



	25°C 298 K	727°C 1000 K
$k(\text{M}^{-1}\text{s}^{-1})$	3.82×10^{-11}	2.64×10^3
K	4.65×10^{-13}	49.85

← from ΔH° & S° (at 25°C)
and ΔG° and K @ 1000K.
If ΔH° and S° @ 1000K,
 $\Delta G^\circ = -36$ and $K = 75.95$

$$A = 2 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$$

$$E_a = 112.55 \text{ kJ mol}^{-1}$$

at 25°C

$$\Delta H^\circ = 114.1 \text{ kJ mol}^{-1}$$

$$\Delta S^\circ = 147 \text{ J mol}^{-1} \text{ K}^{-1}$$

$$\Delta G^\circ(1000\text{K}) = -32.5 \text{ kJ mol}^{-1}$$

at 1000K

$$\Delta H^\circ = 116.9 \text{ kJ mol}^{-1}$$

$$\Delta S^\circ = 153 \text{ J mol}^{-1} \text{ K}^{-1}$$

$$\Delta G^\circ(1000\text{K}) = -36 \text{ kJ mol}^{-1}$$

Find equilibrium concentrations at 1000K $[\text{NO}_2] = 1.0 \text{ M}$

	$2\text{NO}_2(\text{g})$	$2\text{NO}(\text{g})$	$\text{O}_2(\text{g})$
I	1.0	0	0
C	-2x	+2x	+x
E	$1.0 - 2x$	2x	x

$$\frac{[\text{NO}]^2 [\text{O}_2]}{[\text{NO}_2]^2} = K$$

$$\frac{(2x)^2 (x)}{(1.0 - 2x)^2} = 49.85$$

small x approx

$$4x^3 = 49.85$$

$$x = 2.318$$

← unphysical!
but will test anyway

Test x

$$\frac{2(2.318)}{1.0} \times 100\% = 463\% \text{ TOO BIG!}$$

$$[\text{NO}_2]_{\text{eq}} = 1.0 - 2(0.456)$$

$$= 0.088 \text{ M}$$

$$[\text{NO}]_{\text{eq}} = 2(0.456)$$

$$= 0.912 \text{ M}$$

$$[\text{O}_2]_{\text{eq}} = 0.456 \text{ M}$$

$$4x^3 = 49.85 (1.0 - 4x + 4x^2)$$

$$4x^3 = 49.85 - 199.4x + 199.4x^2$$

$$4x^3 - 199.4x^2 + 199.4x - 49.85 = 0$$

$$x_1 = 0.456$$

$$x_2 = 0.559$$

$$x_3 = 48.83$$

Can we still avoid the cubic even though small 'x' did not work?
Try starting with all products! (convert all reactants to products). So...

	$2\text{NO}_2(\text{g})$	$2\text{NO}(\text{g})$	$\text{O}_2(\text{g})$
I	0	1.0	0.5
C	+2x	-2x	-x
E	2x	$1.0 - 2x$	$0.5 - x$

$$\frac{[\text{NO}]^2 [\text{O}_2]}{[\text{NO}_2]^2} = K$$

$$\frac{(1.0 - 2x)^2 (0.5 - x)}{(2x)^2} = 49.85$$

$$(1.0 - 4x + 4x^2)(0.5 - x) = 199.4x^2$$

$$0.5 - x - 2x - 4x^2 + 2x^3 - 4x^3 = 199.4x^2$$

$$4x^3 + 201.4x^2 + 3x - 0.5 = 0$$

$$x_1 = -50.3 \quad x_2 = -0.05 \quad x_3 = 0.0429$$

small x approx

$$\frac{(1.0)^2 (0.5)}{(2x)^2} = 49.85$$

$$0.5 = 49.85(4x^2)$$

$$0.5 = 199.4x^2$$

$$x = 0.0500$$

Test x (<5%)

$$\frac{2(0.0500)}{1} \times 100\% = 10\% \text{ TOO BIG!}$$

$$\frac{2(0.0500)}{0.5} \times 100\% = 20\% \text{ TOO BIG!}$$

STILL DID NOT WORK ☹️