

Appendix1. Expressions for chemical potentials of components of (Zn,Fe)S *sph*, (Ag,Cu)<sub>16</sub>(Sb,As)<sub>2</sub>S<sub>11</sub> *plb-prc*, (Ag,Cu)<sub>3</sub>(Sb,As)<sub>3</sub> *prg-prs*, (Cu,Ag)<sub>3</sub>SbS<sub>3</sub> *skn*, (Cu,Ag)<sub>10</sub>(Fe,Zn)<sub>2</sub>(Sb,As)<sub>4</sub>S<sub>13</sub> *fah*, Ag(Sb,Bi)S<sub>2</sub> *β-mia*, *arm* and *mat*, and Pb<sub>2</sub>S<sub>2</sub>-AgSbS<sub>2</sub>-AgBiS<sub>2</sub> *gn* solutions after Balabin and Sack (2000), Harlov and Sack (1994), Harlov and Sack (1995a), Ghosal and Sack (1995), Sack et al. (1987), Ghosal and Sack (1999) and Chutas (2004).

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$$\begin{aligned} \mu_{\text{ZnS}}^{\text{Sph}} &= \mu_{\text{ZnS}}^{\text{O Sph}} + RT \ln (X_{\text{ZnS}}) + (X_{\text{FeS}})^2 \left[ A_0 + A_1 (3 - 4 X_{\text{FeS}}) + A_2 (5 - 16 X_{\text{FeS}} + 12 X_{\text{FeS}}^2) + A_3 (7 - 36 X_{\text{FeS}} + 60 X_{\text{FeS}}^2 \right. \\ &\quad \left. - 32 X_{\text{FeS}}^3) + A_4 (9 - 64 X_{\text{FeS}} + 168 X_{\text{FeS}}^2 - 192 X_{\text{FeS}}^3 + 80 X_{\text{FeS}}^4) \right] \end{aligned}$$


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$$\begin{aligned} \mu_{\text{FeS}}^{\text{Sph}} &= \mu_{\text{FeS}}^{\text{O Sph}} + RT \ln (X_{\text{FeS}}) + (X_{\text{ZnS}})^2 \left[ A_0 - A_1 (3 - 4 X_{\text{ZnS}}) + A_2 (5 - 16 X_{\text{ZnS}} + 12 X_{\text{ZnS}}^2) - A_3 (7 - 36 X_{\text{ZnS}} + 60 X_{\text{ZnS}}^2 \right. \\ &\quad \left. - 32 X_{\text{ZnS}}^3) + A_4 (9 - 64 X_{\text{ZnS}} + 168 X_{\text{ZnS}}^2 - 192 X_{\text{ZnS}}^3 + 80 X_{\text{ZnS}}^4) \right] \end{aligned}$$


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$$\begin{aligned} \mu_{\text{Ag}_{16}\text{Sb}_2\text{S}_{11}}^{\text{Plb-Prc}} &= \mu_{\text{Ag}_{16}\text{Sb}_2\text{S}_{11}}^{\text{O Plb}} + RT \left[ 4 \ln (X_{\text{Ag}}^{\text{A}}) + 4 \ln (X_{\text{Ag}}^{\text{B}}) + 8 \ln (X_{\text{Ag}}^{\text{C}}) + 2 \ln (1 - X_3) \right] - \Delta \bar{G}_{34}^{\text{O}}(X_3)(X_4) + W_{\text{AsSb}}^{\text{SM}}(X_3^2) + \left[ W_{\text{AgCu}}^{\text{A}} + W_{\text{AgCu}}^{\text{B}} \right. \\ &\quad \left. + W_{\text{AgCu}}^{\text{C}} - \frac{1}{2} \Delta \bar{G}_{4s}^* - \frac{1}{2} \Delta \bar{G}_{4t}^* - \frac{1}{2} \Delta \bar{G}_{st}^* \right] (X_4^2) - \left[ -\frac{7}{32} \Delta \bar{G}_{4s}^* + \frac{1}{32} \Delta \bar{G}_{4t}^* + \frac{1}{32} \Delta \bar{G}_{st}^* - \frac{1}{16} W_{\text{AgCu}}^{\text{A}} - \frac{9}{16} W_{\text{AgCu}}^{\text{B}} - \frac{1}{16} W_{\text{AgCu}}^{\text{C}} \right] (s^2) \\ &\quad - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* - \frac{3}{8} \Delta \bar{G}_{4t}^* + \frac{1}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} - \frac{1}{4} W_{\text{AgCu}}^{\text{B}} - \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (t^2) - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* + \frac{3}{8} \Delta \bar{G}_{4t}^* - \frac{3}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} + \frac{3}{4} W_{\text{AgCu}}^{\text{B}} \right. \\ &\quad \left. + \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (s)(t) - \frac{1}{4} \Delta \bar{G}_{3s}^*(X_3)(s) - \frac{1}{4} \left[ \Delta \bar{G}_{3t}^* + \Delta \bar{G}_{34}^* \right] (X_3)(t) - \left[ -\frac{3}{4} \Delta \bar{G}_{4s}^* + \frac{1}{4} \Delta \bar{G}_{4t}^* + \frac{1}{4} \Delta \bar{G}_{st}^* - \frac{1}{2} W_{\text{AgCu}}^{\text{A}} + \frac{3}{2} W_{\text{AgCu}}^{\text{B}} \right. \end{aligned}$$

