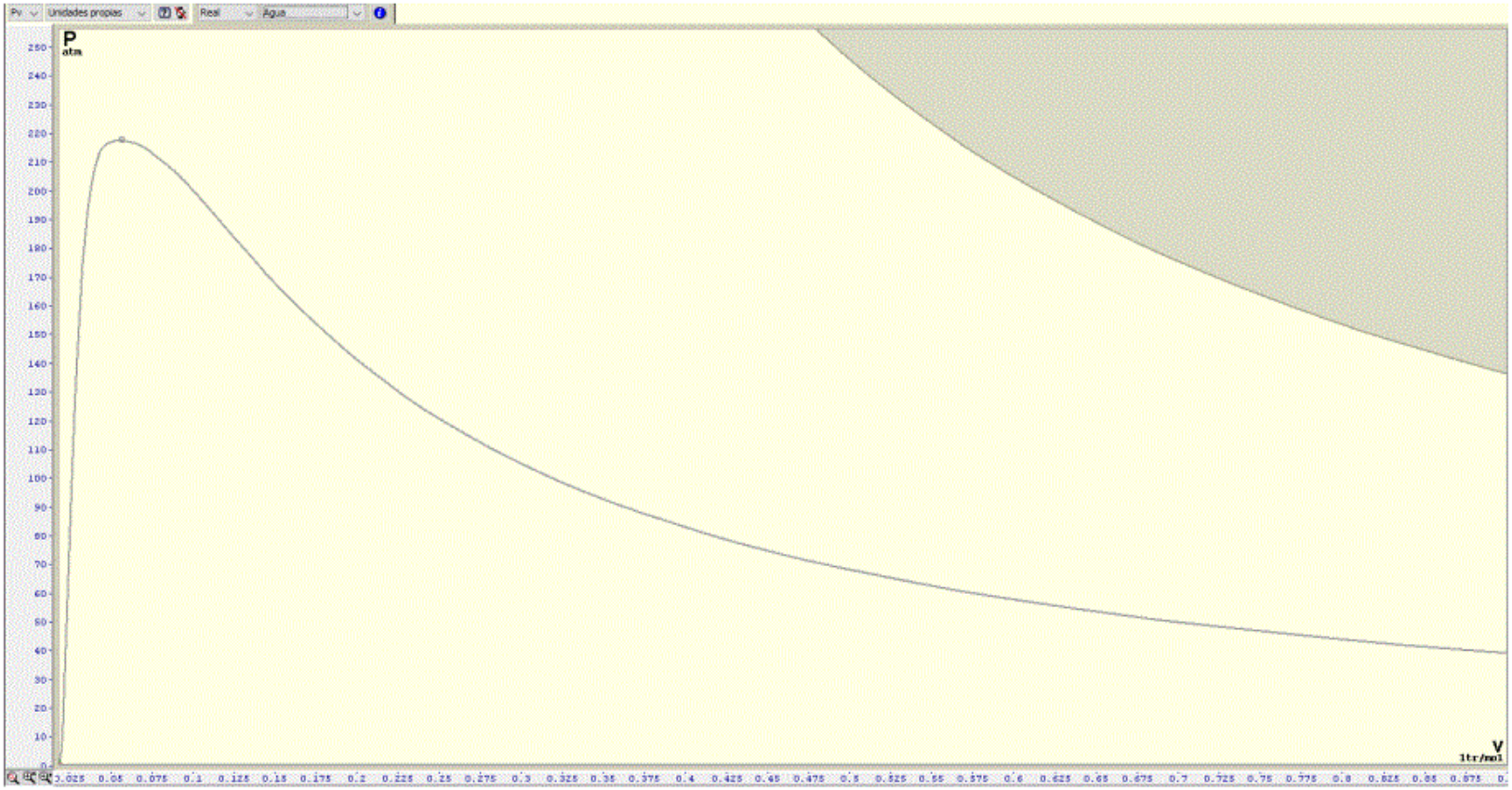
