Gibbs Energy of Formation of Ammonia

Here, we calculate the Gibbs energy of formation of ammonia (NH_3), given the reaction

$$N_2\,(g) + 3\,H_2\,(g) \rightarrow 2\,NH_3\,(g)$$

Values of the Gibbs energy of formation tabulated in the literature are normally only given at standard temperature, or for a small number of temperatures. However, the ThermophysicalData:-Chemicals package contains curve fits for experimental values of enthalpy and entropy of N_2, H_2 and NH_3, correlated against temperature.

This means that Maple will help you calculate the Gibbs energy of formation of ammonia at any temperature (assuming that the enthalpy and entropy are within the bounds of the fitted data).

```
> restart:
  with(ThermophysicalData:-Chemicals) :
```

Temperature

```
> T := 298.15 K :
```

Enthalpy

```
> h_N2 := Property("Hmolar", "N2", "temperature" = T);
  h_H2 := Property("Hmolar", "H2", "temperature" = T);
  h_NH3 := Property("Hmolar", "NH3", "temperature" = T);
```

$$9.92 \times 10^{-6}\ \frac{\mathrm{J}}{\mathrm{mol}}$$

$$-4.96 \times 10^{-6}\ \frac{\mathrm{J}}{\mathrm{mol}}$$

$$-45.94 \times 10^{3}\ \frac{\mathrm{J}}{\mathrm{mol}} \qquad \mathbf{(1)}$$

Entropy

```
> s_N2 := Property("Smolar", "N2", "temperature" = T);
  s_H2 := Property("Smolar", "H2", "temperature" = T);
  s_NH3 := Property("Smolar", "NH3", "temperature" = T);
```

$$191.61 \frac{J}{mol\,K}$$

$$130.68 \frac{J}{mol\,K}$$

$$192.77 \frac{J}{mol\,K} \tag{2}$$

Change in enthalpy and entropy per mole of NH_3

> $DeltaH := 0.5\,(2\,h\_NH3 - (h\_N2 + 3\,h\_H2))$;
> $DeltaS := 0.5\,(2\,s\_NH3 - (s\_N2 + 3\,s\_H2))$;

$$-45.94 \frac{kJ}{mol}$$

$$-99.06 \frac{J}{mol\,K} \tag{3}$$

Hence the Gibbs Energy of Formation

> $DeltaG := DeltaH - T \cdot DeltaS$

$$-16.41 \frac{kJ}{mol} \tag{4}$$