UNIVERSITI TEKNOLOGI PETRONAS

FINAL EXAMINATION
JANUARY 2025 SEMESTER

COURSE	:	CEB2023/CFB2023 - CHEMICAL ENGINEERING THERMODYNAMICS II
DATE	:	19 APRIL 2025 (SATURDAY)
TIME	:	2.30 PM - 5.30 PM (3 HOURS)

INSTRUCTIONS TO CANDIDATES

1. Answer **ALL** questions in the Answer Booklet.
2. Begin **EACH** answer on a new page in the Answer Booklet.
3. Indicate clearly answers that are cancelled, if any.
4. Where applicable, show clearly steps taken in arriving at the solutions and indicate **ALL** assumptions, if any.
5. **DO NOT** open this Question Booklet until instructed.

Note :

i. There are **TWELVE (12)** pages in this Question Booklet including the cover page and appendices.

ii. **DOUBLE-SIDED** Question Booklet.

1. a. An ideal gas at 30°C and 5 bar, undergoes the following mechanically reversible cyclic processes in a closed system as below:

(1) constant pressure heating to 200°C

(2) adiabatic expansion to 1 bar

(3) isothermal compression to its original state

The following heat capacities for air may be assumed independent of temperature: heat capacity at constant volume, $C_V = (5/2)R$ and heat capacity at constant pressure, $C_P = (7/2)R$.

i. Sketch the processes on a single pressure-volume (P-V) diagram.

[4 marks]

ii. Determine the heat transferred, Q (J), work required, W (J), change in internal energy, ΔU (J) and change in enthalpy, ΔH (J) for each process.

[12 marks]

b. The Second Law of Thermodynamics introduces entropy as a key property in energy transformations. State the Second Law of Thermodynamics in terms of entropy and explain its significance in spontaneous processes. Write the mathematical expression for the entropy change of a reversible process and describe how entropy changes for an isolated system.

[8 marks]

2. a. Accurate estimation of thermodynamic properties such as residual volume is crucial in chemical engineering applications, particularly in the design and operation of high-pressure steam systems.

   i. Define residual volume, V^R and explain its significance in real gas behaviour compared to ideal gas assumptions.

   [6 marks]

   ii. Steam is stored in a pressurized vessel at 70 bar and 360°C. Estimate the molar residual volume V^R (m^3/mol) using steam table and compare the results obtained using Redlich/Kwong cubic equation of state. Limit the computation to four iterations including the initial guess.

   [10 marks]

   iii. Based on **part (a) (ii)**, estimate the residual Gibbs energy and the residual enthalpy of the steam.

   [6 marks]

b. Define latent heat of vaporization and latent heat of fusion.

[4 marks]

3. a. The enthalpies (J/mol) of a binary liquid system of *n*-pentane (1) and *n*-hexanol (2) are expressed by the equation below:

$$H = x_1 x_2 [2326 - 1417(x_1 - x_2)]$$

i. Determine expressions for partial enthalpies for n-pentane and n-hexanol in terms of x_1.

[4 marks]

ii. Calculate the enthalpy for pure *n*-pentane (H_1) and *n*-hexanol (H_2) as well as the partial enthalpies ($\overline{H_1}$ and $\overline{H_2}$) at x_1=0.5. Estimate the infinite dilution partial enthalpies ($\overline{H_1^\infty}$ and $\overline{H_2^\infty}$).

[6 marks]

iii. Differentiate between excess enthalpy and partial molar enthalpy.

[4 marks]

b. A system contains pentane and hexane at 195°C and 50 bar. The experimental virial coefficients for pure pentane, pure hexane and mixture of pentane-hexane are −59.892 cm^3/mol, −159.43 cm^3/mol and −99.181 cm^3/mol, respectively. Estimate the mixture compressibility factor and fugacity of each component if the mixture contains 40 mol% hexane.

