UNIVERSITY
OF
JOHANNESBURG

PROGRAM	:	NATIONAL DIPLOMA *CHEMICAL ENGINEERING*
SUBJECT	:	**THERMODYNAMICS:** **CHEMICAL ENGINEERING III**
CODE	:	**CIT 3111**
DATE	:	WINTER SSA EXAMINATION 2015 15 JULY 2015
DURATION	:	(SESSION 3) 15:00 - 18:00
WEIGHT	:	40 : 60
TOTAL MARKS	:	100

EXAMINER	:	DR T.A. MAMVURA
MODERATOR	:	DR H. RUTTO
NUMBER OF PAGES	:	5 PAGES + TABLES (7 PAGES)

INSTRUCTIONS	:	QUESTION PAPERS MUST BE HANDED IN.
REQUIREMENTS	:	CALCULATOR PERMITED
	:	GRAPH PAPER (ONE PER STUDENT)
	:	ALL REQUIRED FORMULAE AND TABLES PROVIDED

INSTRUCTIONS TO CANDIDATES:
PLEASE ANSWER ALL THE QUESTIONS.

QUESTION 1

1.1. One cubic metre of an ideal gas at 600 K and 1000 kPa expands to five times its initial volume as follows:

(a) By a mechanically reversible, isothermal process.

(b) By a mechanically reversible, adiabatic process.

For each case calculate the final T, P, U, H, Q and W if $C_p = 21$ J/mol-K. (15)

1.2. Using the Maxwell relations, determine a relation for $(\partial S/\partial V)_T$ for a gas whose equation of state is $\left(P - {}^{a}/_{V^2}\right)(V - b) = RT$ (5)

20 MARKS

QUESTION 2

Ethane gas at 850 K and 10 bar undergoes a reversible adiabatic expansion to 4 bar. Assuming ethane to be an ideal gas at these conditions, determine its final temperature. Assume starting temperature of 800 K.

20 MARKS

QUESTION 3

Two reversible heat engines operate in series between a source at 527 °C and a sink at 17 °C. If the engines have equal efficiencies and the first rejects 400 kJ to the second, calculate:

(i) Draw a diagram to show the representation

(ii) The temperature at which heat is supplied to the second engine

(iii) The heat taken from the source

(iv) The work done by each engine

Assume that each engine operates on the Carnot cycle

20 MARKS

QUESTION 4

Assuming Raoult's law to be valid for the following system: Toluene(l)/Water(2), prepare a P-x-y diagram for a temperature of 343.15 K (70°C). The Antoinne equations for toluene and water are:

For Toluene: $\ln P_i^{sat} = 14.0098 - \frac{3103.01}{T+219.79}$ T in K and P in kPa

For Water: $\ln P_i^{sat} = 16.2620 - \frac{3799.89}{T+226.35}$ T in K and P in kPa

20 MARKS

QUESTION 5

Calculate Z, H^R and S^R by the Redlich/Kwong equation for cyclohexane at 650 K and 50 bar. For the Redlick/Kwong equation: $\Omega = 0.08664$; $\psi = 0.42748$; $\alpha(T_r) = T_r^{-1/2}$; $\sigma = 1$; $\epsilon = 0$ and & $Z_c = {}^1/_3$

20 MARKS

FORMULAE

To solve these questions you may need basic equations provided:

Mechanically reversible closed processes:

1. Constant V: $Q = n\Delta U = n\int_{T_1}^{T_2} C_v dT = nC_v\Delta T$
2. Constant P: $Q = n\Delta H = n\int_{T_1}^{T_2} C_p dT = nC_p\Delta T;\ W = -R(T_2 - T_1)$
3. Constant T: $Q = -W = RT_1 \ln\frac{V_2}{V_1} = -RT_1 \ln\frac{P_2}{P_1} = P_1V_1 \ln\frac{V_2}{V_1} = -P_1V_1 \ln\frac{P_2}{P_1}$
4. Adiabatic: $W = \Delta U = C_V\Delta T = \frac{R\Delta T}{\gamma-1} = \frac{R(T_2-T_1)}{\gamma-1} = \frac{P_2V_2-P_1V_1}{\gamma-1} = \frac{P_1V_1}{\gamma-1}\left[\left(\frac{P_2}{P_1}\right)^{\gamma-1/\gamma} - 1\right] = \frac{RT_1}{\gamma-1}\left[\left(\frac{P_2}{P_1}\right)^{\gamma-1/\gamma} - 1\right];\qquad \gamma = \frac{C_P}{C_V}$
5. Adiabatic: $\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{R/C_V};\qquad \frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{R/C_P};\qquad \frac{P_2}{P_1} = \left(\frac{V_1}{V_2}\right)^{C_P/C_V}$