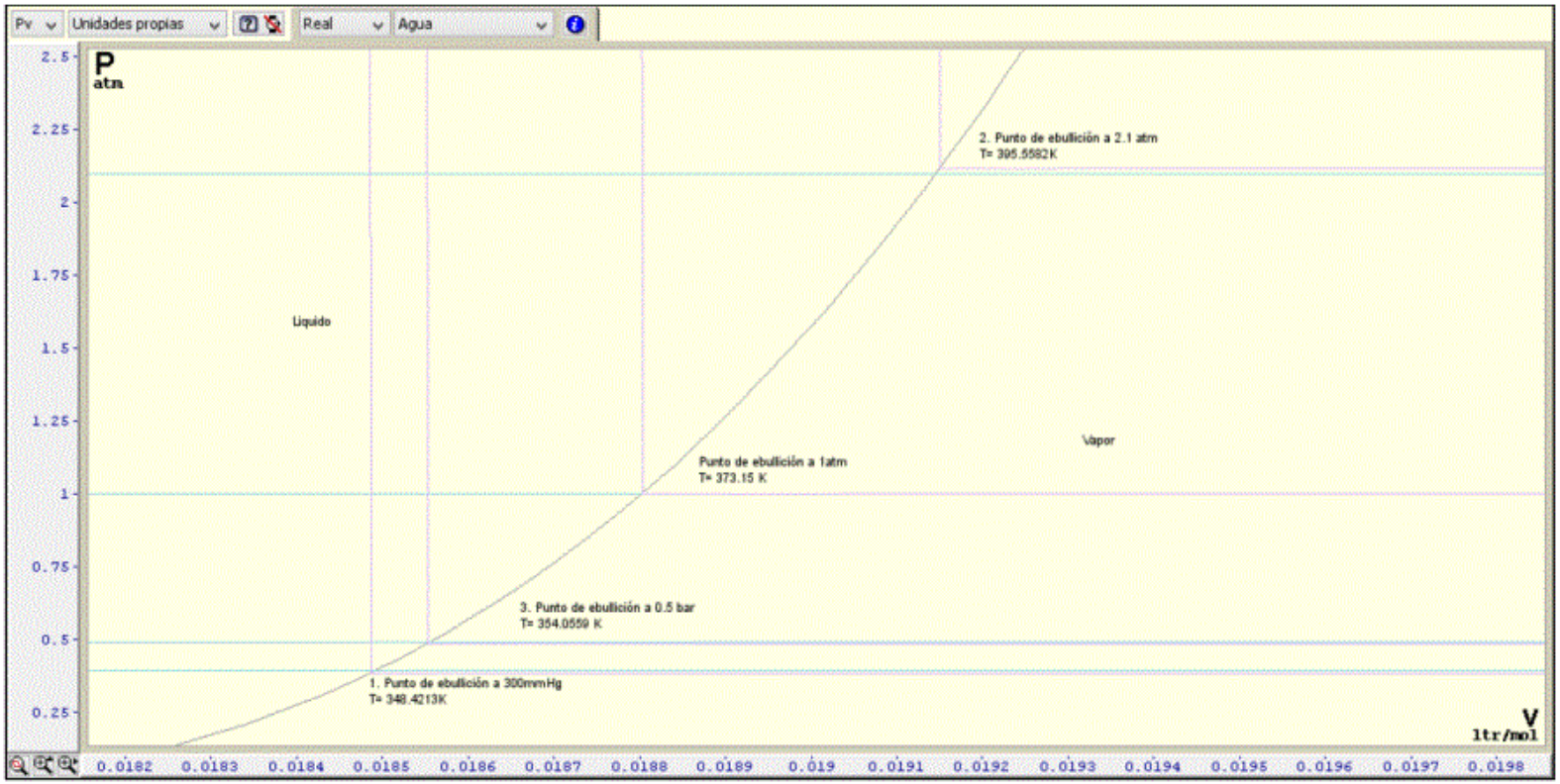
