

Stoichiometry to atom fraction

In[4]:= **A1**[S0_, S1_, S2] = S1 / (S0 + S1 + S2)

$$\text{Out[4]} = \frac{S1}{S0 + S1 + S2}$$

In[139]:= **den** = S0 + S1 + S2

$$\text{Out[139]} = S0 + S1 + S2$$

In[142]:= **Simplify**[D[A1[S0, S1, S2], S1] == (1 - S1 / den) / den]

Out[142]= True

In[143]:= **Simplify**[D[A1[S0, S1, S2], S2] == (0 - S1 / den) / den]

Out[143]= True

Atom fraction to mass fraction

In[7]:= **C1**[A0_, A1_, A2_, W0_, W1_, W2_] = (A1 W1) / (A0 W0 + A1 W1 + A2 W2)

$$\text{Out[7]} = \frac{A1 W1}{A0 W0 + A1 W1 + A2 W2}$$

In[144]:= **den** = A0 W0 + A1 W1 + A2 W2

$$\text{Out[144]} = A0 W0 + A1 W1 + A2 W2$$

In[149]:= **D**[C1[A0, A1, A2, W0, W1, W2], A1]

$$\text{Out[149]} = -\frac{A1 W1^2}{(A0 W0 + A1 W1 + A2 W2)^2} + \frac{W1}{A0 W0 + A1 W1 + A2 W2}$$

In[150]:= **Simplify**[D[C1[A0, A1, A2, W0, W1, W2], A1] == $\frac{W1}{den} (1 - A1 W1 / den)$]

Out[150]= True

In[151]:= **D**[C1[A0, A1, A2, W0, W1, W2], A2]

$$\text{Out[151]} = -\frac{A1 W1 W2}{(A0 W0 + A1 W1 + A2 W2)^2}$$

In[154]:= **Simplify**[D[C1[A0, A1, A2, W0, W1, W2], A2] == $\frac{W1}{den} (0 - A1 W2 / den)$]

Out[154]= True

In[10]:= **D**[C1[A0, A1, A2, W0, W1, W2], W1] /. {A0 W0 + A1 W1 + A2 W2 → dc1}

$$\text{Out[10]} = \frac{A1}{dc1} - \frac{A1^2 W1}{dc1^2}$$

$$\text{In[156]:= Simplify}\left[D[C1[A0, A1, A2, W0, W1, W2], W1] == \frac{A1}{\text{den}} \left(1 - \frac{A1 W1}{\text{den}}\right)\right]$$

Out[156]= True

$$\text{In[11]:= D}[C1[A0, A1, A2, W0, W1, W2], W2] /. \{A0 W0 + A1 W1 + A2 W2 \rightarrow \text{dc1}\}$$

$$\text{Out[11]= } -\frac{A1 A2 W1}{\text{dc1}^2}$$

$$\text{In[159]:= Simplify}\left[D[C1[A0, A1, A2, W0, W1, W2], W2] == \frac{A1}{\text{den}} \left(0 - \frac{A2 W1}{\text{den}}\right)\right]$$

Out[159]= True

Mass fraction to normalized mass fraction

$$\text{In[12]:= N1}[C0_, C1_, C2_] = C1 / (C0 + C1 + C2)$$

$$\text{Out[12]= } \frac{C1}{C0 + C1 + C2}$$

$$\text{In[160]:= den} = C0 + C1 + C2$$

$$\text{Out[160]= } C0 + C1 + C2$$

$$\text{In[13]:= D}[N1[C0, C1, C2], C1] /. \{C0 + C1 + C2 \rightarrow \text{dn1}\}$$

$$\text{Out[13]= } -\frac{C1}{\text{dn1}^2} + \frac{1}{\text{dn1}}$$

$$\text{In[162]:= Simplify}\left[D[N1[C0, C1, C2], C1] == \frac{1}{\text{den}} \left(1 - \frac{C1}{\text{den}}\right)\right]$$

Out[162]= True

$$\text{In[14]:= D}[N1[C0, C1, C2], C2] /. \{C0 + C1 + C2 \rightarrow \text{dn1}\}$$

$$\text{Out[14]= } -\frac{C1}{\text{dn1}^2}$$

$$\text{In[163]:= Simplify}\left[D[N1[C0, C1, C2], C2] == \frac{1}{\text{den}} \left(0 - \frac{C1}{\text{den}}\right)\right]$$