   PVT relations: $\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$
6. Ideal gas equation: $PV = nRT$
7. $\frac{dm_{cv}}{dt} = \Delta m = \dot{m}_{out} - \dot{m}_{in}$
8. $\Delta\dot{m}\left(H + \frac{1}{2}u^2 + gh\right) = \dot{Q} + \dot{W}_s$
9. Interpolation formula: $M = \left(\frac{X_2-X}{X_2-X_1}\right)M_1 + \left(\frac{X-X_1}{X_2-X_1}\right)M_2$ or $M = \frac{M_1(X_2-X)+M_2(X-X_1)}{X_2-X_1}$
10. For the Virial equation truncated to second term: $\frac{PV}{RT} = 1 + \frac{B}{V} + \frac{C}{V^2}$
11. Generalized correlations for Gases (Lee/Kesler):

    $Z = Z^o + \omega Z^1$
12. Generalized Pitzer correlation:

    $Z = 1 + (B^0 + \omega B^1)\frac{P_r}{T_r}$

    $B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}\qquad B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$
13. Enthalpy of reaction: $\Delta H = R\int_{T_o}^{T}\frac{C_P}{R}dT = nR\left[\Delta AT_o(\tau-1) + \frac{\Delta B}{2}T_o^2(\tau^2-1) + \frac{\Delta C}{3}T_o^3(\tau^3-1) + \frac{\Delta D}{T_o}\left(\frac{\tau-1}{\tau}\right)\right]$
14. Enthalpy of reaction: $Q = n\Delta H = n\langle C_P\rangle_H(T - T_o)$

    For $\langle C_P\rangle_H = R\left[A + \frac{B}{2}T_o(\tau+1) + \frac{C}{3}T_o^2(\tau^2+\tau+1) + \frac{D}{\tau T_o^2}\right]$

    And also: $\langle C_P\rangle_H = R\left[\Delta A + \frac{\Delta B}{2}T_o(\tau+1) + \frac{\Delta C}{3}T_o^2(\tau^2+\tau+1) + \frac{\Delta D}{\tau T_o^2}\right]$

15. Clapeyron equation: $\Delta H = T\Delta V \frac{dP^{sat}}{dT}$

16. For a Carnot engine: $\eta = \frac{|W_{net}|}{|Q_H|} = 1 - \frac{|Q_c|}{|Q_H|} = 1 - \frac{T_c}{T_H}$

17. General entropy change: $\Delta S = C_p \ln \frac{T_2}{T_1} - ln \frac{P_2}{P_1}$

18. Entropy change for an ideal gas: $\frac{\Delta S}{R} = \frac{\left\langle C_p^{ig} \right\rangle_S}{R} \ln \frac{T}{T_o} - \ln \frac{P}{P_o}$, for

For $\frac{\left\langle C_p^{ig} \right\rangle_S}{R} = A + \left[BT_o + \left(CT_o^2 + \frac{D}{\tau^2 T_o^2}\right)\left(\frac{\tau+1}{\tau}\right)\right]\left(\frac{\tau-1}{\ln \tau}\right)$

19. Maxwell relations: (i) $\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$; (ii) $\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$; (iii) $\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T$;

(iv) $\left(\frac{\partial V}{\partial T}\right)_P = -\left(\frac{\partial S}{\partial P}\right)_T$

20. $\frac{H^R}{RT_c} = P_r\left[\left(0.083 - \frac{1.097}{T_r^{1.6}}\right) + \omega\left(0.139 - \frac{0.894}{T_r^{4.2}}\right)\right]$

21. $\frac{S^R}{R} = -P_r\left[\frac{0.675}{T_r^{2.6}} + \omega\left(\frac{0.722}{T_r^{5.2}}\right)\right]$

22. For Redlich/Kwong equation of state: $\beta = \Omega\frac{P_r}{T_r}$; $q = \frac{\psi\alpha(T_r)}{\Omega T_r} = \frac{\psi}{\Omega T_r^{1.5}}$