$$-\frac{1}{2} W_{\text{AgCu}}^{\text{C}} ](X_4)(s) - \left[ -\frac{1}{2} \Delta \bar{G}_{4s}^* + \frac{1}{2} \Delta \bar{G}_{4t}^* + \frac{1}{2} \Delta \bar{G}_{st}^* - W_{\text{AgCu}}^{\text{A}} - W_{\text{AgCu}}^{\text{B}} + W_{\text{AgCu}}^{\text{C}} \right] (X_4)(t)$$

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$$\begin{aligned} \mu_{\text{Ag}_{16}\text{As}_2\text{S}_{11}}^{\text{Pb-Prc}} &= \mu_{\text{Ag}_{16}\text{As}_2\text{S}_{11}}^{\text{o Prc}} + RT \left[ 4 \ln (X_{\text{Ag}}^{\text{A}}) + 4 \ln (X_{\text{Ag}}^{\text{B}}) + 8 \ln (X_{\text{Ag}}^{\text{C}}) + 2 \ln (X_3) \right] + \Delta \bar{G}_{34}^0 (1 - X_3)(X_4) + W_{\text{AsSb}}^{\text{SM}} (1 - X_3)^2 + \left[ W_{\text{AgCu}}^{\text{A}} + W_{\text{AgCu}}^{\text{B}} \right. \\ &+ W_{\text{AgCu}}^{\text{C}} - \frac{1}{2} \Delta \bar{G}_{4s}^* - \frac{1}{2} \Delta \bar{G}_{4t}^* - \frac{1}{2} \Delta \bar{G}_{st}^* \left. \right] (X_4^2) - \left[ -\frac{7}{32} \Delta \bar{G}_{4s}^* + \frac{1}{32} \Delta \bar{G}_{4t}^* + \frac{1}{32} \Delta \bar{G}_{st}^* - \frac{1}{16} W_{\text{AgCu}}^{\text{A}} - \frac{9}{16} W_{\text{AgCu}}^{\text{B}} - \frac{1}{16} W_{\text{AgCu}}^{\text{C}} \right] (s^2) \\ &- \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* - \frac{3}{8} \Delta \bar{G}_{4t}^* + \frac{1}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} - \frac{1}{4} W_{\text{AgCu}}^{\text{B}} - \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (t^2) - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* + \frac{3}{8} \Delta \bar{G}_{4t}^* - \frac{3}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} + \frac{3}{4} W_{\text{AgCu}}^{\text{B}} \right. \\ &+ \left. \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (s)(t) + \frac{1}{4} \Delta \bar{G}_{3s}^* (1 - X_3)(s) + \frac{1}{4} \left[ \Delta \bar{G}_{3t}^* + \Delta \bar{G}_{34}^* \right] (1 - X_3)(t) - \left[ -\frac{3}{4} \Delta \bar{G}_{4s}^* + \frac{1}{4} \Delta \bar{G}_{4t}^* + \frac{1}{4} \Delta \bar{G}_{st}^* - \frac{1}{2} W_{\text{AgCu}}^{\text{A}} + \frac{3}{2} W_{\text{AgCu}}^{\text{B}} \right. \\ &\left. - \frac{1}{2} W_{\text{AgCu}}^{\text{C}} \right] (X_4)(s) - \left[ -\frac{1}{2} \Delta \bar{G}_{4s}^* + \frac{1}{2} \Delta \bar{G}_{4t}^* + \frac{1}{2} \Delta \bar{G}_{st}^* - W_{\text{AgCu}}^{\text{A}} - W_{\text{AgCu}}^{\text{B}} + W_{\text{AgCu}}^{\text{C}} \right] (X_4)(t) \end{aligned}$$


