APPROVED SOLUTION

CADET ____________________ SECTION ______ TIME OF DEPARTURE ________

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2023-2024
WRITTEN PARTIAL REVIEW III
15 November 2023, A-Hour

TEXT: Smith, Van Ness, & Abbott
SCOPE: Lessons 22-32
TIME: 55 Minutes

References Permitted: Open notes, book, internet, CHEMCAD, Mathematica, Excel.

INSTRUCTIONS

1. Do not mark this exam or open it until "begin work" is given.
2. You have 55 minutes to complete the exam.
3. There are 3 problems on 3 pages in this exam (not including the cover page). Write your name on the top of each sheet.
4. Solve the problems in the space provided and in Mathematica. Show all work to receive full credit.
5. Laptops are not authorized for referencing only. Desktop PCs must be used for all calculations.
6. Save Mathematica and CHEMCAD files on your desktop and re-save frequently.
7. When finished, upload all electronic work files to Canvas.

(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	40	
B	100	
C	60	
TOTAL CUT		
TOTAL GRADE	200	

APPROVED SOLUTION

Cadet:______________________

Problem: A

Weight: 40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate ΔH^{ig} and ΔS^{ig} for *ideal* gas-phase nitrogen compressed and heated from 298.15 K and 1 bar to 1000 K and 40 bar. Report your answers for ΔH^{ig} and ΔS^{ig} in J/mol and J/(mol·K), respectively.

Solution:

```
In[•]:= Quit[];

In[1]:= (*Nitrogen*)
        p = 40.00; (*bar*)
        t = 1000.; (*K*)

        R = 8.314; (*J/(mol*K)*)

        a = 3.280;
        b = 0.593*10^-3;
        d = 0.040*10^5;
        Cp = a + b*T + d*T^-2;

        (*enthalpy*)
        Hig = R*Integrate[Cp, {T, 298.15, t}] (*eq 2.21*)

        (*entropy*)
        Sig = R*(Integrate[Cp/T, {T, 298.15, t}] - Log[p/1]) (*eq 5.10*)

Out[8]= 21463.64826
Out[9]= 5.962273108
```

$$Hig = R*\int_{298.15}^{t} Cp\, dT$$

$$Sig = R*\left(\int_{298.15}^{t} \frac{Cp}{T}\, dT - Log\left[\frac{p}{1}\right]\right)$$

Out[8]= 21463.64826 J/mol — ANS, ΔH_{ig}

Out[9]= 5.962273108 J/(mol·K) — ANS, ΔS_{ig}

APPROVED SOLUTION

Cadet:______________________

Problem: Weight:
B 100

Use the Peng-Robinson equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z, H^R, and S^R) for nitrogen at 1000 K and 40 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for H^R and S^R in J/mol and J/(mol·K), respectively.

Solution:

```
In[12]:= (*Table B.1, p.665*)
tc = 126.2; (*K*)
pc = 34.00; (*bar*)
ω = 0.038;

(*Reduced t and p*)
tr = t / tc;  pr = p / pc;

(*Table 3.1 page 100*)
ϵ = 1 - √2 ; σ = 1 + √2 ; Ω = 0.07780; Ψ = 0.45724;
α[x_] = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω^2) * (1 - √x ))^2;

β = Ω * pr / tr; (*eq 3.50*)
q[x_] = (Ψ * α[x]) / (Ω * x); (*eq 3.51*)
eq1 = Z == 1 + β - q[tr] * β * (Z - β) / ((Z + ϵ * β) * (Z + σ * β)); (*eq 3.48*)
ans = Quiet[Solve[eq1, Z, Reals]];
Z1 = Z /. ans[[3]];
I = 1 / (σ - ϵ) * Log[(Z1 + σ * β) / (Z1 + ϵ * β)];  (*eq 13.72*)
Hr[x_] = (Z1 - 1 + x * ∂x q[x] * I) * R * t ; (*13.75*)
Sr[x_] = (Log[Z1 - β] + (q[x] + x * ∂x q[x]) * I) * R ; (*13.76*)

In[25]:= Z1
Hr[tr]
Sr[tr]

Out[25]= 1.011174588
Out[26]= 71.50932885
Out[27]= -0.02132500073
```

Out[25]= 1.011174588 — ANS, Z

Out[26]= 71.50932885 J/mol — ANS, H^R

Out[27]= −0.02132500073 J/(mol·K) — ANS, S^R

APPROVED SOLUTION

Cadet:________________________

Problem: Weight:
C 60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of nitrogen at 1000 K and 40 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

	Ideal	Residual	Total
Enthalpy, J/mol	21,463.65	71.51	21,535.16 //ANS
Entropy, J/mol·K	5.96	-0.02	5.94 //ANS

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of nitrogen at 1000 K and 40 bar using the Peng-Robinson equation of state.

(c) Give two reasons for the difference between the answers in parts (a) and (b).

