Lab 12: two routes and one pressure change

Guide page 1 | Worksheet D, p. 4 | Setup at slide 19, demonstration at 20, independent work at 21.

Open the Chemical equilibrium Lab

Select **Reset synthetic example**. This restores defaults, including Cp=30 and a corrected van't Hoff route. Change the two settings below explicitly. Keep the reaction $A_2 \rightleftharpoons 2A$ and formal atom counts supplied by the example.

Field / control	Required setting
Evaluation temperature / K	350
Reference temperature / K	350
Gas standard pressure p° / kPa	100
Observation and extent pressure / kPa	100 for 12A; 400 for 12B
Nonreacting ideal gas in extent feed / mol	0
Direct ΔrG° / kJ per mol of reaction	−4; its data temperature remains 350 K
ΔrH°(Tref) / kJ mol^{-1}	50
ΔrS°(Tref) / J mol^{-1} K^{-1}	154.28571428571428
Constant ΔrCp° / J mol^{-1} K^{-1}	Change 30 to 0
Reference K input convention / value	ln Kref / 1.3745412004882978
K source for extent and driving force	Direct ΔrG° at its supplied T
Initial amounts in the species table	A_2: 1 mol; A: 0 mol

12A: reference state and route check

1. Click **Compare K methods**. Inspect the method table, then **From K to equilibrium composition**. Record K, ξ, equilibrium mole fractions and the atom-balance residual.

2. Select **ΔH°/ΔS° · constant values** as K source. Recalculate and compare at 350 K. Return to **Direct ΔrG°**, recalculate, and click **Export complete study**. Name the downloaded file 12A or identify it clearly in your records.

12B: change only actual total pressure

3. Set actual pressure to **400 kPa**, leaving p°=100 kPa and T=350 K. Recalculate, record and export 12B. Compare with your hand calculation. Input changes invalidate old results.

Two different Q contexts: Observed activities uses independent input mole fractions 0.2 and 0.8. At 100 kPa these give Q=3.2, which differs from K. Use the **equilibrium composition** table for your solver Q=K check. Do not change the equilibrium assertion just to force agreement.

Lab 12: a temperature law and a restored study

Guide page 2 | Worksheet F, p. 5 | Attempt at slide 29. Demonstration and check at slide 30.

12C: raise temperature at the baseline pressure

1. Starting from your reference data, select **van ’t Hoff · constant ΔH°** for **K source for extent and driving force**. Set **Evaluation temperature=400 K** and actual **pressure=100 kPa**. Keep Cp=0, inert gas=0 and p°=100 kPa.

2. Keep Tref=350 K, lnKref=1.3745412004882978, Href=50 kJ/mol and Sref=154.28571428571428 J mol^{-1} K^{-1}. The direct and formation Gibbs-data temperature labels stay at 350 K. Their point-data routes will be unavailable at 400 K. This is an applicability check, not a missing zero.

3. Click **Compare K methods**. Read the selected van't Hoff K and the equilibrium composition. Record 12C in the worksheet. Independently check Q and the atom inventory. Export the complete study as 12C.

Reopen an actual exported calculator study

4. In **Restore calculator study JSON**, choose your 12A complete-study file. This calculator control restores inputs and automatically recalculates. Verify 350 K, 100 kPa, direct Gibbs source, Cp=0, the initial amounts and the fresh result. Record one matching value.

5. Keep the three files and your worksheet. A restored record does not prove the physical model. It demonstrates that the saved settings can reproduce the calculation.

If you use Study workspace instead

Study workspace also imports studies or comparison JSON files. Its **Restore** action loads inputs; click **Compare K methods** afterward to obtain a fresh result. The two restore controls behave differently. A comparison file is optional for this lesson.

Troubleshooting and scope

If Export is disabled, recalculate after changing inputs. If extent is unavailable at 400 K, check that the selected K source is the constant-enthalpy van't Hoff route. Do not relabel the direct 350 K property as a 400 K property.

The extent solver assumes one neutral ideal-gas reaction at fixed T and total P. It excludes charged gas species, multiple reactions, nonideal EOS effects and phase splitting. Gas activity coefficients in the independent observations panel are not an EOS for this solver.

The temperature graph uses T on its horizontal axis and the selected logarithm of K on the vertical axis. With Cp=0 and mutually consistent reference data, some curves overlap. The reaction graph uses ξ / mol and [G(ξ)−G(0)]/(RT) / mol. Neither is a kinetic time trace.

Stop rule: use the worksheet pause budgets. If blocked, write the exact step or error, retain your hand calculations and continue. Bring the question on 13 November.