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$$\begin{aligned} \mu_{\text{Cu}_{16}\text{Sb}_2\text{S}_{11}}^{\text{Pb-Prc}} &= \mu_{\text{Cu}_{16}\text{Sb}_2\text{S}_{11}}^{\text{o Plb}} + RT \left[ 4 \ln (X_{\text{Cu}}^{\text{A}}) + 4 \ln (X_{\text{Cu}}^{\text{B}}) + 8 \ln (X_{\text{Cu}}^{\text{C}}) + 2 \ln (1 - X_3) \right] + \Delta \bar{G}_{34}^0 (X_3)(1 - X_4) + W_{\text{AsSb}}^{\text{SM}} (X_3^2) + \left[ W_{\text{AgCu}}^{\text{A}} + W_{\text{AgCu}}^{\text{B}} \right. \\ &+ W_{\text{AgCu}}^{\text{C}} - \frac{1}{2} \Delta \bar{G}_{4s}^* - \frac{1}{2} \Delta \bar{G}_{4t}^* - \frac{1}{2} \Delta \bar{G}_{st}^* \left. \right] (1 - X_4^2) - \left[ -\frac{7}{32} \Delta \bar{G}_{4s}^* + \frac{1}{32} \Delta \bar{G}_{4t}^* + \frac{1}{32} \Delta \bar{G}_{st}^* - \frac{1}{16} W_{\text{AgCu}}^{\text{A}} - \frac{9}{16} W_{\text{AgCu}}^{\text{B}} - \frac{1}{16} W_{\text{AgCu}}^{\text{C}} \right] (s^2) \\ &- \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* - \frac{3}{8} \Delta \bar{G}_{4t}^* + \frac{1}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} - \frac{1}{4} W_{\text{AgCu}}^{\text{B}} - \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (t^2) - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* + \frac{3}{8} \Delta \bar{G}_{4t}^* - \frac{3}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} + \frac{3}{4} W_{\text{AgCu}}^{\text{B}} \right. \\ &+ \left. \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (s)(t) - \frac{1}{4} \Delta \bar{G}_{3s}^* (X_3)(s) - \frac{1}{4} \left[ \Delta \bar{G}_{3t}^* + \Delta \bar{G}_{34}^* \right] (X_3)(t) + \left[ -\frac{3}{4} \Delta \bar{G}_{4s}^* + \frac{1}{4} \Delta \bar{G}_{4t}^* + \frac{1}{4} \Delta \bar{G}_{st}^* - \frac{1}{2} W_{\text{AgCu}}^{\text{A}} + \frac{3}{2} W_{\text{AgCu}}^{\text{B}} \right. \end{aligned}$$

$$-\frac{1}{2} W_{\text{AgCu}}^{\text{C}} ](1 - X_4)(s) + \left[ -\frac{1}{2} \Delta \bar{G}_{4s}^* + \frac{1}{2} \Delta \bar{G}_{4t}^* + \frac{1}{2} \Delta \bar{G}_{st}^* - W_{\text{AgCu}}^{\text{A}} - W_{\text{AgCu}}^{\text{B}} + W_{\text{AgCu}}^{\text{C}} \right] (1 - X_4)(t)$$

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$$\begin{aligned} \mu_{\text{Cu}_{16}\text{As}_2\text{S}_{11}}^{\text{Plb-Prs}} &= \mu_{\text{Cu}_{16}\text{As}_2\text{S}_{11}}^{\text{o Prs}} + RT \left[ 4 \ln (X_{\text{Cu}}^{\text{A}}) + 4 \ln (X_{\text{Cu}}^{\text{B}}) + 8 \ln (X_{\text{Cu}}^{\text{C}}) + 2 \ln (X_3) \right] - \Delta \bar{G}_{34}^0 (1 - X_3)(1 - X_4) + W_{\text{AsSb}}^{\text{SM}} (1 - X_3)^2 + \left[ W_{\text{AgCu}}^{\text{A}} \right. \\ &+ W_{\text{AgCu}}^{\text{B}} + W_{\text{AgCu}}^{\text{C}} - \frac{1}{2} \Delta \bar{G}_{4s}^* - \frac{1}{2} \Delta \bar{G}_{4t}^* - \frac{1}{2} \Delta \bar{G}_{st}^* \left. \right] (1 - X_4)^2 - \left[ -\frac{7}{32} \Delta \bar{G}_{4s}^* + \frac{1}{32} \Delta \bar{G}_{4t}^* + \frac{1}{32} \Delta \bar{G}_{st}^* - \frac{1}{16} W_{\text{AgCu}}^{\text{A}} - \frac{9}{16} W_{\text{AgCu}}^{\text{B}} \right. \\ &- \frac{1}{16} W_{\text{AgCu}}^{\text{C}} \left. \right] (s^2) - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* - \frac{3}{8} \Delta \bar{G}_{4t}^* + \frac{1}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} - \frac{1}{4} W_{\text{AgCu}}^{\text{B}} - \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \right] (t^2) - \left[ \frac{1}{8} \Delta \bar{G}_{4s}^* + \frac{3}{8} \Delta \bar{G}_{4t}^* - \frac{3}{8} \Delta \bar{G}_{st}^* - \frac{1}{4} W_{\text{AgCu}}^{\text{A}} \right. \\ &+ \frac{3}{4} W_{\text{AgCu}}^{\text{B}} + \frac{1}{4} W_{\text{AgCu}}^{\text{C}} \left. \right] (s)(t) - \frac{1}{4} \Delta \bar{G}_{3s}^* (X_3)(s) - \frac{1}{4} \left[ \Delta \bar{G}_{3t}^* + \Delta \bar{G}_{34}^* \right] (X_3)(t) + \\ &+ \frac{1}{4} W_{\text{AgCu}}^{\text{C}} ] (s)(t) + \frac{1}{4} \Delta \bar{G}_{3s}^* (1 - X_3)(s) + \frac{1}{4} \left[ \Delta \bar{G}_{3t}^* + \Delta \bar{G}_{34}^* \right] (1 - X_3)(t) + \left[ -\frac{3}{4} \Delta \bar{G}_{4s}^* + \frac{1}{4} \Delta \bar{G}_{4t}^* + \frac{1}{4} \Delta \bar{G}_{st}^* - \frac{1}{2} W_{\text{AgCu}}^{\text{A}} + \frac{3}{2} W_{\text{AgCu}}^{\text{B}} \right. \\ &\left. - \frac{1}{2} W_{\text{AgCu}}^{\text{C}} \right] (1 - X_4)(s) + \left[ -\frac{1}{2} \Delta \bar{G}_{4s}^* + \frac{1}{2} \Delta \bar{G}_{4t}^* + \frac{1}{2} \Delta \bar{G}_{st}^* - W_{\text{AgCu}}^{\text{A}} - W_{\text{AgCu}}^{\text{B}} + W_{\text{AgCu}}^{\text{C}} \right] (1 - X_4)(t) \end{aligned}$$

