In[1979]:=

```
(*
Lab: Equations of State M8
Author: Jared Frazier
Description:

Reproduce isotherm and compressibility factor figures from Physical Chemistry: A Molecular Approac

Course: CHEM 4361
*)
Clear["Global`*"]

(**********************)
(*Question 2: Isotherms*)
(**********************)
(*Gas constant in (L * bar)/(mol * K)*)
universalGasConstR = 0.083145;

pressureVdwFuncOfVandT[a_, b_, temp_, vol_] := (

(*
The van der Wals equation P (V, T)
:param a: Gas constant 'a' (L^2 bar/mol^2)
:param b: Gas constant 'b' (L/mol)
:param temp: Temperature (K)
:param vol: Volume (liter)
:return: Pressure (bar)
*)
  (universalGasConstR * temp)/(vol - b) - a/(vol * vol)
)

pressureIdealGas[temp_, vol_] := (

(*
The pressure for an ideal gas
:param temp: Temperature (K)
:param vol: Volume (L)
:return: Pressure (bar)
*)
  (universalGasConstR * temp)/vol
)

(*Gas constants for CO2*)
vdwConstsForCO2 = ChemicalData["CarbonDioxide", "VanDerWaalsConstants"] ;
aConstCO2 = vdwConstsForCO2[[1, 1]];
bConstCO2 = vdwConstsForCO2[[2, 1]];
```

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(*Pressure Volume Plots*)

(*For both plots*)
volumeListForPlot = Range[1, 25];
t1 = 303;
t2 = 350;
t3 = 400;

(*Plot Pvdw*)
t1Pressures = pressureVdwFuncOfVandT[aConstCO2, bConstCO2, t1, volumeListForPlot];
t2Pressures = pressureVdwFuncOfVandT[aConstCO2, bConstCO2, t2, volumeListForPlot];
t3Pressures = pressureVdwFuncOfVandT[aConstCO2, bConstCO2, t3, volumeListForPlot];
ListLinePlot[
    {t1Pressures, t2Pressures, t3Pressures},
    PlotLabel→"Question 2a: Isotherm Pressure-Volume Curve for CO2",
    AxesLabel→{"Volume (L)", "Pressure (Bar)"},
    PlotLegends→{"T1 = 303 K", "T2 = 350 K", "T3 = 400 K"},
    PlotStyle→{Dotted, Dashed, Thick},
    PlotRange→Full,
    ImageSize→Large
]

(*Plot Pvdw - Pideal*)
t1PressuresIdeal = pressureIdealGas[t1, volumeListForPlot];
t2PressuresIdeal = pressureIdealGas[t2, volumeListForPlot];
t3PressuresIdeal = pressureIdealGas[t3, volumeListForPlot];
ListLinePlot[
    {t1Pressures - t1PressuresIdeal, t2Pressures - t2PressuresIdeal, t3Pressures - t3PressuresIde
    PlotLabel→"Question 2b: Isotherm Pressure-Volume Curve for CO2",
    AxesLabel→{"Volume (L)", "Pvdw - Pideal (Bar)"},
    PlotLegends→{"T1 = 303 K", "T2 = 350 K", "T3 = 400 K"},
    PlotStyle→{Dotted, Dashed, Thick},
    PlotRange→Full,
    ImageSize→Large
]
(******************************************)
(*Question 3: Function for Molar Volume*)
(******************************************)
vdwExpression = (P + a/V^2)*(V - b) - R*T;   (*From eq (7) in the handout*)
vdwVolumeExpression = Solve[vdwExpression==0, V];  (*Set to 0 and solve for Volume*)
realVdwVolumeExpression = V/. vdwVolumeExpression[[1, 1]];  (*The only real solution expression*)
molarVolumeRealFunction[a_, b_, P_, R_, T_] := (
(*
Given several gas arguments, return the real molar volume of the gas.
:param a: Gas Constant.
:param b: Gas Constant.
:param P: Pressure (Bar).
:param R: Universal Gas Constant.
:param T: Temperature (K).
```

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:return: The real molar volume of the gas.
*)
    Evaluate[realVdwVolumeExpression]
)
molarVolumeIdealFunction[P_, R_, T_] := (

(*
Return the ideal molar volume of a gas.
:param P: Pressure (Bar).
:param R: Universal Gas Constant.
:param T: Temperature (K).
:return: The ideal molar volume of the gas.
