Problem 1 (15 points total)
A pure gas is held at 50 bar and 300 K. The compressibility factor is measured to be 0.85. Using only this available data, calculate as accurately as possible the fugacity of the gas. Clearly show your logic.

Problem 1 Solution
The compressibility factor is defined as

$$z = \frac{Pv_i}{RT} \tag{1}$$

The definition for pure species fugacity is

$$g_i - g_i^o = \int_{P_{low}}^{P} v_i dP = RT \ln\left[\frac{f_i^v}{P_{low}}\right] \qquad \text{at constant T} \tag{2}$$

Substituting into (2) using (1)

$$g_i - g_i^o = \int_{P_{low}}^{P} \frac{zRT}{P} dP = RT \ln\left[\frac{f_i^v}{P_{low}}\right] \tag{3}$$

In integrating this expression, we treat z as a constant in the range of interest (P_{low} to 50 bar). This assumption is necessary to get an estimate of fugacity.

Simplifying Equation 3,

$$z \int_{P_{low}}^{P} \frac{1}{P} dP = \ln\left[\frac{f_i^v}{P_{low}}\right] \tag{4}$$

Integrating both sides, we get

$$z \ln\left[\frac{P}{P_{low}}\right] = \ln\left[\frac{f_i^v}{P_{low}}\right] \tag{5}$$

Adding ln (P_{low}) to both sides,

$$\ln\left[f_i^v\right] = z \ln P \tag{6}$$

Substituting in for z and P,

$$f_i^v = \exp(0.85 \ln[50 bar]) \tag{8}$$

$$f_i^v = 27.8\,bar \tag{9}$$

An alternative route to a fugacity estimate:

$$\ln\left[\varphi_i\right] = \int_{P_{low}}^{P} (z-1)\frac{dP}{P}$$

Again treating z_i as a constant and integrating

$$\ln\left[\varphi_i\right] = (z_i - 1)\ln\frac{P}{P_{low}}$$

Letting $P_{low} \rightarrow$ 1 bar

$$\ln\left[\frac{f_i^v}{P}\right] = (z_i - 1)\ln\left[P\right]$$

$$\ln\left[f_i^v\right] = \ln P + (z_i - 1)\ln\left[P\right]$$

Substituting in for P and z_i,

$$f_i^v = 27.8\;bar$$

Grading Scheme for Method 1

1. 1 point for $z = \dfrac{Pv_i}{RT}$
2. 3 points for $\displaystyle\int_{P_{low}}^{P} \frac{z}{P}dP = \ln\left[\frac{f_i^v}{P_{low}}\right]$
3. 3 points for stating that the pressure dependence of z is neglected
4. 5 points for $\ln\left[f_i^v\right] = z\ln P$
5. 3 points for $f_i^v = 27.8\,bar$ (2 points if no units)

Grading Scheme for Method 2

1. 3 points for $\displaystyle\ln\left[\varphi_i\right] = \int_{P_{low}}^{P} (z-1)\frac{dP}{P}$
2. 3 points for stating that the pressure dependence of z is neglected
3. 2 points for stating P_{low} is assumed to be 1 bar (Pressure at which gas behaves ideally)
4. 4 points for $\ln\left[\dfrac{f_i^v}{P}\right] = (z_i - 1)\ln\left[P\right]$
5. 3 points for $f_i^v = 27.8\,bar$ (2 points if no units)