Solution, part (a):

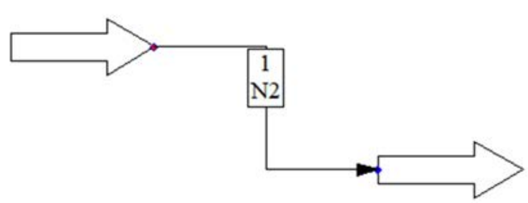
```
In[26]:= (*Table C.4, p.671*)
         ΔHfo = 0;
         ΔGfo = 0;
         ΔSfo = (ΔHfo - ΔGfo)/298.15;

         H = ΔHfo + Hig + Hr[tr] (*6.50*)
         S = ΔSfo + Sig + Sr[tr] (*6.51*)
Out[29]= 21535.15759
Out[30]= 5.940948108
```

21535.15759 J/mol //ANS — ANS, H

5.940948108 J/(mol·K) //ANS — ANS, S

Solution, part (b):

Stream No.	1
Name	N2
- - Overall - -	
Temp K	1000.0000
Pres bar	40.0000
Enth J/sec	21536. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	5.962 //ANS



Solution, part (c):

The answers are different because of the following: (1) different heat capacity polynomial, (2) different T_c, P_c, and ω, and (3) different numerical methods. //ANS

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PROBLEM	VALUE	CUT
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B	100	
C	60	
TOTAL CUT		
TOTAL GRADE	200	

Cadet: **APPROVED SOLUTION**

Problem: Weight:
A 40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate ΔH^{ig} and ΔS^{ig} for *ideal* gas-phase oxygen being compressed and heated from 298.15 K and 1 bar to 1225 K and 60 bar. Report your answers for ΔH^{ig} and ΔS^{ig} in J/mol and J/(mol·K), respectively.

Solution:

```
In[∘]:= Quit[];

In[1]:= (*oxygen*)
p = 60.; (*bar*)
t = 1225.; (*K*)

R = 8.314;

a = 3.639;
b = 0.506*10^-3;
d = -0.227*10^5;
Cp = a + b*T + d*T^-2;

(*enthalpy*)
Hig = R*∫_298.15^t Cp dT (*eq 2.21*)

(*entropy*)
Sig = R*(∫_298.15^t Cp/T dT - Log[p/1]) (*eq 5.10*)

Out[8]= 30532.08151
Out[9]= 11.61293535
```

$$\text{Hig} = R \int_{298.15}^{t} Cp \, dT$$

$$\text{Sig} = R\left(\int_{298.15}^{t} \frac{Cp}{T} \, dT - \text{Log}\left[\frac{p}{1}\right]\right)$$

Out[8]= 30532.08151 J/mol — ANS, ΔH_{ig}

Out[9]= 11.61293535 J/(mol·K) — ANS, ΔS_{ig}

Cadet: **APPROVED SOLUTION**

Problem: B   Weight: 100

Use the Peng-Robinson equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z, H^R, and S^R) for oxygen at 1225 K and 60 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for H^R and S^R in J/mol and J/(mol·K), respectively.

Solution:

```
(*Table B.1, p.665*)
tc = 154.6; (*K*)
pc = 50.43; (*bar*)
ω = 0.022;

(*Reduced t and p*)
tr = t / tc;  pr = p / pc;

(*Table 3.1 page 100*)
ϵ = 1 - √2 ;  σ = 1 + √2 ;  Ω = 0.07780;  Ψ = 0.45724;
α[x_] = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω^2) * (1 - √x))^2;

β = Ω * pr / tr; (*eq 3.50*)
q[x_] = (Ψ * α[x]) / (Ω * x); (*eq 3.51*)
eq1 = Z == 1 + β - q[tr] * β * (Z - β) / ((Z + ϵ * β) * (Z + σ * β)); (*eq 3.48*)
ans = Quiet[Solve[eq1, Z, Reals]];
Z1 = Z /. ans[[3]];
I = 1 / (σ - ϵ) * Log[(Z1 + σ * β) / (Z1 + ϵ * β)];  (*eq 13.72*)
Hr[x_] = (Z1 - 1 + x * ∂x q[x] * I) * R * t ; (*13.75*)
Sr[x_] = (Log[Z1 - β] + (q[x] + x * ∂x q[x]) * I) * R ; (*13.76*)


In[25]:= Z1
         Hr[tr]
         Sr[tr]

Out[25]= 1.011127697
Out[26]= 81.88931287
Out[27]= -0.02556163333
```

1.011127697 — ANS, Z

81.88931287 J/mol — ANS, H^R

-0.02556163333 J/(mol·K) — ANS, S^R

Cadet: **APPROVED SOLUTION**

Problem:	Weight:
C	60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of oxygen at 1225 K and 60 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

	Ideal	Residual	Total
Enthalpy, J/mol	30,532.08	81.89	30,613.97 //ANS
Entropy, J/mol·K	11.61	-0.03	11.58 //ANS

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of oxygen at 1225 K and 60 bar using the Peng-Robinson equation of state.

(c) Give two reasons for the difference between the answers in parts (a) and (b).

Solution, part (a):

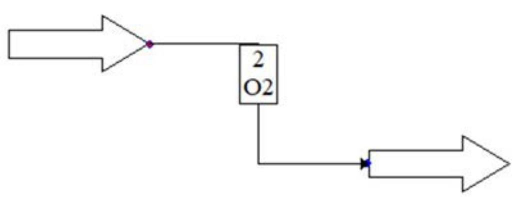
```
In[26]:= (*Table C.4, p.671*)
         ΔHfo = 0;
         ΔGfo = 0;
         ΔSfo = (ΔHfo - ΔGfo)/298.15;

         H = ΔHfo + Hig + Hr[tr] (*6.50*)
         S = ΔSfo + Sig + Sr[tr] (*6.51*)
Out[29]= 30613.97082
Out[30]= 11.58737372
```

$H = 30613.97082$ J/mol //ANS
ANS, H

$S = 11.58737372$ J/(mol·K) //ANS
ANS, S

Solution, part (b):

Stream No.	2
Name	O2
- - Overall - -	
Temp K	1225.0000
Pres bar	60.0000
Enth J/sec	30727. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	11.61 //ANS



Solution, part (c):

The answers are different because of the following: (1) different heat capacity polynomial, (2) different T_c, P_c, and ω, and (3) different numerical methods. //ANS