Out[163]= True

Mass fraction to atom fraction

$$\text{In[15]:= A1}[C0_, C1_, C2_, W0_, W1_, W2_] = (C1 / W1) / (C0 / W0 + C1 / W1 + C2 / W2)$$

$$\text{Out[15]= } \frac{C1}{W1 \left(\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}\right)}$$

In[126]:= **den = C0 / W0 + C1 / W1 + C2 / W2**

Out[126]= $\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}$

In[127]:= **Simplify[D[A1[C0, C1, C2, W0, W1, W2], C1] == $\left(\frac{1}{\text{den } W1}\right) \left(1 - \frac{C1}{\text{den } W1}\right)$]**

In[131]:= **D[A1[C0, C1, C2, W0, W1, W2], C2]**

Out[131]= $-\frac{C1}{W1 \left(\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}\right)^2 W2}$

In[130]:= **Simplify[D[A1[C0, C1, C2, W0, W1, W2], C2] == $\left(\frac{1}{\text{den } W1}\right) \left(0 - \frac{C1}{\text{den } W2}\right)$]**

Out[130]= **True**

In[132]:= **D[A1[C0, C1, C2, W0, W1, W2], W1]**

Out[132]= $\frac{C1^2}{W1^3 \left(\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}\right)^2} - \frac{C1}{W1^2 \left(\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}\right)}$

In[136]:= **Simplify[D[A1[C0, C1, C2, W0, W1, W2], W1] == $\left(\frac{C1}{\text{den } W1^2}\right) \left(\frac{C1}{W1 \text{ den}} - 1\right)$]**

Out[136]= **True**

In[137]:= **D[A1[C0, C1, C2, W0, W1, W2], W2]**

Out[137]= $\frac{C1 C2}{W1 \left(\frac{C0}{W0} + \frac{C1}{W1} + \frac{C2}{W2}\right)^2 W2^2}$

In[138]:= **Simplify[D[A1[C0, C1, C2, W0, W1, W2], W2] == $\left(\frac{C2}{\text{den } W2^2}\right) \left(\frac{C1}{W1 \text{ den}} - 0\right)$]**

Out[138]= **True**

Mixtures to mass fractions

Let's say we have masses M_i with element j . Within each mass the mass fraction is $C_{i,j}$ and the mean atomic weight is $W_{i,j}$. Each mass has $N_{i,j}$ atoms of j with mass $C_{i,j} M_i$. $N_{i,j} = C_{i,j} M_i / W_{i,j}$

In[85]:= **C1[C00_, C01_, C02_, C10_, C11_, C12_,
A00_, A01_, A02_, A10_, A11_, A12_, M0_, M1_] = M0 C01 + M1 C11**

Out[85]= **C01 M0 + C11 M1**

In[116]:= **CC1 = C1[C00, C01, C02, C10, C11, C12, A00, A01, A02, A10, A11, A12, M0, M1]**

Out[116]= **C01 M0 + C11 M1**

In[117]:= **D[CC1, C01]**

Out[117]= **M0**

In[118]:= **D[CC1, M0]**

Out[118]= **C01**

In[89]:= **A1[C00_, C01_, C02_, C10_, C11_, C12_, A00_, A01_, A02_, A10_, A11_, A12_, M0_, M1_] =**

$$(C01 M0 + C11 M1) / \left(\frac{C01 M0}{A01} + \frac{C11 M1}{A11} \right)$$

Out[89]=
$$\frac{C01 M0 + C11 M1}{\frac{C01 M0}{A01} + \frac{C11 M1}{A11}}$$

In[93]:= **AA1 = A1[C00, C01, C02, C10, C11, C12, A00, A01, A02, A10, A11, A12, M0, M1]**

Out[93]=
$$\frac{C01 M0 + C11 M1}{\frac{C01 M0}{A01} + \frac{C11 M1}{A11}}$$

In[119]:= **Simplify[D[AA1, M0] == (AA1 (1 - AA1 / A01)) $\frac{C01}{CC1}$]**

Out[119]= **True**

In[120]:= **Simplify[D[AA1, C01] == (AA1 (1 - AA1 / A01)) $\frac{M0}{CC1}$]**

Out[120]= **True**

In[121]:= **D[AA1, A01] (CC1 / AA1²)**

Out[121]=
$$\frac{C01 M0}{A01^2}$$

In[125]:= **Simplify[D[AA1, A01] == $\left(\frac{AA1}{A01}\right)^2 \left(\frac{C01}{CC1}\right) M0]$**

Out[125]= **True**