$Z = 1 + \beta - q\beta\frac{Z-\beta}{(Z+\epsilon\beta)(Z+\sigma\beta)}$ where you iterate for Z;

$I = \ln\left(\frac{Z+\beta}{Z}\right)$; $\ln \alpha(T_r) = -\frac{1}{2}\ln T_r$; $d\ln\frac{\alpha(T_r)}{d\ln T_r = -1/2}$

$\frac{H^R}{RT} = Z - 1 + \left[\frac{d\ ln\ \alpha(T_r)}{d\ ln\ T_r} - 1\right]qI = Z - 1 + (-\frac{1}{2} - 1)qI$;

$\frac{S^R}{R} = ln(Z-\beta) + \frac{d\ ln\ \alpha(T_r)}{d\ ln\ T_r}qI = \ln(Z-\beta) + \left(-\frac{1}{2}\right)qI$

23. $P = x_i P_i^{sat}$

24. Raoult's law: $y_i = \frac{x_i P_i^{sat}}{P}$

25. Activity coefficient: $\ln \phi = (B^0 + \omega B^1)\frac{P_r}{T_r}$

26. Residual Gibbs energy: $G^R = RT \ln \phi$

27.

Table A.1 Conversion Factors

Quantity	Conversion
Length	1 m = 100 cm = 3.280 84 (ft) = 39.3701 (in)
Mass	1 kg = 10^3 g = 2.204 62 (lb_m)
Force	1 N = 1 kg m s^{-2} = 10^5 (dyne) = 0.224 809 (lb_f)
Pressure	1 bar = 10^5 kg m^{-1} s^{-2} = 10^5 N m^{-2} = 10^5 Pa = 10^2 kPa = 10^6 dyne cm^{-2} = 0.986 923 atm = 14.5038 (psia) = 750.061 torr
Volume	1 m^3 = 10^6 cm^3 = 35.3147 $(ft)^3$ = 264.172 (gal)
Density	1 g cm^{-3} = 10^3 kg m^{-3} = 62.4278 $(lb_m)(ft)^{-3}$
Energy	1 J = 1 kg m^2 s^{-2} = 1 N m = 1 m^3 Pa = 10^{-5} m^3 bar = 10 cm^3 bar = 9.869 23 cm^3 atm = 10^7 dyne cm = 10^7 erg = 0.239 006 (cal) = 5.121 97 x 10^{-3} $(ft)^3(psia)$ = 0.737 562 $(ft)(lb_f)$ = 9.478 31 x 10^{-4} (Btu)
Power	1 kW = 10^3 W = 10^3 kg m^2 s^{-3} = 10^3 J s^{-1} = 239.006 (cal) s^{-1} = 737.562 $(ft)(lb_f)$ s^{-1} = 0.947 831 (Btu) s^{-1} = 1.341 02 (hp)

Table A.2 Values of the Universal Gas Constant

R = 8.314 J mol^{-1} K^{-1} = 8.314 m^3 Pa mol^{-1} K^{-1}
= 83.14 cm^3 bar mol^{-1} K^{-1} = 8314 cm^3 kPa mol^{-1} K^{-1}
= 82.06 cm^3 atm mol^{-1} K^{-1} = 82 363.95 cm^3 torr mol^{-1} K^{-1} = 0.082 06 m^3 atm $kmol^{-1}K^{-1}$
= 1.9872 (cal) mol^{-1} K^{-1} = 1.986 (Btu)(lb mole)$^{-1}$(R)$^{-1}$
= 0.7302 $(ft)^3$(atm)(lb mol)$^{-1}$(R)$^{-1}$ = 10.73 $(ft)^3$(psia)(lb mol)$^{-1}$(R)$^{-1}$
= 1545 (ft)(lb_f)(lb mol)$^{-1}$(R)$^{-1}$

Appendix B

Properties of Pure Species

Listed here for various chemical species are values for the molar mass (molecular weight), acentric factor ω, critical temperature T_c, critical pressure P_c, critical compressibility factor Z_c, critical molar volume V_c, and normal boiling point T_n. Abstracted from Project 801, DIPPR®, Design Institute for Physical Property Data of the American Institute of Chemical Engineers, they are reproduced with permission. The full data compilation is published by T. E. Daubert, R. P. Danner, H. M. Sibul, and C. C. Stebbins, *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation,* Taylor & Francis, Bristol, PA, 1,405 chemicals, extant 1995. Included are values for 26 physical constants and regressed values of parameters in equations for the temperature dependence of 13 thermodynamic and transport properties.