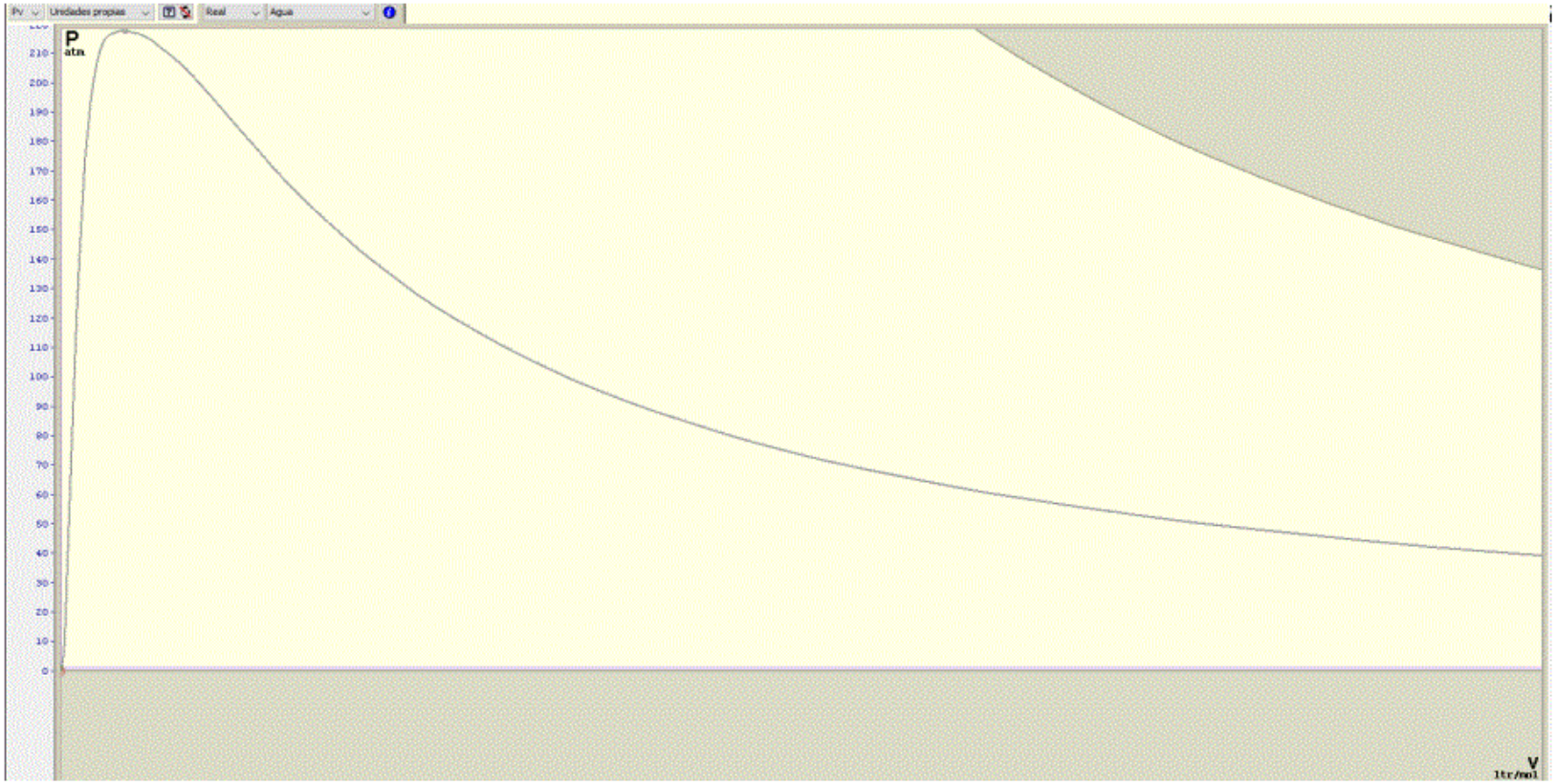
