Problem Set 2

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```
r_jmolk=8.31441
r_barcm3molk=83.1441
r_calmolk=1.987
```

Question 1

Calculate $\bar{V}_{H_2O}$ at $T = 800C$ and $P = 1000bars$ from figure of the compressibility factor as a function of P and T. For reference $P_{crit} = 220.4bar$ and $T_{crit} = 647.3K$ for pure H2O.

Reduced pressure:

```
p=1000
p_crit=220.4
press_reduced=p/p_crit
print(press_reduced)
```

```
## [1] 4.537205
```

Reduced temperature:

```
t=800+273.15
t_crit=647.3
t_reduced=t/t_crit
print(t_reduced)
```

```
## [1] 1.657887
```

From the figure: $Z = 0.88$

$Z \equiv \frac{P\bar{V}}{RT}$ so $\bar{V} = \frac{ZRT}{P}$

```
z=0.88
molar_volume=z*t*r_barcm3molk/p
print(molar_volume)
```

```
## [1] 78.51896
```

We get $78.52cm^3$ as the molar volume of pure water at 800C and 1000 bars.

Question 2

Calculate $\bar{V}_{H_2O}$ and $f^{P,T}_{H_2O}$ at $T = 800C$ and $P = 1000bars$ from the modified Redlich-Kwong equation of state. Use the following formulations for the attraction coefficient (a) and the excluded volume (b) from Bowers and Helgeson (1983) where T is in C.

```
t_c=800
a=10^6*(111.3+50.7*exp(-0.983*10^(-2)*t_c))
b=14.6
```

Question 3

Question 4

Question 5