Delta_{diss} H^\circ (298.15 \text{ K}, I=0)$ for this diprotic weak acid

calcGHSdiss[fructose16phossp, 1, 0]

{37.96, -1.8, -133.356}

calcGHSdiss[fructose16phossp, 2, 0]

{34.53, -1.8, -121.851}