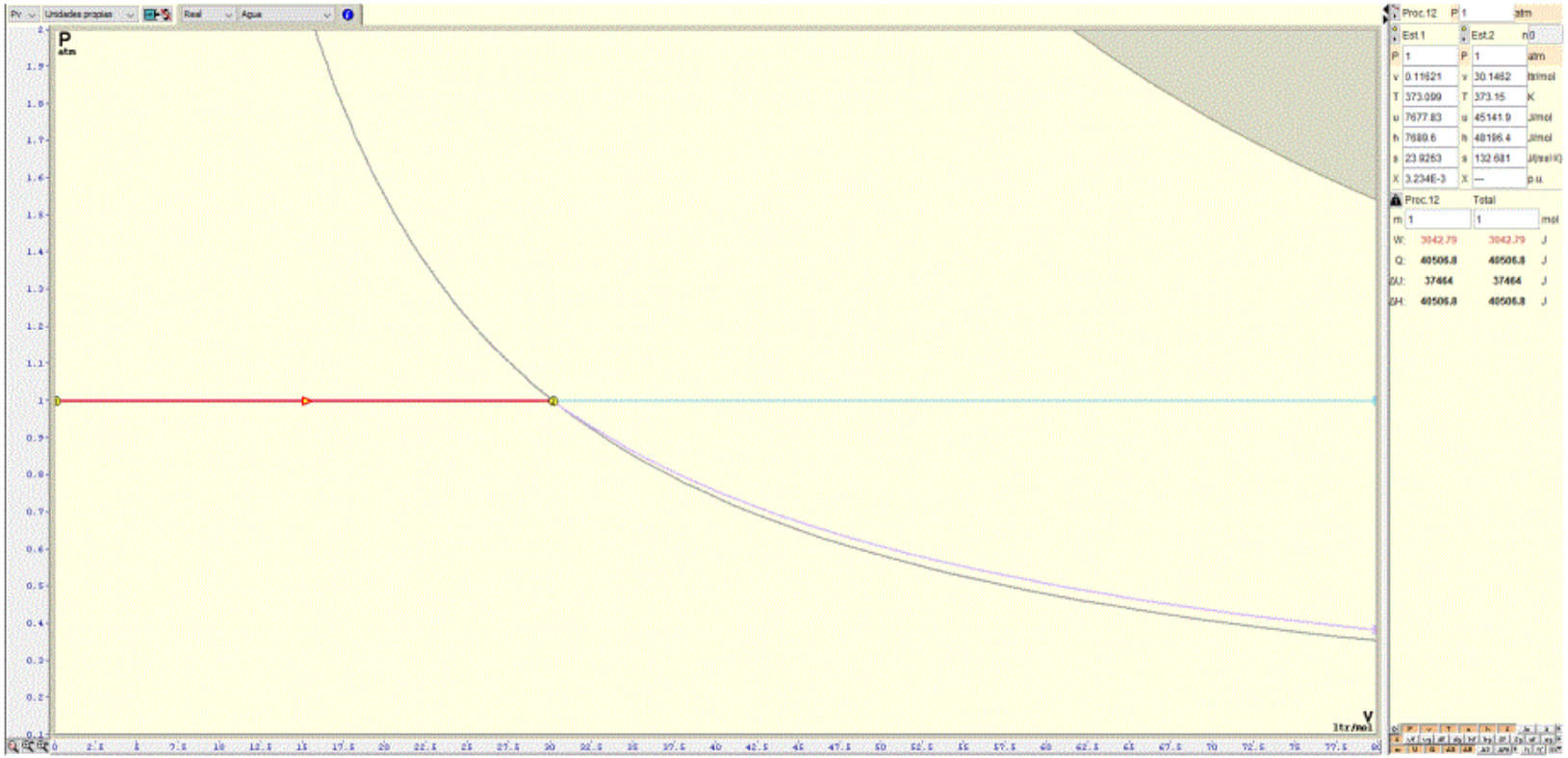
Clase 82 18 Enero 2021