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$$\begin{aligned} \mu_{\text{Ag}_3\text{SbS}_3}^{\text{Prg-Prs}} &= \mu_{\text{Ag}_3\text{SbS}_3}^{\text{o Prg}} + RT \ln \left[ (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^3 (1 - X_{\text{As}}^{\text{Prg-Prs}}) \right] + W_{\text{AsSb}}^{\text{Prg-Prs}} (X_{\text{As}}^{\text{Prg-Prs}})^2 + \left[ W_{\text{CuAg}}^{\text{Prg-Prs}} + \Delta W (1 - 2 X_{\text{Cu}}^{\text{Prg-Prs}}) \right] (X_{\text{Cu}}^{\text{Prg-Prs}})^2 \\ &+ \left[ (\Delta \bar{H}_{\text{DAgPrg-AgPrg}}^0 - T \Delta \bar{S}_{\text{DAgPrg-AgPrg}}^0) - (\Delta \bar{H}_{\text{DCuPyr-CuPyr}}^0 - T \Delta \bar{S}_{\text{DCuPrg-CuPrg}}^0) \right] (X_{\text{Cu}}^{\text{Prg-Prs}})^2 \end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Cu}_3\text{SbS}_3}^{\text{Prg-Prs}} &= \left[ \mu_{\text{Cu}_3\text{SbS}_3}^{\circ \text{Skn}} - \Delta \bar{G}_{\text{CuSkn-Prg}}^{\circ} \right] + RT \ln \left[ (X_{\text{Cu}}^{\text{Prg-Prs}})^3 (1 - X_{\text{As}}^{\text{Prg-Prs}}) \right] + W_{\text{AsSb}}^{\text{Prg-Prs}} (X_{\text{As}}^{\text{Prg-Prs}})^2 \\
&+ \left[ W_{\text{CuAg}}^{\text{Prg-Prs}} - 2 \Delta W (X_{\text{Cu}}^{\text{Prg-Prs}}) \right] (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^2 + (\Delta \bar{H}_{\text{DAgPrg-AgPrg}}^{\circ} - T \Delta \bar{S}_{\text{DAgPrg-AgPrg}}^{\circ}) (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^2 \\
&+ (\Delta \bar{H}_{\text{DCuPyr-CuPyr}}^{\circ} - T \Delta \bar{S}_{\text{DCuPrg-CuPrg}}^{\circ}) \left[ 2 X_{\text{Cu}}^{\text{Prg-Prs}} - (X_{\text{Cu}}^{\text{Prg-Prs}})^2 \right]
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Ag}_3\text{AsS}_3}^{\text{Prg-Prs}} &= \mu_{\text{Ag}_3\text{AsS}_3}^{\circ \text{Prg}} + RT \ln \left[ (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^3 (X_{\text{As}}^{\text{Prg-Prs}}) \right] + W_{\text{AsSb}}^{\text{Prg-Prs}} (1 - X_{\text{As}}^{\text{Prg-Prs}})^2 + \left[ W_{\text{CuAg}}^{\text{Prg-Prs}} + \Delta W (1 - 2 X_{\text{Cu}}^{\text{Prg-Prs}}) \right] (X_{\text{Cu}}^{\text{Prg-Prs}})^2 \\
&+ \left[ (\Delta \bar{H}_{\text{DAgPrg-AgPrg}}^{\circ} - T \Delta \bar{S}_{\text{DAgPrg-AgPrg}}^{\circ}) - (\Delta \bar{H}_{\text{DCuPyr-CuPyr}}^{\circ} - T \Delta \bar{S}_{\text{DCuPrg-CuPrg}}^{\circ}) \right] (X_{\text{Cu}}^{\text{Prg-Prs}})^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Cu}_3\text{AsS}_3}^{\text{Prg-Prs}} &= \left[ \mu_{\text{Cu}_3\text{SbS}_3}^{\circ \text{Skn}} - \Delta \bar{G}_{\text{CuSkn-Prg}}^{\circ} + \mu_{\text{Ag}_3\text{AsS}_3}^{\circ \text{Prg}} - \mu_{\text{Ag}_3\text{SbS}_3}^{\circ \text{Prg}} \right] + RT \ln \left[ (X_{\text{Cu}}^{\text{Prg-Prs}})^3 (X_{\text{As}}^{\text{Prg-Prs}}) \right] + W_{\text{AsSb}}^{\text{Prg-Prs}} (1 - X_{\text{As}}^{\text{Prg-Prs}})^2 \\
&+ \left[ W_{\text{CuAg}}^{\text{Prg-Prs}} - 2 \Delta W (X_{\text{Cu}}^{\text{Prg-Prs}}) \right] (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^2 + (\Delta \bar{H}_{\text{DAgPrg-AgPrg}}^{\circ} - T \Delta \bar{S}_{\text{DAgPrg-AgPrg}}^{\circ}) (1 - X_{\text{Cu}}^{\text{Prg-Prs}})^2 \\
&+ (\Delta \bar{H}_{\text{DCuPyr-CuPyr}}^{\circ} - T \Delta \bar{S}_{\text{DCuPrg-CuPrg}}^{\circ}) \left[ 2 X_{\text{Cu}}^{\text{Prg-Prs}} - (X_{\text{Cu}}^{\text{Prg-Prs}})^2 \right]
\end{aligned}$$