[10 marks]

4. Propionaldehyde is produced by the catalytic dehydrogenation of isopropanol as shown below:

$$(CH_3)_2CHOH\ (g) \rightarrow CH_3CH_2CHO\ (g) + H_2\ (g)$$

The data for the standard heat of formation, ΔH_f° and standard Gibbs energy of formation, ΔG_f° of isopropanol and propionaldehyde at 298.15 K are given in **TABLE Q4.**

TABLE Q4: Standard heat and standard Gibbs of formation at 298.15 K

	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)
$(CH_3)_2CHOH$ (g)	-261.31	-159.94
CH_3CH_2CHO (g)	-205.79	-142.19

a. Determine the equilibrium constant, K at 500 K. Assume heat of reaction is constant.

[8 marks]

b. Calculate the equilibrium composition at 500 K and 1 bar for a feedstock with 1 mol of pure isopropanol. Assume the reaction mixture behaves as an ideal gas.

[8 marks]

c. Based on **part (b)**, propose **TWO (2)** methods to increase the production of propionaldehyde. Justify your answer with suitable calculations.

[10 marks]

\- END OF PAPER -

APPENDIX A

List of Formula

1. **Generic Cubic Equations of State: Vapor and Vapor-Like Roots**

$$Z = 1 + \beta - q\beta \frac{Z - \beta}{(Z + \varepsilon\beta)(Z + \sigma\beta)}$$

$$\beta = \Omega \frac{P_r}{T_r}$$

$$q = \frac{\Psi \alpha(T_r)}{\Omega T_r}$$

Case I: $\epsilon \neq \sigma,\ I = \frac{1}{\sigma - \epsilon} \ln\left(\frac{Z + \sigma\beta}{Z + \epsilon\beta}\right)$

Case II: $\epsilon = \sigma,\ I = \frac{\beta}{Z + \epsilon\beta}$

2. **Generic Cubic Equations of State: Liquid and Liquid-Like Roots**

$$Z = \beta + (Z + \epsilon\beta)(Z + \sigma\beta)\left(\frac{1 + \beta - Z}{q\beta}\right)$$

3. **Parameter Assignments for Equations of State**

EOS	$\alpha(T_r)$	σ	ε	Ω	Ψ	Z_C
vdW (1873)	1	0	0	1/8	27/64	3/8
RK (1949)	$T_r^{-1/2}$	1	0	0.086 64	0.427 48	1/3
SRK (1972)	$\alpha_{SRK}(T_r;\omega)^\dagger$	1	0	0.086 64	0.427 48	1/3
PR (1976)	$\alpha_{PR}(T_r;\omega)^\ddagger$	$1+\sqrt{2}$	$1-\sqrt{2}$	0.077 80	0.457 24	0.307 40

$^\dagger \alpha_{SRK}(T_r;\omega) = [1 + (0.480 + 1.574\omega - 0.176\omega^2)(1 - T_r^{1/2})]^2$

$^\ddagger \alpha_{PR}(T_r;\omega) = [1 + (0.374\,64 + 1.542\,26\omega - 0.269\,92\omega^2)(1 - T_r^{1/2})]^2$

4. **Residual Gibbs energy Equations of State**

$$\frac{G^R}{RT} = Z - 1 - \ln(Z - \beta) - qI$$

5. **Residual Gibbs energy Equations of State**

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

6. Generalized Property Correlations for Gases

$$Z = 1 + \hat{B}\frac{P_r}{T_r}$$

$$\hat{B} = B^0 + \omega B^1$$

$$B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}$$

$$B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

7. Adiabatic Equations at Constant Heat Capacities for Ideal Gases

$TV^{\gamma-1}$ = constant

$TP^{(1-\gamma)/\gamma}$ = constant

PV^{γ} = constant

$$\gamma = \frac{C_P}{C_V}$$

8. Partial Properties for Binary Solutions

$$\overline{M}_1 = M + x_2\frac{dM}{dx_1}$$

$$\overline{M}_2 = M - x_1\frac{dM}{dx_1}$$

9. Virial Equation for Gas Mixture

$$Z = 1 + \frac{BP}{RT}$$

$$B = \sum_i \sum_j y_i y_j B_{ij}$$

10. Fugacity Coefficients

$$\ln \hat{\phi}_1 = \frac{P}{RT}(B_{11} + y_2^2\delta_{12})$$

$$\ln \hat{\phi}_2 = \frac{P}{RT}(B_{22} + y_1^2\delta_{12})$$

$$\delta_{12} = 2B_{12} - B_{11} - B_{22}$$

APPENDIX A

List of Formula (Cont'd)

