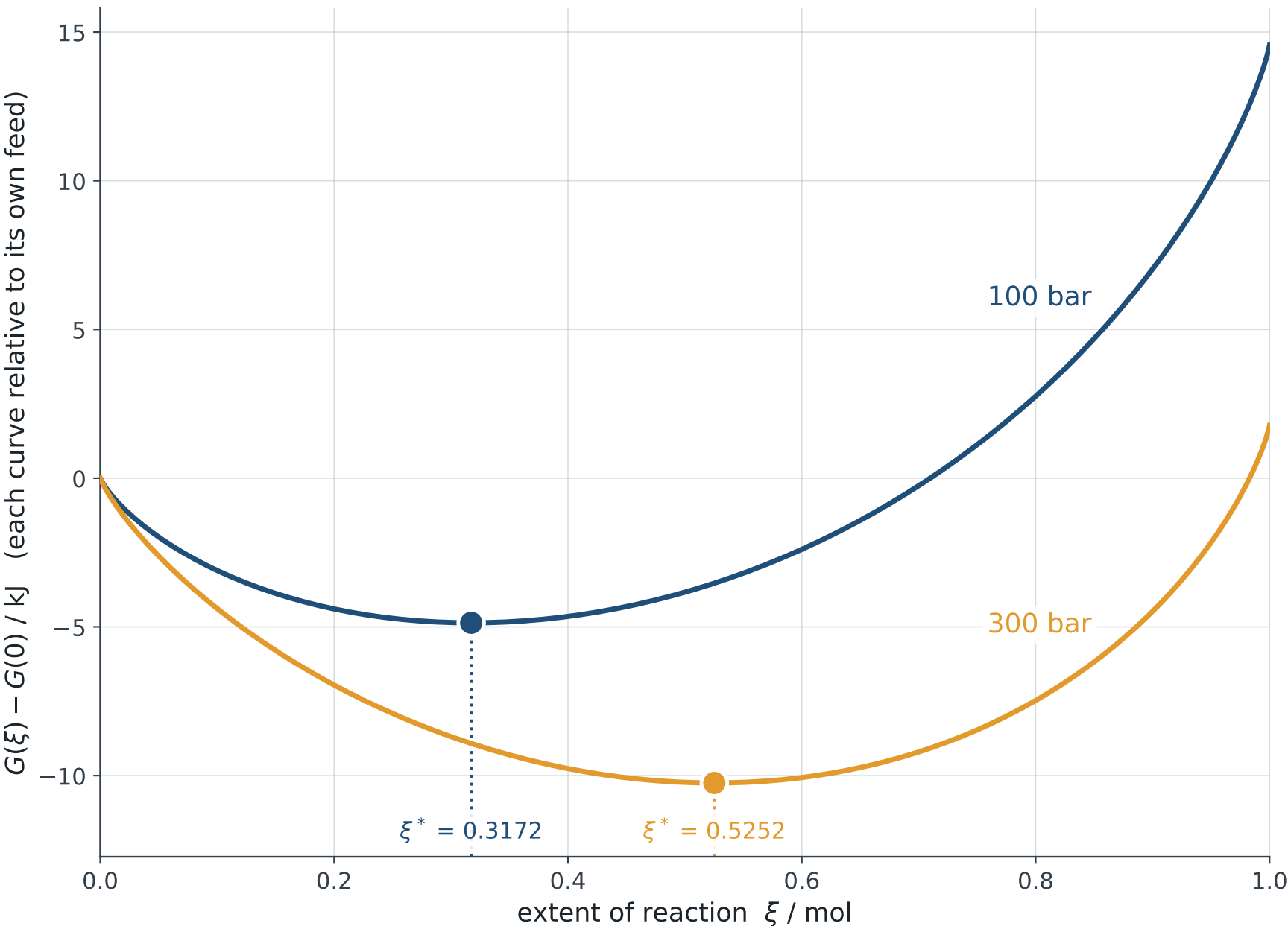


The equilibrium composition is where G is a minimum — and pressure moves it even though K does not



$\text{N}_2 + 3 \text{H}_2 \rightarrow 2 \text{NH}_3$
 feed 1 : 3 : 0 mol, $T = 700 \text{ K}$, ideal gas
 $\Delta H_{298}^\circ = -91.12 \text{ kJ/mol}$ $\Delta G_{298}^\circ = -32.05 \text{ kJ/mol}$
 $\Delta G^\circ(700 \text{ K}) = 55.07 \text{ kJ/mol}$
 $K(700 \text{ K}) = 7.77\text{e-}05$ — the same at both pressures
 feasible window from `extent\_bounds`:
 $\xi = -0.000$ to 1.000 mol

$P = 100 \text{ bar}$
 $\xi^* = 0.31723 \text{ mol}$ $y_{\text{NH}_3} = 0.1885$
 $G(\xi^*) - G(0) = -4.863 \text{ kJ}$
 $|\xi^* \text{ from `solve_extent`} - \xi^* \text{ from min } G|$
 $= 7.9\text{e-}08 \text{ mol}$

$P = 300 \text{ bar}$
 $\xi^* = 0.52517 \text{ mol}$ $y_{\text{NH}_3} = 0.3561$
 $G(\xi^*) - G(0) = -10.248 \text{ kJ}$
 $|\xi^* \text{ from `solve_extent`} - \xi^* \text{ from min } G|$
 $= 7.0\text{e-}08 \text{ mol}$

What is ΔG° worth?
 1 kJ/mol on ΔG° is a factor 1.19 in K at 700 K
 and a factor 1.50 — 50 % — at 298 K.
 It moves ξ^* at 300 bar by +0.0157 / -0.0159 mol.
 `chemicals` gives $\Delta G_{298}^\circ = -32.05$ against the usual
 literature -32.8 kJ/mol : 0.75 kJ/mol, 30 % in K .

Formation properties from `chemicals` via `reaction.from\_chemicals`; nothing typed in.
 Curves are `total\_G`; markers are `solve\_extent`, which solves $K_a(\xi) = K(T)$ and never evaluates G .