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$$\mu_{\text{Cu}_3\text{SbS}_3}^{\text{Skn}} = \mu_{\text{Cu}_3\text{SbS}_3}^{\circ \text{Skn}} + RT \left[ \ln (X_{\text{Cu}}^{\text{A Skn}}) + 2 \ln (X_{\text{Cu}}^{\text{B Skn}}) \right] + (W_{\text{AgCu}}^{\text{A Skn}} + W_{\text{AgCu}}^{\text{B Skn}} - \Delta \bar{G}_{\text{xs}}^*) (1 - X_{\text{Cu}}^{\text{Skn}})^2 + \left( \frac{2}{9} \Delta \bar{G}_{\text{xs}}^* + \frac{4}{9} W_{\text{AgCu}}^{\text{A Skn}} + \frac{1}{9} W_{\text{AgCu}}^{\text{B Skn}} \right) (s)^2$$

$$+ \left( \frac{1}{3} \Delta \bar{G}_{xs}^* - \frac{4}{3} W_{AgCu}^A Skn + \frac{2}{3} W_{AgCu}^B Skn \right) (1 - X_{Cu}^{Skn})(s)$$


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$$\begin{aligned} \mu_{Ag_3SbS_3}^{Skn} &= \mu_{Ag_3SbS_3}^{o Prg} - \Delta \bar{G}_{AgPrg-Skn}^0 + RT \left[ \ln (1 - X_{Cu}^A Skn) + 2 \ln (1 - X_{Cu}^B Skn) \right] + (W_{AgCu}^A Skn + W_{AgCu}^B Skn - \Delta \bar{G}_{xs}^*) (X_{Cu}^{Skn})^2 \\ &+ \left( \frac{2}{9} \Delta \bar{G}_{xs}^* + \frac{4}{9} W_{AgCu}^A Skn + \frac{1}{9} W_{AgCu}^B Skn \right) (s)^2 - \left( \frac{1}{3} \Delta \bar{G}_{xs}^* - \frac{4}{3} W_{AgCu}^A Skn + \frac{2}{3} W_{AgCu}^B Skn \right) (X_{Cu}^{Skn})(s) \end{aligned}$$