Electronic versions by the same authors include:

- *DIPPR® Data Compilation of Pure Compound Properties,* ASCII Files, National Institute of Science and Technology, Standard Reference Data, Gaithersburg, MD, 1458 chemicals, extant 1995.
- *DIPPR® Data Compilation, Student DIPPR Database,* PC-DOS Version, National Institute of Science and Technology, Standard Reference Data, Gaithersburg, MD, 100 common chemicals for teaching purposes, 1995.

Table B.1 Properties of Pure Species

	Molar mass	ω	T_c/K	P_c/bar	Z_c	V_c $cm^3\ mol^{-1}$ or $10^{-3}\ m^3\ kmol^{-1}$	T_n/K
Methane	16.043	0.012	190.6	45.99	0.286	98.6	111.4
Ethane	30.070	0.100	305.3	48.72	0.279	145.5	184.6
Propane	44.097	0.152	369.8	42.48	0.276	200.0	231.1
n-Butane	58.123	0.200	425.1	37.96	0.274	255.	272.7
n-Pentane	72.150	0.252	469.7	33.70	0.270	313.	309.2
n-Hexane	86.177	0.301	507.6	30.25	0.266	371.	341.9
n-Heptane	100.204	0.350	540.2	27.40	0.261	428.	371.6
n-Octane	114.231	0.400	568.7	24.90	0.256	486.	398.8
n-Nonane	128.258	0.444	594.6	22.90	0.252	544.	424.0
n-Decane	142.285	0.492	617.7	21.10	0.247	600.	447.3
Isobutane	58.123	0.181	408.1	36.48	0.282	262.7	261.4
Isooctane	114.231	0.302	544.0	25.68	0.266	468.	372.4
Cyclopentane	70.134	0.196	511.8	45.02	0.273	258.	322.4
Cyclohexane	84.161	0.210	553.6	40.73	0.273	308.	353.9
Methylcyclopentane	84.161	0.230	532.8	37.85	0.272	319.	345.0
Methylcyclohexane	98.188	0.235	572.2	34.71	0.269	368.	374.1
Ethylene	28.054	0.087	282.3	50.40	0.281	131.	169.4
Propylene	42.081	0.140	365.6	46.65	0.289	188.4	225.5
1-Butene	56.108	0.191	420.0	40.43	0.277	239.3	266.9
cis-2-Butene	56.108	0.205	435.6	42.43	0.273	233.8	276.9
trans-2-Butene	56.108	0.218	428.6	41.00	0.275	237.7	274.0
1-Hexene	84.161	0.280	504.0	31.40	0.265	354.	336.3
Isobutylene	56.108	0.194	417.9	40.00	0.275	238.9	266.3
1,3-Butadiene	54.092	0.190	425.2	42.77	0.267	220.4	268.7
Cyclohexene	82.145	0.212	560.4	43.50	0.272	291.	356.1
Acetylene	26.038	0.187	308.3	61.39	0.271	113.	189.4
Benzene	78.114	0.210	562.2	48.98	0.271	259.	353.2
Toluene	92.141	0.262	591.8	41.06	0.264	316.	383.8
Ethylbenzene	106.167	0.303	617.2	36.06	0.263	374.	409.4
Cumene	120.194	0.326	631.1	32.09	0.261	427.	425.6
o-Xylene	106.167	0.310	630.3	37.34	0.263	369.	417.6
m-Xylene	106.167	0.326	617.1	35.36	0.259	376.	412.3
p-Xylene	106.167	0.322	616.2	35.11	0.260	379.	411.5
Styrene	104.152	0.297	636.0	38.40	0.256	352.	418.3
Naphthalene	128.174	0.302	748.4	40.51	0.269	413.	
Biphenyl	154.211	0.365	789.3	38.50	0.295	502.	528.2
Formaldehyde	30.026	0.282	408.0	65.90	0.223	115.	254.1
Acetaldehyde	44.053	0.291	466.0	55.50	0.221	154.	294.0
Methyl acetate	74.079	0.331	506.6	47.50	0.257	228.	330.1
Ethyl acetate	88.106	0.366	523.3	38.80	0.255	286.	350.2
Acetone	58.080	0.307	508.2	47.01	0.233	209.	329.4
Methyl ethyl ketone	72.107	0.323	535.5	41.50	0.249	267.	352.8
Diethyl ether	74.123	0.281	466.7	36.40	0.263	280.	307.6
Methyl t-butyl ether	88.150	0.266	497.1	34.30	0.273	329.	328.4
Methanol	32.042	0.564	512.6	80.97	0.224	118.	337.9