Título de la nota 17/01/2021




Pv
Unidades propias
Real
Agua
P
atm
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
Liquido
Vapor
2. Punto de ebullición a 2.1 atm
T= 395.5582K
Punto de ebullición a 1atm
T= 373.15 K
3. Punto de ebullición a 0.5 bar
T= 354.0559 K
1. Punto de ebullición a 300mmHg
T= 348.4213K
V
ltr/mol
0.0182
0.0183
0.0184
0.0185
0.0186
0.0187
0.0188
0.0189
0.019
0.0191
0.0192
0.0193
0.0194
0.0195
0.0196
0.0197
0.0198

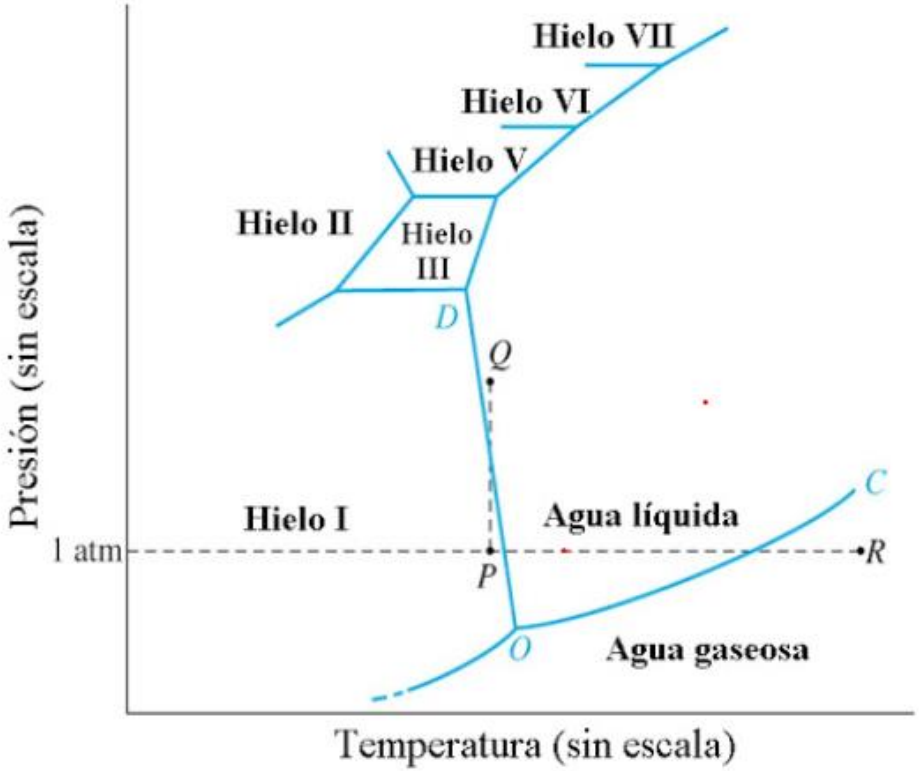

Pv
Unidades propias
Real
Agua
P
atm
V
ltr/mol

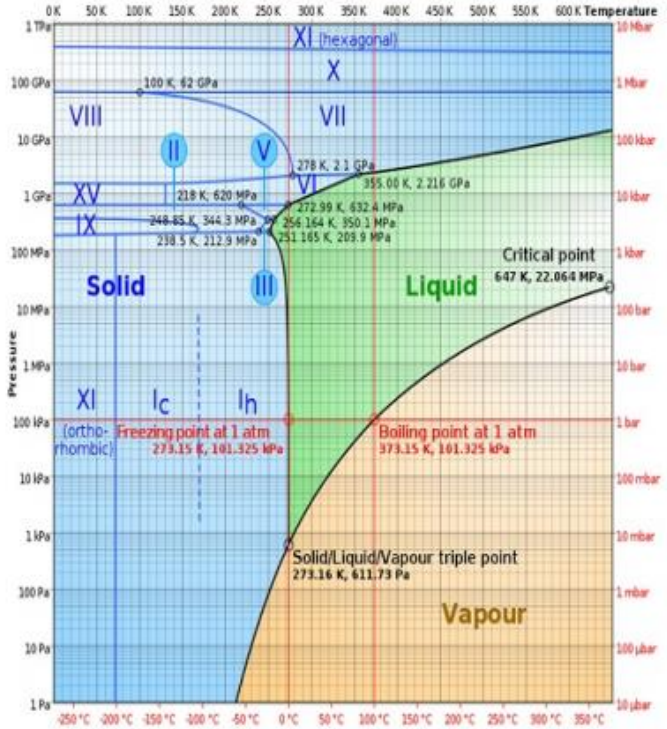