*)
    Return[(R * T)/P]
)

(****************************************)
(*Question 4: Compressibility Factor      *)
(****************************************)

(*Gas constants*)
(*Helium gas (He)*)
vdwConstsForHe = ChemicalData["Helium", "VanDerWaalsConstants"] ;
aConstHe = vdwConstsForHe[[1, 1]];
bConstHe = vdwConstsForHe[[2, 1]];
(*Nitrogen gas (N2)*)
vdwConstsForN2 = ChemicalData["Dinitrogen", "VanDerWaalsConstants"];
aConstN2 = vdwConstsForN2[[1, 1]];
bConstN2 = vdwConstsForN2[[2, 1]];
(*Methane gas (CH4)*)
vdwConstsForCH4 = ChemicalData["Methane", "VanDerWaalsConstants"];
aConstCH4 = vdwConstsForCH4[[1, 1]];
bConstCH4 = vdwConstsForCH4[[2, 1]];

(*Pressure list for plot*)
pressureListForPlot = Range[1, 1000];

(*V̅_0 and V_some_gas*)
heMolarVolumeRealData = molarVolumeRealFunction[aConstHe, bConstHe, pressureListForPlot, universa
n2MolarVolumeRealData = molarVolumeRealFunction[aConstN2, bConstN2, pressureListForPlot, universa
ch4MolarVolumeRealData = molarVolumeRealFunction[aConstCH4, bConstCH4, pressureListForPlot, unive
molarVolumeOfIdealGas = molarVolumeIdealFunction[pressureListForPlot, universalGasConstR, 300];

(*Compressibility Data for Plot*)
zHe = heMolarVolumeRealData / molarVolumeOfIdealGas;
zN2 = n2MolarVolumeRealData / molarVolumeOfIdealGas;