Table B.1 (Continued)

	Molar mass	ω	T_c/K	P_c/bar	Z_c	V_c cm^3 mol^{-1} or 10^{-3} m^3 kmol^{-1}	T_n/K
Ethanol	46.069	0.645	513.9	61.48	0.240	167.	351.4
1-Propanol	60.096	0.622	536.8	51.75	0.254	219.	370.4
1-Butanol	74.123	0.594	563.1	44.23	0.260	275.	390.8
1-Hexanol	102.177	0.579	611.4	35.10	0.263	381.	430.6
2-Propanol	60.096	0.668	508.3	47.62	0.248	220.	355.4
Phenol	94.113	0.444	694.3	61.30	0.243	229.	455.0
Ethylene glycol	62.068	0.487	719.7	77.00	0.246	191.0	470.5
Acetic acid	60.053	0.467	592.0	57.86	0.211	179.7	391.1
n-Butyric acid	88.106	0.681	615.7	40.64	0.232	291.7	436.4
Benzoic acid	122.123	0.603	751.0	44.70	0.246	344.	522.4
Acetonitrile	41.053	0.338	545.5	48.30	0.184	173.	354.8
Methylamine	31.057	0.281	430.1	74.60	0.321	154.	266.8
Ethylamine	45.084	0.285	456.2	56.20	0.307	207.	289.7
Nitromethane	61.040	0.348	588.2	63.10	0.223	173.	374.4
Carbon tetrachloride	153.822	0.193	556.4	45.60	0.272	276.	349.8
Chloroform	119.377	0.222	536.4	54.72	0.293	239.	334.3
Dichloromethane	84.932	0.199	510.0	60.80	0.265	185.	312.9
Methyl chloride	50.488	0.153	416.3	66.80	0.276	143.	249.1
Ethyl chloride	64.514	0.190	460.4	52.70	0.275	200.	285.4
Chlorobenzene	112.558	0.250	632.4	45.20	0.265	308.	404.9
Tetrafluoroethane	102.030	0.327	374.2	40.60	0.258	198.0	247.1
Argon	39.948	0.000	150.9	48.98	0.291	74.6	87.3
Krypton	83.800	0.000	209.4	55.02	0.288	91.2	119.8
Xenon	131.30	0.000	289.7	58.40	0.286	118.0	165.0
Helium 4	4.003	−0.390	5.2	2.28	0.302	57.3	4.2
Hydrogen	2.016	−0.216	33.19	13.13	0.305	64.1	20.4
Oxygen	31.999	0.022	154.6	50.43	0.288	73.4	90.2
Nitrogen	28.014	0.038	126.2	34.00	0.289	89.2	77.3
Air[†]	28.851	0.035	132.2	37.45	0.289	84.8	
Chlorine	70.905	0.069	417.2	77.10	0.265	124	239.1
Carbon monoxide	28.010	0.048	132.9	34.99	0.299	93.4	81.7
Carbon dioxide	44.010	0.224	304.2	73.83	0.274	94.0	
Carbon disulfide	76.143	0.111	552.0	79.00	0.275	160.	319.4
Hydrogen sulfide	34.082	0.094	373.5	89.63	0.284	98.5	212.8
Sulfur dioxide	64.065	0.245	430.8	78.84	0.269	122.	263.1
Sulfur trioxide	80.064	0.424	490.9	82.10	0.255	127.	317.9
Nitric oxide (NO)	30.006	0.583	180.2	64.80	0.251	58.0	121.4
Nitrous oxide (N_2O)	44.013	0.141	309.6	72.45	0.274	97.4	184.7
Hydrogen chloride	36.461	0.132	324.7	83.10	0.249	81.	188.2
Hydrogen cyanide	27.026	0.410	456.7	53.90	0.197	139.	298.9
Water	18.015	0.345	647.1	220.55	0.229	55.9	373.2
Ammonia	17.031	0.253	405.7	112.80	0.242	72.5	239.7
Nitric acid	63.013	0.714	520.0	68.90	0.231	145.	356.2
Sulfuric acid	98.080	...	924.0	64.00	0.147	177.	610.0

[†]Pseudoparameters for $y_{N_2} = 0.79$ and $y_{O_2} = 0.21$. See Eqs. (6.88)–(6.90).