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$$\begin{aligned} \mu_{Cu_{10}Fe_2Sb_4S_{13}}^{Fah} &= \mu_{Cu_{10}Fe_2Sb_4S_{13}}^{o Fah} + RT \ln \left[ (1 - X_4 - \frac{2}{5} s)^6 \left( \frac{2}{3} [1 - X_4] + \frac{2}{5} s \right)^4 \left( \frac{3}{2} \right)^4 (1 - X_2)^2 (1 - X_3)^4 \right] - \Delta \bar{G}_{23}^0 (X_2)(X_3) - \Delta \bar{G}_{24}^0 (X_2)(X_4) \\ &- \Delta \bar{G}_{34}^0 (X_3)(X_4) + W_{FeZn}^{TET} (X_2)^2 + W_{AsSb}^{SM} (X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{AgCu}^{TET} + W_{AgCu}^{TRG}) (X_4)^2 - \Delta \bar{G}_{2s}^* (X_2)(s) - \Delta \bar{G}_{3s}^* (X_3)(s) \\ &- \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{AgCu}^{TET} - 4 W_{AgCu}^{TRG}) (X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{AgCu}^{TET} - 4 W_{AgCu}^{TRG}) (s)^2 \end{aligned}$$


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$$\begin{aligned} \mu_{Cu_{10}Zn_2Sb_4S_{13}}^{Fah} &= \mu_{Cu_{10}Zn_2Sb_4S_{13}}^{o Fah} + RT \ln \left[ (1 - X_4 - \frac{2}{5} s)^6 \left( \frac{2}{3} [1 - X_4] + \frac{2}{5} s \right)^4 \left( \frac{3}{2} \right)^4 (X_2)^2 (1 - X_3)^4 \right] + \Delta \bar{G}_{23}^0 (1 - X_2)(X_3) + \Delta \bar{G}_{24}^0 (1 - X_2)(X_4) \\ &- \Delta \bar{G}_{34}^0 (X_3)(X_4) + W_{FeZn}^{TET} (1 - X_2)^2 + W_{AsSb}^{SM} (X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{AgCu}^{TET} + W_{AgCu}^{TRG}) (X_4)^2 + \Delta \bar{G}_{2s}^* (1 - X_2)(s) - \Delta \bar{G}_{3s}^* (X_3)(s) \\ &- \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{AgCu}^{TET} - 4 W_{AgCu}^{TRG}) (X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{AgCu}^{TET} - 4 W_{AgCu}^{TRG}) (s)^2 \end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Cu}_{10}\text{Fe}_2\text{As}_4\text{S}_{13}}^{\text{Fah}} &= \mu_{\text{Cu}_{10}\text{Fe}_2\text{As}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (1 - X_4 - \frac{2}{5}s)^6 \left( \frac{2}{3}[1 - X_4] + \frac{2}{5}s \right)^4 \left( \frac{3}{2} \right)^4 (1 - X_2)^2 (X_3)^4 \right] + \Delta \bar{G}_{23}^{\circ} (X_2)(1 - X_3) - \Delta \bar{G}_{24}^{\circ} (X_2)(X_4) \\
&+ \Delta \bar{G}_{34}^{\circ} (1 - X_3)(X_4) + W_{\text{FeZn}}^{\text{TET}} (X_2)^2 + W_{\text{AsSb}}^{\text{SM}} (1 - X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}}) (X_4)^2 - \Delta \bar{G}_{2s}^* (X_2)(s) + \Delta \bar{G}_{3s}^* (1 - X_3)(s) \\
&- \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (s)^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Ag}_{10}\text{Fe}_2\text{Sb}_4\text{S}_{13}}^{\text{Fah}} &= \mu_{\text{Ag}_{10}\text{Fe}_2\text{Sb}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (X_4 + \frac{2}{5}s)^6 \left( \frac{2}{3}X_4 - \frac{2}{5}s \right)^4 \left( \frac{3}{2} \right)^4 (1 - X_2)^2 (1 - X_3)^4 \right] - \Delta \bar{G}_{23}^{\circ} (X_2)(X_3) + \Delta \bar{G}_{24}^{\circ} (X_2)(1 - X_4) \\
&+ \Delta \bar{G}_{34}^{\circ} (X_3)(1 - X_4) + W_{\text{FeZn}}^{\text{TET}} (X_2)^2 + W_{\text{AsSb}}^{\text{SM}} (X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}}) (1 - X_4)^2 - \Delta \bar{G}_{2s}^* (X_2)(s) - \Delta \bar{G}_{3s}^* (X_3)(s) \\
&+ \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (1 - X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (s)^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Cu}_{10}\text{Zn}_2\text{As}_4\text{S}_{13}}^{\text{Fah}} &= \mu_{\text{Cu}_{10}\text{Zn}_2\text{As}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (1 - X_4 - \frac{2}{5}s)^6 \left( \frac{2}{3}[1 - X_4] + \frac{2}{5}s \right)^4 \left( \frac{3}{2} \right)^4 (X_2)^2 (X_3)^4 \right] - \Delta \bar{G}_{23}^{\circ} (1 - X_2)(1 - X_3) + \Delta \bar{G}_{24}^{\circ} (1 - X_2)(X_4) \\
&+ \Delta \bar{G}_{34}^{\circ} (1 - X_3)(X_4) + W_{\text{FeZn}}^{\text{TET}} (1 - X_2)^2 + W_{\text{AsSb}}^{\text{SM}} (1 - X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}}) (X_4)^2 + \Delta \bar{G}_{2s}^* (1 - X_2)(s) \\
&+ \Delta \bar{G}_{3s}^* (1 - X_3)(s) - \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}}) (s)^2
\end{aligned}$$


