

24.11: The Standard Gibbs Free Energy for $H_2(g)$, $I_2(g)$, and $HI(g)$

For many diatomic molecules, the data needed to calculate G_{IG}^o are readily available in various compilations. For illustration, we consider the molecules H_2 , I_2 , and HI . The necessary experimental data are summarized in Table 2.

Table 2: Data for the calculation of partition functions for $H_2(g)$, $I_2(g)$, and $HI(g)$

Compound	Molar mass, g	D_0 , kJ mol ⁻¹	ν , hertz	$r_X Y$, m
H_2	2.016	432.073	1.31948×10^{14}	7.4144×10^{-11}
I_2	253.82	148.81	6.43071×10^{12}	2.666×10^{-10}
HI	127.918	294.67	6.69227×10^{13}	1.60916×10^{-10}

The terms in the simplified equation for the standard Gibbs free energy at 298.15 K are given in Table 3.

Table 3: Gibbs free energy components

Compound	$\ln \left[\left(\frac{2\pi mkT}{h^2} \right)^{3/2} \frac{kT}{p_o} \right]$	$\ln \left(\frac{8\pi^2 I kT}{\sigma h^2} \right)$	$-\ln(1 - e^{-h\nu/kT})$	$\frac{D_0}{RT}$
H_2	126.23929	0.6312*	0.0000	174.295
I_2	133.49256	7.932	0.4388	60.0289
HI	132.46470	3.4604	0.00002	118.868

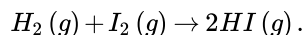
*Calculated as a sum of terms (see Table 1) rather than as the integral approximation.

Finally, the standard molar Gibbs Free Energies at 298.15 K are summarized in Table 4.

Table 4: Calculated Gibbs free energies

Compound	G_{298K}^o , kJ mole ⁻¹
H_2	-746.577
I_2	-500.471
HI	-631.622

These results can be used to calculate the standard Gibbs free energy change, at 298.15 K, for the reaction



We find

$$\Delta_r G_{298}^o = 2G^o(HI, g, 298.15 \text{ K}) - G^o(H_2, g, 298.15 \text{ K}) - G^o(I_2, g, 298.15 \text{ K}) = -16.20 \text{ kJ}$$

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