R: check phases, pressure and adsorption

Solution page 1 | Read only after attempting R1-R2. All values are synthetic teaching definitions.

R1. Fixed temperature and free volume

1. ncap=(10 kPa)(1 L)/[(8.314462618 kPa L mol^{-1} K^{-1})(300 K)]=**0.004009079 mol**.

2. Only 0.002 mol is available. Since this is less than ncap, all the volatile solid disappears: ngas=0.002 mol and nsolid=0.

3. PA=(0.002)(8.314462618)(300)/1=**4.988678 kPa**. The partial pressure is below Psub because the inventory is insufficient to saturate the gas.

4. Adding 0.002 mol inert at the same T and V gives Pinert=4.988678 kPa and **Ptotal=9.977355 kPa**. PA stays 4.988678 kPa under these ideal-gas, nonreacting, nonadsorbing assumptions.

The presence or absence of solid does not establish ideal-gas behavior. Ideal-gas behavior is an assumption of the model. At nA=ncap exactly, ngas=ncap, nsolid=0 and PA=Psub at the phase boundary.

R2. Check the candidate pressure independently

1. At PA=10 kPa, ngas=10×1/(8.314462618×300)=**0.004009079 mol**.

2. q=qs bPA/(1+bPA)=2×0.1×10/(1+0.1×10)=**1 mol/kg**. Thus nads=0.010 kg×1 mol/kg=**0.010000 mol**.

3. ngas+nads=**0.014009079 mol**, exceeding the specified 0.010 mol feed. Therefore 10 kPa is not the equilibrium pressure for this feed.

4. A numerical root of 0.010=PA/(R·300)+0.010[2×0.1PA/(1+0.1PA)] is **PA=6.080248 kPa**. It gives ngas=0.002437619 mol and nads=0.007562381 mol.

The final sum equals 0.010 mol, and both amounts satisfy their own equations at the same pressure. Simply defining nads=feed−ngas would close the sum without checking the isotherm.

A-B: quotient, driving force and two K routes

Solution page 2 | Checks for worksheet pp. 2-3. Use a consistent reaction and standard-state basis.

A1-A3. Mole table and dimensionless quotient

With $f=\xi/(1\ \text{mol})$: $n_{A_2}=(1-f)$ mol, $n_A=2f$ mol and $n_{total}=(1+f)$ mol. Nonnegative amounts require $0\le f\le 1$. The atom inventory is $2(1-f)+2f=2$ mol of atoms.

$y_{A_2}=(1-f)/(1+f)$, $y_A=2f/(1+f)$. For ideal gases $a_i=y_iP/p^\circ$, so **$Q=[4f^2/(1-f^2)](P/p^\circ)$**. This expression is finite and positive for $0<f<1$.

At $f=0.50$: $n_{A_2}=0.50$ mol, $n_A=1.00$ mol, $y_{A_2}=1/3$ and $y_A=2/3$. $Q=4/3$ at $P/p^\circ=1$ and $Q=16/3$ at $P/p^\circ=4$. These trial states have not yet been required to satisfy $Q=K$.

B1. Driving force at 350 K

At $Q=1$, $\Delta_rG=-4000+RT\ln 1=$ **-4000 J/mol**: increasing extent is favored.

At $Q=10$, $\Delta_rG=-4000+(8.314462618)(350)\ln 10=$ **$+2700.665$ J/mol**: decreasing extent is favored.

B2. Direct Gibbs route

Convert -4.000 kJ/mol to -4000 J/mol. $\ln K=-(-4000)/(8.314462618\times 350)=$ **1.3745412**. $K=\exp(1.3745412)=$ **3.9532626**. K is dimensionless.

B3-B4. Enthalpy-entropy route and interpretation

$\Delta_rG^\circ=50000-350(54000/350)=50000-54000=$ **-4000 J/mol**. Substituting into the same Gibbs relation gives the same $\ln K$ and K.

The synthetic inputs were defined to agree at the reference temperature. Agreement checks consistent signs, units and reaction basis. It does not independently validate real-compound properties or the ideal-gas approximation.

K depends on temperature for a fixed reaction and standard-state convention. It is not the current reaction quotient unless the specified composition is at equilibrium.

C: solve the equilibrium and change pressure

Solution page 3 | Checks for worksheet pp. 3-4. Initial amounts: 1 mol A_2 and no A or inert gas.

C1. Rearrange Q=K

Write $p=P/p^\circ$. $K(1-f^2)=4pf^2$, so $K=f^2(K+4p)$. Therefore **$f=\sqrt{[K/(K+4p)]}$**. The positive root lies between 0 and 1 for $K>0$ and $p>0$.

C2-C3. Reference case at 350 K and 100 kPa

Here $p=1$ and $K=3.9532626$. $f=\sqrt{[3.9532626/(3.9532626+4)]}=$**0.7050261**. Hence $\xi=0.7050261$ mol.