P
atm
V
ltr/mol
Proc.12 P 1 atm
Est.1 Est.2 n0
P 1 P 1 atm
v 0.11621 v 30.1462 ltr/mol
T 373.099 T 373.15 K
u 7677.83 u 45141.9 J/mol
h 7689.6 h 48196.4 J/mol
s 23.9263 s 132.681 J/(mol·K)
X 3.234E-3 X --- p.u.
Proc.12 Total
m 1 1 mol
W: 3842.79 3842.79 J
Q: 40506.8 40506.8 J
ΔU: 37464 37464 J
ΔH: 40506.8 40506.8 J

Presión 1 (mmHg)	Presión 2 (mmHg)	Punto de ebullición (K)
760	300	348.407
	1,596	395.54
	375.03	354.042

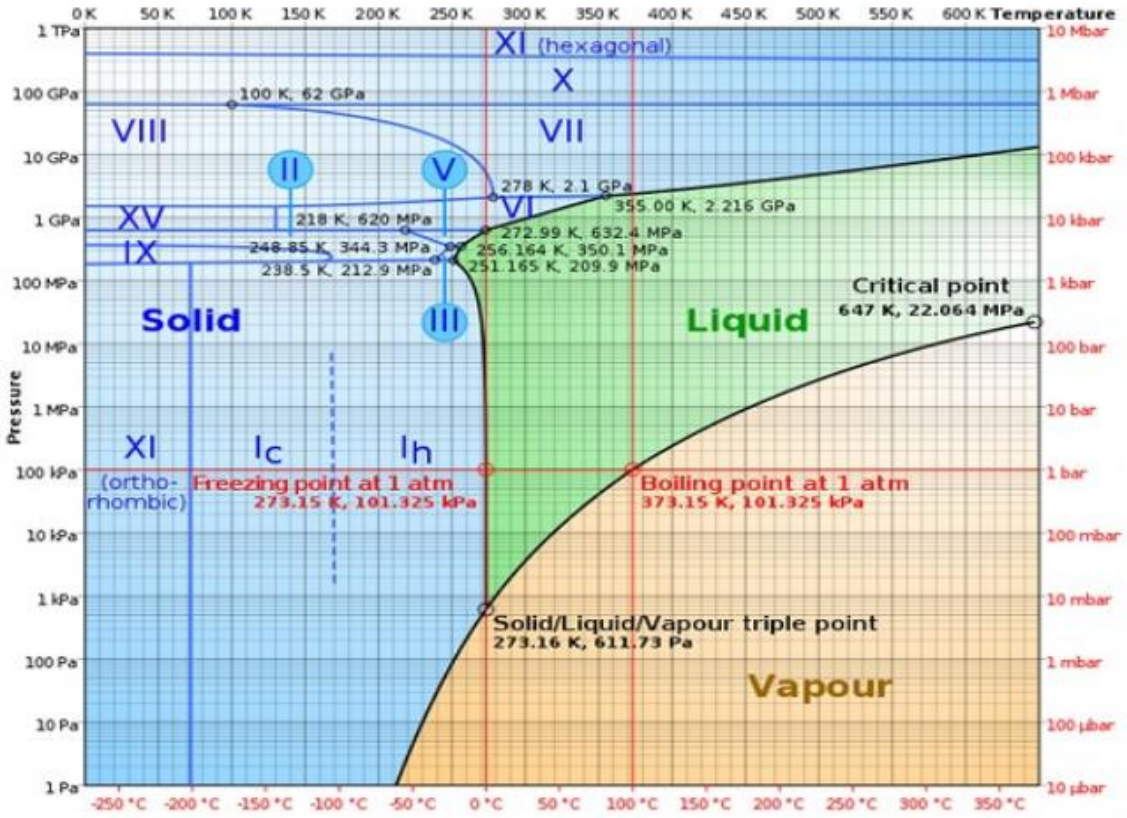
Presión 1 (mmHg)	Presión 2 (mmHg)	Punto de ebullición (K)
760	300	348.972
	1,596	395.308
	375.03	354.436