zCH4 = ch4MolarVolumeRealData / molarVolumeOfIdealGas;
idealGas = ConstantArray[1, 1000];
```

```
(*Plot the compressibility factors*)
ListLinePlot[
    {zHe, zN2, zCH4, idealGas},
    PlotLabel→"Question 4: Compressibility Factor",
    AxesLabel→{"Pressure (bar)", "Z = V̄/V̄₀"},
    PlotLegends→{"He", "N₂", "CH₄", "Ideal Gas"},
    PlotStyle→{Dotted, Dashed, Thick, DotDashed},
    PlotRange→Full,
    ImageSize→Large
]

(*****************************************)
(*Question 5: VDW to Virial             *)
(*****************************************)
(*Import data*)
pathToIsothermData = FileNameJoin[{NotebookDirectory[], "isotherm.dat"}];
isothermData= Import[pathToIsothermData, "FieldSeparators"→"\t"];

(*Make list of volumes*)
volumeList = {};
For[row=2, row ≤ Length[isothermData], row++,
    AppendTo[volumeList, isothermData[[row,1]]]
]

(*Make list of P(T₁)*)
pT1List = {};
For[row=2, row ≤ Length[isothermData], row++,
    If[isothermData[[row, 2]] == "NULL",
        AppendTo[pT1List, Null],
        AppendTo[pT1List, ToExpression[isothermData[[row,2]]]]
        ]
]

(*Make list of P(T₂)*)
pT2List = {};
For[row=2, row ≤ Length[isothermData], row++,
    AppendTo[pT2List, ToExpression[isothermData[[row, 3]]]]
]

(*Make list of P(T₃)*)
pT3List = {};
For[row=2, row ≤ Length[isothermData], row++,