Quantity	Value
nA_2 / mol	0.294973941
nA / mol	1.410052118
ntotal / mol	1.705026059
yA_2	0.173002600
yA	0.826997400
$Q = (yA^2/yA_2)(P/p^\circ)$	3.953262552

The atom check gives $2\times0.294973941+1.410052118=2.000000000$ mol of atoms. Total molecular moles increase because one A_2 molecule produces two A molecules. Conserving total molecular moles would contradict the stoichiometry.

C4. Same temperature, four times the pressure

At P=400 kPa, $p=4$ while K remains 3.9532626. $f=\sqrt{[K/(K+16)]}=$**0.4451136**, so $\xi=0.4451136$ mol.

$nA_2=0.554886393$ mol, $nA=0.890227214$ mol, $yA_2=0.383974236$ and $yA=0.616025764$. Recomputed Q remains 3.9532626 and the atom amount remains 2 mol.

At a fixed trial composition, Q is proportional to pressure for $\Delta\nu=+1$. Compression raises Q above the unchanged K, so the reverse reaction reduces extent until Q=K. This is a fixed-total-pressure equilibrium comparison, distinct from adding inert gas at fixed volume.

D: read the calculator and keep the right evidence

Solution page 4 | Worksheet p. 4. The guide provides exact controls, export and restore instructions.

D1-D3. Reference controls and the pressure comparison

Reset the synthetic example, then explicitly set Cp from 30 to **0** and the extent K source to **Direct ΔrG° at its supplied T**. Keep the standard pressure at 100 kPa. At 350 K, the direct Gibbs and constant H/S routes agree. Return to direct Gibbs before saving 12A and 12B.

Case	T / K	P / kPa	K	ξ / mol
12A	350	100	3.953263	0.705026
12B	350	400	3.953263	0.445114

D4. Q and a conserved amount

For 12B, $Q=(0.616025764^2/0.383974236)\times4=3.9532626$. The atom check gives $2\times0.554886393+0.890227214=2.0000000$ mol of A atoms.

The reaction graph has ξ / mol on the horizontal axis and [G(ξ)−G(0)]/(RT) / mol on the vertical axis. The marked state is the minimum of this one-reaction ideal-gas model at fixed T and P. The relative energy reference can shift vertically without changing the minimum location.

A separate panel contains separate observations

The default observation table has $yA_2=0.2$ and $yA=0.8$. At 100 kPa it gives $Q=0.8^2/0.2=$**3.2**, which differs from K=3.953263. At 400 kPa the same fractions give Q=12.8. This is expected for independent trial inputs.

The extent solver returns a different composition that satisfies Q=K. Do not interpret a nonzero driving force in the supplied-observation panel as failure of the equilibrium solver. Read the selected K-source label and the equilibrium-composition table.

What the checks establish

Agreement, a small lnQ−lnK residual and atom conservation support the calculation within the specified model. They do not validate real property data, the ideal-gas assumption, or the absence of additional reactions and phases.

If a run was blocked, retain the error and the independent calculation. A missing calculator value is not zero and is not evidence of a successful Lab run.

E-F: temperature law, restored evidence and completion

Solution page 5 | Worksheet pp. 5-6. Constant ΔH°=50 kJ/mol and ΔCp°=0 over 350-400 K.

E1. Integrated van't Hoff calculation

ln[K400/K350]=(50000/8.314462618)(1/350−1/400)=**2.1477206**. Add lnK350=1.3745412 to obtain **lnK400=3.5222618**, then **K400=33.8609295**.

E2. Consistent thermal cross-check

With the same constant H and S definitions: ΔrG°(400)=50000−400(54000/350)=**−11714.2857 J/mol**. Thus −ΔrG°/(R·400)=3.5222618. This agreement relies on ΔCp°=0 and the consistent reference values.

E3. Composition at 400 K and 100 kPa

f=√[33.8609295/(33.8609295+4)]=**0.9457009**. ξ=0.9457009 mol, nA_2=0.054299101 mol, nA=1.891401798 mol, yA_2=0.027907219 and yA=0.972092781. The atom amount stays 2 mol and Q=33.8609295.

F1-F3. Read, export and restore

For 12C, select **van ’t Hoff · constant ΔH°**, T=400 K and P=100 kPa. Keep Tref=350 K and Cp=0. The direct and formation Gibbs energies supplied at 350 K are unavailable at 400 K because no new point property has been provided.

Use **Restore calculator study JSON** with your 12A file. It restores and recalculates automatically. Recovered settings should include 350 K, 100 kPa, direct Gibbs source and Cp=0. The expected fresh result is K=3.953263 and ξ=0.705026 mol.

12A→12B changes the composition-dependent Q relation through pressure while K is unchanged. 12A→12C changes the standard Gibbs energy and K through the specified temperature law. Both comparisons retain the same reaction, standard states and initial inventory.

G. Exit ticket and feedback

Give your own explanation and one numerical check, with units and conditions. Report actual time and one exact unresolved step if any. Submit once and wait for the receipt. Keep corrections and exported studies for the classroom discussion on 13 November. No additional required assignment follows.