T_2 (calculada) K	T_2 (Termograph) K
348.42131	348.97
395.5582	395.308
354.0559	354.434





Presión (atm)	0.1	1500	0.7
Punto de fusión (K)	273.1564	262.572	273.152


0 K
50 K
100 K
150 K
200 K
250 K
300 K
350 K
400 K
450 K
500 K
550 K
600 K
Temperature
1 TPa
100 GPa
10 GPa
1 GPa
100 MPa
10 MPa
1 MPa
100 kPa
10 kPa
1 kPa
100 Pa
10 Pa
1 Pa
Pressure
10 Mbar
1 Mbar
100 kbar
10 kbar
1 kbar
100 bar
10 bar
1 bar
100 mbar
10 mbar
1 mbar
100 µbar
10 µbar
-250 °C
-200 °C
-150 °C
-100 °C
-50 °C
0 °C
50 °C
100 °C
150 °C
200 °C
250 °C
300 °C
350 °C
XI (hexagonal)
X
VII
VIII
II
V
VI
XV
IX
III
100 K, 62 GPa
278 K, 2.1 GPa
355.00 K, 2.216 GPa
218 K, 620 MPa
272.99 K, 632.4 MPa
248.85 K, 344.3 MPa
256.164 K, 350.1 MPa
238.5 K, 212.9 MPa
251.165 K, 209.9 MPa
Solid
Liquid
Critical point
647 K, 22.064 MPa
XI
(ortho-
rhombic)
Ic
Ih
Freezing point at 1 atm
273.15 K, 101.325 kPa
Boiling point at 1 atm
373.15 K, 101.325 kPa
Solid/Liquid/Vapour triple point
273.16 K, 611.73 Pa
Vapour

Curva de calentamiento

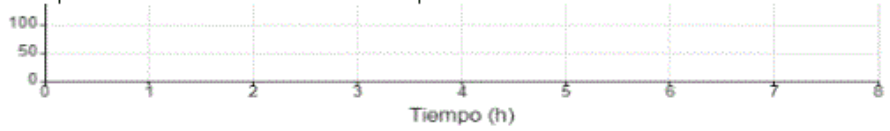
Insertar en las celdas de color amarillo los valores correspondientes

T_1	(K)	268.15	Cp Hielo	(cal/gK)	0.50	Cp vapor	Constantes
T_2	(K)	273.15	ΔH_f	(cal/g)	80.00		(300-2500)K
T_3	(K)	373.15	Cp agua	(cal/gK)	1.00	a	7.19e+000
T_4	(K)	413.15	ΔH_v	(cal/g)	540.00	b	2.37e-003
m	(g)	1.50e+5	n	(mol)	8.33e+3	c	2.08e-007
M	(g/mol)	18.00				d	0.00e+000