    AppendTo[pT3List, ToExpression[isothermData[[row, 4]]]]
]

(*Make list of P(T₄)*)
pT4List = {};
```

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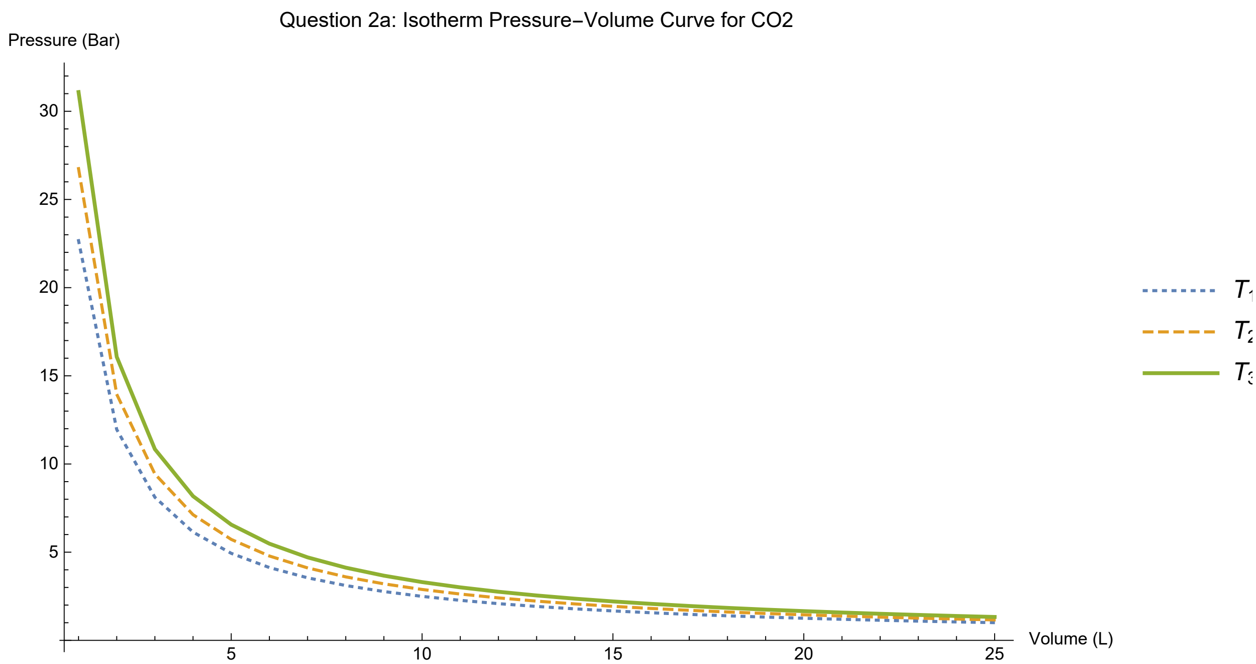
For[row=2, row ≤ Length[isothermData], row++,
    AppendTo[pT4List, ToExpression[isothermData[[row, 5]]]]
]
(*Join lists*)
dataT1 = Transpose @ {volumeList, pT1List};
dataT2 = Transpose @ {volumeList, pT2List};
dataT3 = Transpose @ {volumeList, pT3List};
dataT4 = Transpose @ {volumeList, pT4List};
(*Plot data*)
ListLinePlot[
    {dataT1, dataT2, dataT3, dataT4},
    PlotLabel→"Question 5b: (V̄ - P) Plots for CO2",
    AxesLabel→{"Volume (L)", "P(Tj)"},
    PlotLegends→{"@ T1", "@ T2", "@ T3", "@ T4"},
    PlotStyle→{Dotted, Dashed, Thick, DotDashed},
    PlotRange→Full,
    ImageSize→Large
]

(*Derive parameters for non-linear fit*)
virialEOS = universalGasConstR * ((1/V) + (B2/V^2) + (B3/V^3));  (*Tj is omitted for now as it is
nlm1 = NonlinearModelFit[dataT1[[4;;23]], virialEOS, {B2, B3}, V]["BestFitParameters"];  (*For on
nlm2 = NonlinearModelFit[dataT2, virialEOS, {B2, B3}, V]["BestFitParameters"];
nlm3 = NonlinearModelFit[dataT3, virialEOS, {B2, B3}, V]["BestFitParameters"];
nlm4 = NonlinearModelFit[dataT4, virialEOS, {B2, B3}, V]["BestFitParameters"];

