KMM 102E
Introduction to Computer Programming in Python
2021 - 2022 Spring

Homework Assignment #: 5

Equations of states have been developed to characterize the real PVT behavior of the pure substances and their mixtures. There are more than 25 million chemicals, leading to an infinite number of different mixtures. Among the equations of state, the **Redlich–Kwong equation of state** is written as follows:

$$P = \frac{RT}{V-b} - \frac{a}{V\,(V+b)}$$

Rearrangement of this relation yields molar volume:

$$V_{i+1} = \frac{R.T}{P} + b - \frac{a.(V_i - b)}{P.V_i.(V_i + b)}$$

where V is molar volume, P is pressure, T is temperature in Kelvin, and a and b are the constants specific to the species. a and b values could be calculated based on the following relations:

$$a = 0.42748\left(\frac{R^2 T_C^2}{P_C}\right)\alpha,\;\; b = 0.08664\left(\frac{RT_C}{P_C}\right), \text{ and } \; T_r = \frac{T}{T_C}, \quad \alpha = \frac{1}{T_r^{0.5}}$$

In these equations, Tc is the critical temperature (in absolute terms), Pc is the critical pressure, and Tr is the 'reduced' temperature (the absolute temperature divided by the critical temperature). The α is particular to the Redlich–Kwong equation of state.

Write the **shortest** computer program in Python evaluating the molar volume of specified pure species. Your program must meet the following requirements:

- Generate a variable called DATA in two dimensional list structure form whose each element contains the substance name, its critical temperature (Tc) and its critical pressure (Pc) information for the given substances available within the **PureSpecies.txt** file.
- Lists the substance names available within the DATA variable properly, and then let the user choose a substance whose molar volumes need to be determined.
- Let user enter a temperature value (in kelvin).
- A user-defined function called as "**redlichkwong**" in which $\boldsymbol{a}$ and $\boldsymbol{b}$ *constants* of Redlich–Kwong equation of state are evaluated must be created properly.
- Use list comprehension structure to create a variable named P containing the pressure values ranged from 1 to 20 bar with increments by 2.
- Use list comprehension structure to create a variable named Vi whose elements containing the initial molar volumes based on the following ideal gas equation of state for a given temperature and pressures:

$$P.V = R.T$$

- Calculate the molar volumes and store them in a list-structured variable named *MolarVolume*. For the calculation of molar volume, start with an initial value of V_i calculated for each pressure and then perform the evaluations properly until $|V_{i+1} - V_i| \leq$ 1E-4 is satisfied.

Homework Given Date	:	31.05.2022
Homework Due Date	:	8.06.2022 (*Ninova*) Wednesday
	:	Hard copy until 9.06.2022 Thursday.

Prepared by:

Number	Name	Signature

P.S. You must submit the **hardcopy** of the codes with the **output** results. **The codes must be the same as the files uploaded to Ninova! Both must be submitted**, otherwise your homework will not be evaluated.

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- For a given user-entered temperature value, display a and b constants of Redlich–Kwong equation of state in 4 digits. $P(kPa)$ and $V\ (m^3/kmol)$ values in a suitable tabulated form must also be displayed in 0 and 4 digits, respectively.
- Plot $V\ (m^3/kmol)$ vs $P(kPa)$ for the chosen substance using matplotlib module of Python.

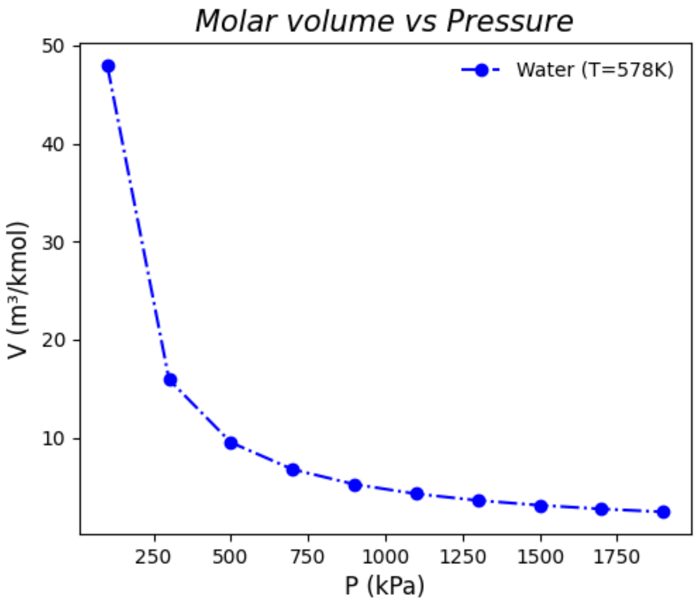
Your output should look like the following:

```
List of substances:
 ===============
1 Methane
2 Ethane
3 Propane
4 Isobutane
5 Isooctane
6 Ethylene
7 Propylene
8 Benzene
9 Acetylene
10 Toluene
11 Acetone
12 Methylamine
13 Ethylamine
14 Chloroform
15 Argon
16 Oxygen
17 Nitrogen
18 Chlorine
19 Water
20 Ammonia
===============
Choose one of the substance: 19
Enter the temperature (K): 578

Redlich Kwong constants of Water are:
a = 593.6564 kPa.m⁶/kmol²
b = 0.0211 m³/kmol

P(kPa)  V(m³/kmol)

 100     47.9547
 300     15.9162
 500      9.5083
 700      6.7618
 900      5.2359
1100      4.2647
1300      3.5922
1500      3.0990
1700      2.7217
1900      2.4238
```



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