11. Standard Gibbs Energy Change on Reaction

$$K = \exp\left(-\frac{\sum v_i \Delta G_f^{\,0}}{RT}\right)$$

12. Temperature Dependence of Reaction Equilibrium Constant

$$-\frac{\Delta H_{rxn}^{\,0}}{R}\left[\frac{1}{T_2}-\frac{1}{T_1}\right] = \ln\left[\frac{K_2}{K_1}\right]$$

13. Relation of Equilibrium constant to composition

$$\prod_i (y_i)^{v_i} = \left(\frac{P}{P_0}\right)^{-v} K$$

14. Values of the Universal Gas Constant

$$\begin{aligned} R &= 8.314\ \mathrm{J\ mol^{-1}\ K^{-1}} = 8.314\ \mathrm{m^3\ Pa\ mol^{-1}\ K^{-1}} \\ &= 83.14\ \mathrm{cm^3\ bar\ mol^{-1}\ K^{-1}} = 8314\ \mathrm{cm^3\ kPa\ mol^{-1}\ K^{-1}} \\ &= 82.06\ \mathrm{cm^3\ atm\ mol^{-1}\ K^{-1}} = 62356\ \mathrm{cm^3\ Torr\ mol^{-1}\ K^{-1}} \\ &= 1.987\ \mathrm{(cal)\ mol^{-1}\ K^{-1}} = 1.986\ \mathrm{(Btu)(lb\ mol)^{-1}(^\circ R)^{-1}} \\ &= 1545\ \mathrm{(ft)(lb_f)(lb\ mol)^{-1}(^\circ R)^{-1}} \end{aligned}$$

15. Interpolation

$$M = \left(\frac{X_2 - X}{X_2 - X_1}\right)M_1 + \left(\frac{X - X_1}{X_2 - X_1}\right)M_2$$

$$M = \left[\left(\frac{X_2 - X}{X_2 - X_1}\right)M_{1,1} + \left(\frac{X - X_1}{X_2 - X_1}\right)M_{1,2}\right]\frac{Y_2 - Y}{Y_2 - Y_1} + \left[\left(\frac{X_2 - X}{X_2 - X_1}\right)M_{2,1} + \left(\frac{X - X_1}{X_2 - X_1}\right)M_{2,2}\right]\frac{Y - Y_1}{Y_2 - Y_1}$$

APPENDIX B

Table of Units

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 = 10^3 liters = 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 × 10^{-3} $(ft)^3$ (psia) = 0.737 562 (ft) (lb_f) = 9.478 31 × 10^{-4} (Btu) = 2.777 78 × 10^{-7} kWh
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)

APPENDIX C

Characteristic Properties of Pure Species

	Molar mass	ω	T_C/K	P_C/bar	Z_C	V_C cm^3 mol^{-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	42.23	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.	491.2
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

APPENDIX C

Characteristic Properties of Pure Species (Cont'd)

	Molar mass	ω	T_C/K	P_C/bar	Z_C	V_C cm^3 mol^{-1}	T_n/K
Methanol	32.042	0.564	512.6	80.97	0.224	118.	337.9
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	75.6	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

APPENDIX D

Steam Tables: Superheated Steam

V = SPECIFIC VOLUME $cm^3\ g^{-1}$
U = SPECIFIC INTERNAL ENERGY $kJ\ kg^{-1}$
H = SPECIFIC ENTHALPY $kJ\ kg^{-1}$
S = SPECIFIC ENTROPY $kJ\ kg^{-1}\ K^{-1}$

TEMPERATURE: t°C
(TEMPERATURE: T kelvins)

