Finding K from ΔG at 727°C

$$2NO_2(g) \rightleftharpoons 2NO(g) + O_2(g)$$

	$\Delta H°$ (kJ mol^{-1} @ 25°C)	$S°$ (J mol^{-1} K^{-1} @ 25°C)
$NO_2(g)$	33.2	240.1
$NO(g)$	90.25	210.8
$O_2(g)$	0	205.2

$\Delta H°_{rxn} = 114.1$ kJ mol^{-1}

$\Delta S°_{rxn} = 147$ J mol^{-1} K^{-1}

Try ① Find $\Delta G°$ (@ 25°C)

$$\Delta G° = \Delta H° - T\Delta S$$

$$\Delta G° = (114.1 \text{ kJ mol}^{-1}) - (298.15 \text{ K} \cdot 0.147 \text{ kJ mol}^{-1} \text{ K}^{-1})$$

$$= 70.4 \text{ kJ mol}^{-1}$$

~~Verify~~

Find K @ 1000 K

$$K = e^{\frac{-\Delta G°}{RT}}$$

$$= e^{\frac{-70.4 \text{ kJ mol}^{-1}}{(8.314 \text{ J mol}^{-1} \text{ K}^{-1})\left(\frac{\text{kJ}}{10^3 \text{ J}}\right)(1000 \text{ K})}}$$

$$= 2.10 \times 10^{-4}$$

② Find $\Delta G°$ (@ 1000 K)

$$\Delta G° = \Delta H° - T\Delta S°$$

$$= (114.1 \text{ kJ mol}^{-1}) - (1000 \text{ K} \cdot 0.147 \text{ kJ mol}^{-1} \text{ K}^{-1})$$

$$= -32.5 \text{ kJ mol}^{-1}$$

Find K @ 1000 K

$$K = e^{\frac{-\Delta G°}{RT}}$$

$$= e^{\frac{-(-32.5 \text{ kJ mol}^{-1})}{(8.314)\left(\frac{\text{kJ}}{10^3 \text{ J}}\right)(1000 \text{ K})}}$$

$$= \cancel{49.85} \; 49.85$$

↑
more accurate since ΔG should be negative @ 1000 K!

$$T = \frac{\Delta H}{\Delta S} = \frac{114.1}{0.147} = 776 \text{ K} \quad (\Delta G = 0)$$

③ Most accurate way is to use thermodynamic values as measured at 1000 K!

	$\Delta H°$ (kJ mol^{-1} at 1000 K)	$S°$ (J mol^{-1} K^{-1} at 1000 K)
$NO_2(g)$	32.01	293.9
$NO(g)$	90.44	248.5
$O_2(g)$	0	243.6

$\Delta H°_{rxn} = 116.9$ kJ mol^{-1}

$\Delta S°_{rxn} = 153$ J mol^{-1} K^{-1}

$$\Delta G° = \Delta H° - T\Delta S°$$

$$= (116.9 \text{ kJ mol}^{-1}) - (1000 \text{ K} \cdot 0.153 \text{ J mol}^{-1} \text{ K}^{-1})$$

$$= -36 \text{ kJ mol}^{-1} \rightarrow \text{agrees better with } ②, \text{ not } ①$$

Find K @ 1000 K

$$K = e^{\frac{-\Delta G°}{RT}} = e^{\frac{-(-36)}{8.314/1000 \cdot 1000}}$$

$$= \cancel{} \; 75.95 \rightarrow \text{agrees better with } ②, \text{ not } ①$$