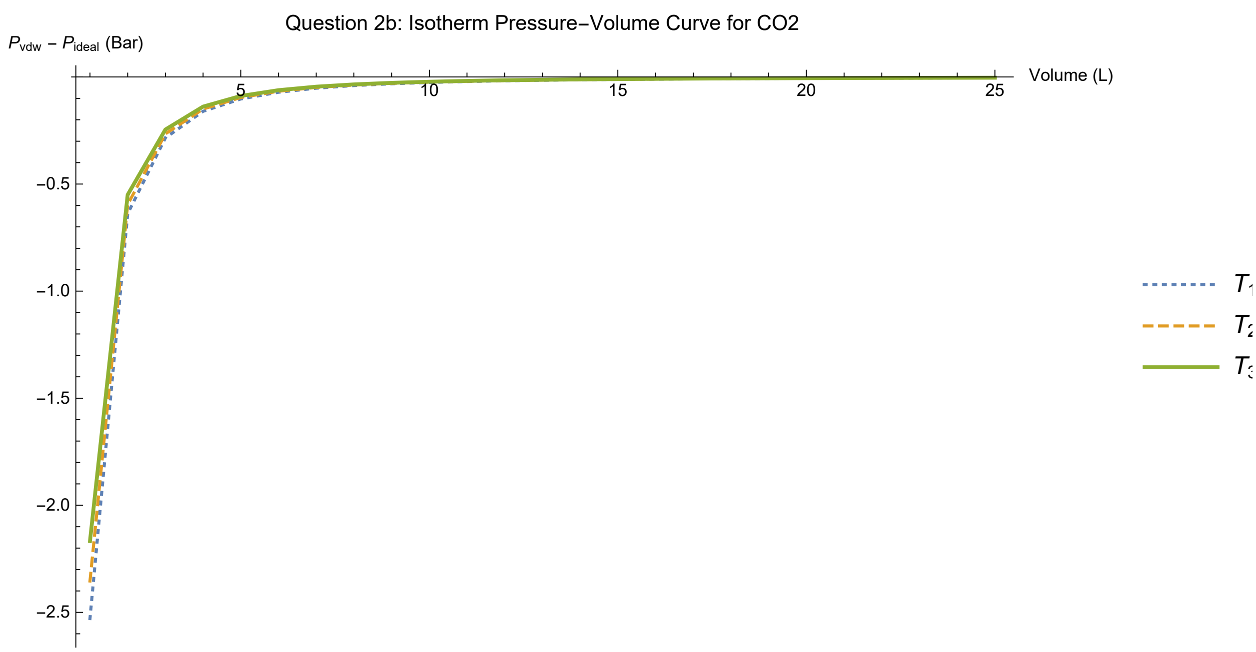
Print["Parameters for T1:", nlm1]
Print["Parameters for T2:", nlm2]
Print["Parameters for T3:", nlm3]
Print["Parameters for T4:", nlm4]
(*Derive the temperature*)
(*Since lim V→inf (PV/R) = T, then the maximum V will be used to estimate the Tj*)
maxVol = Max[volumeList];
indexOfMaxVol = Position[volumeList, maxVol][[1]];
t1 = pT1List[[indexOfMaxVol]] * maxVol / universalGasConstR;
t2 = pT2List[[indexOfMaxVol]] * maxVol / universalGasConstR;
t3 = pT3List[[indexOfMaxVol]] * maxVol / universalGasConstR;
t4 = pT4List[[indexOfMaxVol]] * maxVol / universalGasConstR;

(*Log Results*)
Print[]
Print["Question 5c: Temperatures for each isotherm:"]
Print["T1 = ", t1[[1]], " K"]
Print["T2 = ", t2[[1]], " K"]
Print["T3 = ", t3[[1]], " K"]
Print["T4 = ", t4[[1]], " K"]
```

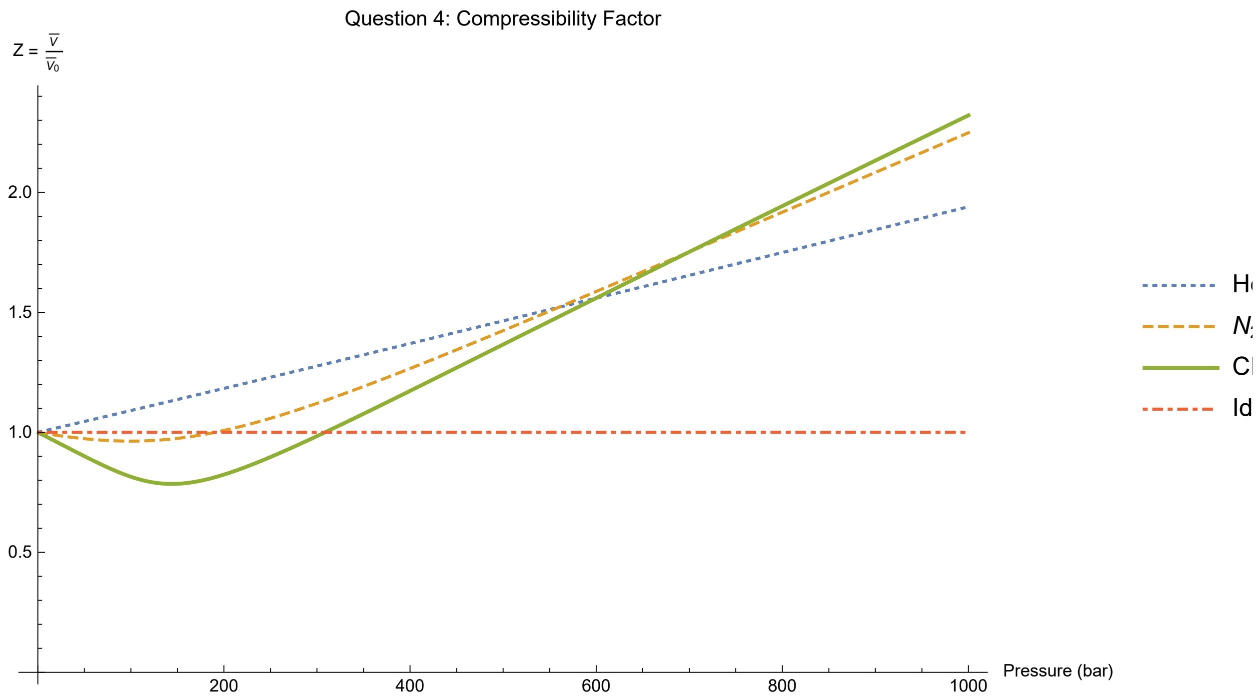
Out[1993]=



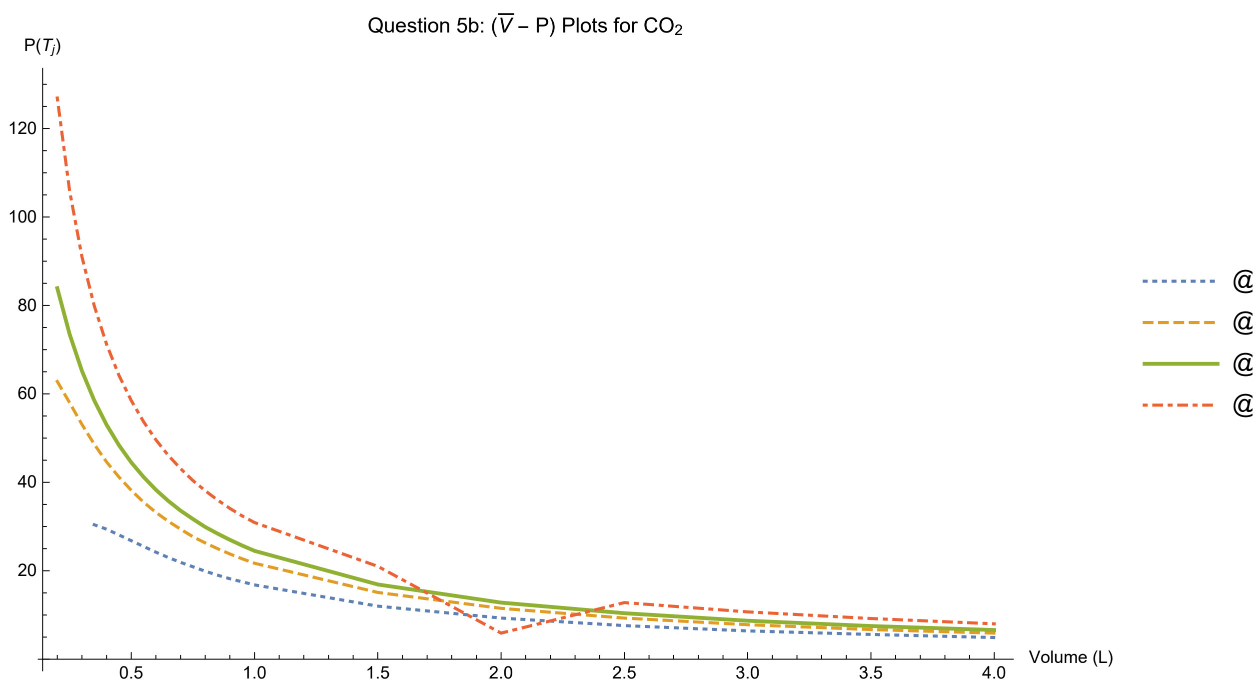
Out[1997]=



Out[2021]=



Out[2038]=



Parameters for T_1:$\{B_2 \to 216.583, B_3 \to -62.6143\}$

Parameters for T_2:$\{B_2 \to 160.26, B_3 \to -26.9935\}$

Parameters for T_3:$\{B_2 \to 184.247, B_3 \to -29.8556\}$

Parameters for T_4:$\{B_2 \to 237.669, B_3 \to -36.6128\}$

Question 5c: Temperatures for each isotherm:

T_1 = 235.733 K

T_2 = 283.841 K

T_3 = 317.518 K

T_4 = 384.87 K