Appendix C

Heat Capacities and Property Changes of Formation

Table C.1 Heat Capacities of Gases in the Ideal-Gas State
Table C.2 Heat Capacities of Solids
Table C.3 Heat Capacities of Liquids
Table C.4 Standard Enthalpies and Gibbs Energies of Formation at 298.15 K (25°C)

Table C.1 Heat Capacities of Gases in the Ideal-Gas State†

Constants in equation $C_P^{ig}/R = A + BT + CT^2 + DT^{-2}$ T (kelvins) from 298.15 to T_{max}

Chemical species		T_{max}	$C_{P_{298}}^{ig}/R$	A	$10^3\,B$	$10^6\,C$	$10^{-5}\,D$
Paraffins:							
Methane	CH_4	1500	4.217	1.702	9.081	−2.164	
Ethane	C_2H_6	1500	6.369	1.131	19.225	−5.561	
Propane	C_3H_8	1500	9.001	1.213	28.785	−8.824	
n-Butane	C_4H_{10}	1500	11.928	1.935	36.915	−11.402	
iso-Butane	C_4H_{10}	1500	11.901	1.677	37.853	−11.945	
n-Pentane	C_5H_{12}	1500	14.731	2.464	45.351	−14.111	
n-Hexane	C_6H_{14}	1500	17.550	3.025	53.722	−16.791	
n-Heptane	C_7H_{16}	1500	20.361	3.570	62.127	−19.486	
n-Octane	C_8H_{18}	1500	23.174	4.108	70.567	−22.208	
1-Alkenes:							
Ethylene	C_2H_4	1500	5.325	1.424	14.394	−4.392	
Propylene	C_3H_6	1500	7.792	1.637	22.706	−6.915	
1-Butene	C_4H_8	1500	10.520	1.967	31.630	−9.873	
1-Pentene	C_5H_{10}	1500	13.437	2.691	39.753	−12.447	
1-Hexene	C_6H_{12}	1500	16.240	3.220	48.189	−15.157	
1-Heptene	C_7H_{14}	1500	19.053	3.768	56.588	−17.847	
1-Octene	C_8H_{16}	1500	21.868	4.324	64.960	−20.521	
Miscellaneous organics:							
Acetaldehyde	C_2H_4O	1000	6.506	1.693	17.978	−6.158	
Acetylene	C_2H_2	1500	5.253	6.132	1.952	.....	−1.299
Benzene	C_6H_6	1500	10.259	−0.206	39.064	−13.301	
1,3-Butadiene	C_4H_6	1500	10.720	2.734	26.786	−8.882	
Cyclohexane	C_6H_{12}	1500	13.121	−3.876	63.249	−20.928	
Ethanol	C_2H_6O	1500	8.948	3.518	20.001	−6.002	
Ethylbenzene	C_8H_{10}	1500	15.993	1.124	55.380	−18.476	
Ethylene oxide	C_2H_4O	1000	5.784	−0.385	23.463	−9.296	
Formaldehyde	CH_2O	1500	4.191	2.264	7.022	−1.877	
Methanol	CH_4O	1500	5.547	2.211	12.216	−3.450	
Styrene	C_8H_8	1500	15.534	2.050	50.192	−16.662	
Toluene	C_7H_8	1500	12.922	0.290	47.052	−15.716	
Miscellaneous inorganics:							
Air		2000	3.509	3.355	0.575	.....	−0.016
Ammonia	NH3	1800	4.269	3.578	3.020	.....	−0.186
Bromine	Br_2	3000	4.337	4.493	0.056	.....	−0.154
Carbon monoxide	CO	2500	3.507	3.376	0.557	.....	−0.031
Carbon dioxide	CO_2	2000	4.467	5.457	1.045	.....	−1.157
Carbon disulfide	CS_2	1800	5.532	6.311	0.805	.....	−0.906
Chlorine	Cl_2	3000	4.082	4.442	0.089	.....	−0.344
Hydrogen	H_2	3000	3.468	3.249	0.422	.....	0.083
Hydrogen sulfide	H_2S	2300	4.114	3.931	1.490	.....	−0.232
Hydrogen chloride	HCl	2000	3.512	3.156	0.623	.....	0.151
Hydrogen cyanide	HCN	2500	4.326	4.736	1.359	.....	−0.725
Nitrogen	N_2	2000	3.502	3.280	0.593	.....	0.040
Nitrous oxide	N_2O	2000	4.646	5.328	1.214	.....	−0.928
Nitric oxide	NO	2000	3.590	3.387	0.629	.....	0.014
Nitrogen dioxide	NO2	2000	4.447	4.982	1.195	.....	−0.792
Dinitrogen tetroxide	N_2O_4	2000	9.198	11.660	2.257	.....	−2.787
Oxygen	O_2	2000	3.535	3.639	0.506	.....	−0.227
Sulfur dioxide	SO_2	2000	4.796	5.699	0.801	.....	−1.015
Sulfur trioxide	SO3	2000	6.094	8.060	1.056	.....	−2.028
Water	H_2O	2000	4.038	3.470	1.450	.....	0.121