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$$\mu_{\text{Ag}_{10}\text{Zn}_2\text{Sb}_4\text{S}_{13}}^{\text{Fah}} = \mu_{\text{Ag}_{10}\text{Zn}_2\text{Sb}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (X_4 + \frac{2}{5}s)^6 \left( \frac{2}{3}X_4 - \frac{2}{5}s \right)^4 \left( \frac{3}{2} \right)^4 (X_2)^2 (1 - X_3)^4 \right] + \Delta \bar{G}_{23}^{\circ} (1 - X_2)(X_3) - \Delta \bar{G}_{24}^{\circ} (1 - X_2)(1 - X_4)$$

$$\begin{aligned}
& + \Delta \bar{G}_{34}^0(X_3)(1 - X_4) + W_{\text{FeZn}}^{\text{TET}}(1 - X_2)^2 + W_{\text{AsSb}}^{\text{SM}}(X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)^2 + \Delta \bar{G}_{2s}^*(1 - X_2)(s) - \Delta \bar{G}_{3s}^*(X_3)(s) \\
& + \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(s)^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Ag}_{10}\text{Fe}_2\text{As}_4\text{S}_{13}}^{\text{Fah}} & = \mu_{\text{Ag}_{10}\text{Fe}_2\text{As}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (X_4 + \frac{2}{5}s)^6 (\frac{2}{3}X_4 - \frac{2}{5}s)^4 (\frac{3}{2})^4 (1 - X_2)^2 (X_3)^4 \right] + \Delta \bar{G}_{23}^0(X_2)(1 - X_3) + \Delta \bar{G}_{24}^0(X_2)(1 - X_4) \\
& - \Delta \bar{G}_{34}^0(1 - X_3)(1 - X_4) + W_{\text{FeZn}}^{\text{TET}}(X_2)^2 + W_{\text{AsSb}}^{\text{SM}}(1 - X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)^2 - \Delta \bar{G}_{2s}^*(X_2)(s) + \Delta \bar{G}_{3s}^*(1 - X_3)(s) \\
& + \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(s)^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{Ag}_{10}\text{Zn}_2\text{As}_4\text{S}_{13}}^{\text{Fah}} & = \mu_{\text{Ag}_{10}\text{Zn}_2\text{As}_4\text{S}_{13}}^{\circ \text{Fah}} + RT \ln \left[ (X_4 + \frac{2}{5}s)^6 (\frac{2}{3}X_4 - \frac{2}{5}s)^4 (\frac{3}{2})^4 (X_2)^2 (X_3)^4 \right] - \Delta \bar{G}_{23}^0(1 - X_2)(1 - X_3) - \Delta \bar{G}_{24}^0(1 - X_2)(1 - X_4) \\
& - \Delta \bar{G}_{34}^0(1 - X_3)(1 - X_4) + W_{\text{FeZn}}^{\text{TET}}(1 - X_2)^2 + W_{\text{AsSb}}^{\text{SM}}(1 - X_3)^2 + (\Delta \bar{G}_{4s}^* + W_{\text{AgCu}}^{\text{TET}} + W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)^2 + \Delta \bar{G}_{2s}^*(1 - X_2)(s) \\
& + \Delta \bar{G}_{3s}^*(1 - X_3)(s) + \frac{1}{5} (\Delta \bar{G}_{4s}^* + 6 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(1 - X_4)(s) - \frac{1}{25} (6 \Delta \bar{G}_{4s}^* - 9 W_{\text{AgCu}}^{\text{TET}} - 4 W_{\text{AgCu}}^{\text{TRG}})(s)^2
\end{aligned}$$