P/kPa (t^{sat}/°C)		sat. liq.	sat. vap.	280 (553.15)	290 (563.15)	300 (573.15)	325 (598.15)	350 (623.15)	375 (648.15)	400 (673.15)	425 (698.15)
6600 (281.84)	V	1.338	29.223	......	30.490	31.911	35.038	37.781	40.287	42.636	44.874
	U	1237.6	2585.5	......	2614.9	2647.7	2719.0	2780.4	2835.8	2887.5	2936.7
	H	1246.5	2778.3	......	2816.1	2858.4	2950.2	3029.7	3101.7	3168.9	3232.9
	S	3.0853	5.8452	......	5.9129	5.9872	6.1442	6.2744	6.3877	6.4894	6.5828
6700 (282.84)	V	1.342	28.741	......	29.850	31.273	34.391	37.116	39.601	41.927	44.141
	U	1242.8	2584.6	......	2610.8	2644.2	2716.4	2778.3	2834.1	2886.1	2935.5
	H	1251.8	2777.1	......	2810.8	2853.7	2946.8	3027.0	3099.5	3167.0	3231.3
	S	3.0946	5.8379	......	5.8980	5.9736	6.1326	6.2640	6.3781	6.4803	6.5741
6800 (283.84)	V	1.345	28.272	......	29.226	30.652	33.762	36.470	38.935	41.239	43.430
	U	1247.9	2583.7	......	2606.6	2640.6	2713.7	2776.2	2832.4	2884.7	2934.3
	H	1257.0	2775.9	......	2805.3	2849.0	2943.3	3024.2	3097.2	3165.1	3229.6
	S	3.1038	5.8306	......	5.8830	5.9599	6.1211	6.2537	6.3686	6.4713	6.5655
7000 (285.79)	V	1.351	27.373	......	28.024	29.457	32.556	35.233	37.660	39.922	42.068
	U	1258.0	2581.8	......	2597.9	2633.2	2708.4	2772.1	2829.0	2881.8	2931.8
	H	1267.4	2773.5	......	2794.1	2839.4	2936.3	3018.7	3092.7	3161.2	3226.3
	S	3.1219	5.8162	......	5.8530	5.9327	6.0982	6.2333	6.3497	6.4536	6.5485
7200 (287.70)	V	1.358	26.522	......	26.878	28.321	31.413	34.063	36.454	38.676	40.781
	U	1267.9	2579.9	......	2589.0	2625.6	2702.9	2767.8	2825.6	2878.9	2929.4
	H	1277.6	2770.9	......	2782.5	2829.5	2929.1	3013.1	3088.1	3157.4	3223.0
	S	3.1397	5.8020	......	5.8226	5.9054	6.0755	6.2132	6.3312	6.4362	6.5319
7400 (289.57)	V	1.364	25.715	......	25.781	27.238	30.328	32.954	35.312	37.497	39.564
	U	1277.6	2578.0	......	2579.7	2617.8	2697.3	2763.5	2822.1	2876.0	2926.9
	H	1287.7	2768.3	......	2770.5	2819.3	2921.8	3007.4	3083.4	3153.5	3219.6
	S	3.1571	5.7880	......	5.7919	5.8779	6.0530	6.1933	6.3130	6.4190	6.5156
7600 (291.41)	V	1.371	24.949	......	......	26.204	29.297	31.901	34.229	36.380	38.409
	U	1287.2	2575.9	......	......	2609.7	2691.7	2759.2	2818.6	2873.1	2924.3
	H	1297.6	2765.5	......	......	2808.8	2914.3	3001.6	3078.7	3149.6	3216.3
	S	3.1742	5.7742	......	......	5.8503	6.0306	6.1737	6.2950	6.4022	6.4996
7800 (293.21)	V	1.378	24.220	......	......	25.214	28.315	30.900	33.200	35.319	37.314
	U	1296.7	2573.8	......	......	2601.3	2685.9	2754.8	2815.1	2870.1	2921.8
	H	1307.4	2762.8	......	......	2798.0	2906.7	2995.8	3074.0	3145.6	3212.9
	S	3.1911	5.7605	......	......	5.8224	6.0082	6.1542	6.2773	6.3857	6.4839
8000 (294.97)	V	1.384	23.525	......	......	24.264	27.378	29.948	32.222	34.310	36.273
	U	1306.0	2571.7	......	......	2592.7	2679.9	2750.3	2811.5	2867.1	2919.3
	H	1317.1	2759.9	......	......	2786.8	2899.0	2989.9	3069.2	3141.6	3209.5
	S	3.2076	5.7471	......	......	5.7942	5.9860	6.1349	6.2599	6.3694	6.4684