†Selected from H. M. Spencer, *Ind.* Eng. Chem., vol. 40, pp. 2152–2154, 1948; K. K. Kelley, *U.S.Bur.* Mines *Bull. 584,* 1960; *L.* B. Pankratz, U.S. *Bur.* Mines *Bull. 672,* 1982.

Table C.2 Heat Capacities of Solids†

Constants for the equation $C_P/R = A + BT + DT^{-2}$ T (kelvins) from 298.15 K to T_{max}

Chemical species	T_{max}	$C_{P_{298}}/R$	A	10^3 B	10^{-5} D
CaO	2000	5.058	6.104	0.443	−1.047
$CaCO_3$	1200	9.848	12.572	2.637	−3.120
$Ca(OH)_2$	700	11.217	9.597	5.435	
CaC_2	720	7.508	8.254	1.429	−1.042
$CaCl_2$	1055	8.762	8.646	1.530	−0.302
C (graphite)	2000	1.026	1.771	0.771	−0.867
Cu	1357	2.959	2.677	0.815	0.035
CuO	1400	5.087	5.780	0.973	−0.874
Fe (α)	1043	3.005	−0.111	6.111	1.150
Fe_2O_3	960	12.480	11.812	9.697	−1.976
Fe_3O_4	850	18.138	9.594	27.112	0.409
FeS	411	6.573	2.612	13.286	
I_2	386.8	6.929	6.481	1.502	
LiCl	800	5.778	5.257	2.476	−0.193
NH_4Cl	458	10.741	5.939	16.105	
Na	371	3.386	1.988	4.685	
NaCl	1073	6.111	5.526	1.963	
NaOH	566	7.177	0.121	16.316	1.948
$NaHCO_3$	400	10.539	5.128	18.148	
S (rhombic)	368.3	3.748	4.114	−1.728	−0.783
SiO_2 (quartz)	847	5.345	4.871	5.365	−1.001

†Selected from K. K. Kelley, *U.S. Bur.* Mines *Bull. 584,* 1960; L. B. Pankratz, *U.S. Bur* Mines *Bull. 672,* 1982.

Table C.3 Heat Capacities of Liquids†

Constants for the equation $C_P/R = A + BT + CT^2$ T from 273.15 to 373.15 K

Chemical species	$C_{P_{298}}/R$	A	10^3 B	10^6 C
Ammonia	9.718	22.626	−100.75	192.71
Aniline	23.070	15.819	29.03	−15.80
Benzene	16.157	−0.747	67.96	−37.78
1,3-Butadiene	14.779	22.711	−87.96	205.79
Carbon tetrachloride	15.751	21.155	−48.28	101.14
Chlorobenzene	18.240	11.278	32.86	−31.90
Chloroform	13.806	19.215	−42.89	83.01
Cyclohexane	18.737	−9.048	141.38	−161.62
Ethanol	13.444	33.866	−172.60	349.17
Ethylene oxide	10.590	21.039	−86.41	172.28
Methanol	9.796	13.431	−51.28	131.13
n-Propanol	16.921	41.653	−210.32	427.20
Sulfur trioxide	30.408	−2.930	137.08	−84.73
Toluene	18.611	15.133	6.79	16.35
Water	9.069	8.712	1.25	−0.18

†Based on correlations presented by J. W. Miller, Jr., G. R. Schon; and C. L. Yaws, Chem. *Eng.*, vol. 83(23), p. 129, 1976.