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$$\begin{aligned}
\mu_{\text{AgSbS}_2}^{\beta} & = \mu_{\text{AgSbS}_2}^{\circ \beta\text{-Mia}} + \frac{1}{5} RT \ln \left[ (1 - X_{\text{Bi}}^{\beta} + \frac{1}{5}s^{\beta})^4 (1 - X_{\text{Bi}}^{\beta} - \frac{4}{5}s^{\beta}) \right] + \frac{1}{5} (\Delta \bar{G}_x^{\circ \beta} + W_{\text{Bi-Sb}}^{\text{I}\beta} + W_{\text{Bi-Sb}}^{\text{II}\beta})(1 - X_{\text{Bi}}^{\beta})^2 \\
& - \frac{1}{5} \left( -\frac{3}{5} \Delta \bar{G}_x^{\circ \beta} + \frac{2}{5} W_{\text{Bi-Sb}}^{\text{I}\beta} - \frac{8}{5} W_{\text{Bi-Sb}}^{\text{II}\beta} \right) (X_{\text{Bi}}^{\beta})(s^{\beta}) - \frac{1}{5} \left( \frac{4}{25} \Delta \bar{G}_x^{\circ \beta} - \frac{1}{25} W_{\text{Bi-Sb}}^{\text{I}\beta} - \frac{16}{25} W_{\text{Bi-Sb}}^{\text{II}\beta} \right)
\end{aligned}$$

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$$\begin{aligned} \mu_{\text{AgBiS}_2}^{\beta} &= \mu_{\text{AgBiS}_2}^{\circ \beta\text{-Mat}} + \frac{1}{5} RT \ln \left[ (X_{\text{Bi}}^{\beta} - \frac{1}{5} s^{\beta})^4 (X_{\text{Bi}}^{\beta} + \frac{4}{5} s^{\beta}) \right] + \frac{1}{5} (\Delta \bar{G}_x^{\circ \beta} + W_{\text{Bi-Sb}}^{\text{I} \beta} + W_{\text{Bi-Sb}}^{\text{II} \beta}) (X_{\text{Bi}}^{\beta})^2 \\ &\quad + \frac{1}{5} \left( -\frac{3}{5} \Delta \bar{G}_x^{\circ \beta} + \frac{2}{5} W_{\text{Bi-Sb}}^{\text{I} \beta} - \frac{8}{5} W_{\text{Bi-Sb}}^{\text{II} \beta} \right) (1 - X_{\text{Bi}}^{\beta}) (s^{\beta}) - \frac{1}{5} \left( \frac{4}{25} \Delta \bar{G}_x^{\circ \beta} - \frac{1}{25} W_{\text{Bi-Sb}}^{\text{I} \beta} - \frac{16}{25} W_{\text{Bi-Sb}}^{\text{II} \beta} \right) \end{aligned}$$


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$$\begin{aligned} \mu_{\text{Pb}_2\text{S}_2}^{\text{Gn}} &= \mu_{\text{Pb}_2\text{S}_2}^{\circ \text{Gn}} + 2 RT \ln (X_{\text{Pb}_2\text{S}_2}^{\text{Gn}}) + W_1 (X_2 - X_1 X_2) + W_2 (X_3 - X_1 X_3) - W_3 (X_2 X_3) + 2 W_4 (X_1 X_2 - X_1^2 X_2) + W_5 (X_2^2 - 2 X_1 X_2^2) \\ &\quad + 2 W_6 (X_1 X_3 - X_1^2 X_3) + W_7 (X_3^2 - 2 X_1 X_3^2) - 2 W_8 (X_2^2 X_3) - 2 W_9 (X_2 X_3^2) + W_{10} ([1 - 2 X_1] X_2 X_3) \end{aligned}$$


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$$\begin{aligned} \mu_{\text{AgSbS}_2}^{\text{Gn}} &= \mu_{\text{AgSbS}_2}^{\circ \alpha\text{-Mia}} + 2 RT \ln (X_{\text{AgSbS}_2}^{\text{Gn}}) + W_1 (X_1 - X_1 X_2) - W_2 (X_1 X_3) + W_3 (X_3 - X_2 X_3) + W_4 (X_1^2 - 2 X_1^2 X_2) \\ &\quad + 2 W_5 (X_1 X_2 - X_1 X_2^2) - 2 W_6 (X_1^2 X_3) - 2 W_7 (X_1 X_3^2) + 2 W_8 (X_2 X_3 - X_2^2 X_3) + W_9 (X_3^2 - 2 X_2 X_3^2) + W_{10} ([1 - 2 X_2] X_1 X_3) \end{aligned}$$


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$$\begin{aligned} \mu_{\text{AgBiS}_2}^{\text{Gn}} &= \mu_{\text{AgBiS}_2}^{\circ \alpha\text{-Mat}} + 2 RT \ln (X_{\text{AgBiS}_2}^{\text{Gn}}) - W_1 (X_1 X_2) + W_2 (X_1 - X_1 X_3) + W_3 (X_2 - X_2 X_3) - 2 W_4 (X_1^2 X_2) - 2 W_5 (X_1 X_2^2) \\ &\quad + W_6 (X_1^2 - 2 X_1^2 X_3) + 2 W_7 (X_1 X_3 - X_1 X_3^2) + W_8 (X_2^2 - 2 X_2^2 X_3) + 2 W_9 (X_2 X_3 - X_2 X_3^2) + W_{10} ([1 - 2 X_3] X_1 X_2) \end{aligned}$$


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