ΔH_1	(cal)	3.75e+5
ΔH_2	(cal)	1.20e+7
ΔH_3	(cal)	1.50e+7
ΔH_4	(cal)	8.10e+7
ΔH_5	(cal)	2.72e+6
ΔH total	(cal)	1.11e+8

	Tiempo (h)	T (K)
Etapa I	0	268.15
	0.5	273.15
Etapa II	0.5	273.15
	2	273.15
Etapa III	2	273.15
	4	373.15
Etapa IV	4	373.15
	6	373.15
Etapa V	6	373.15
	7	413.15

	Proceso	Energía para cambio de estado (cal)
1	ΔH_I, del punto 1 al 2	3.75×10^5
2	ΔH_{II}, del punto 2 al 3	1.2×10^7
3	ΔH_{III}, del punto 3 al 4	1.5×10^7
4	ΔH_{IV}, del punto 4 al 5	8.1×10^7
5	ΔH_V, del punto 5 al 6	2.71×10^6



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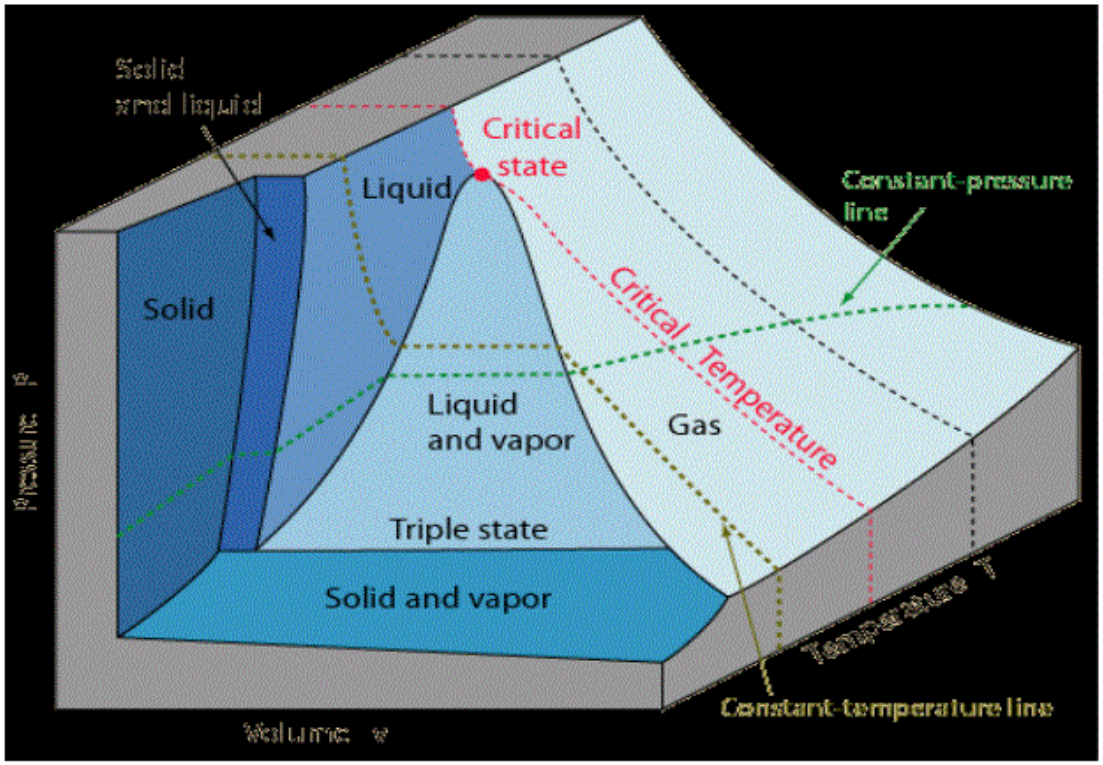
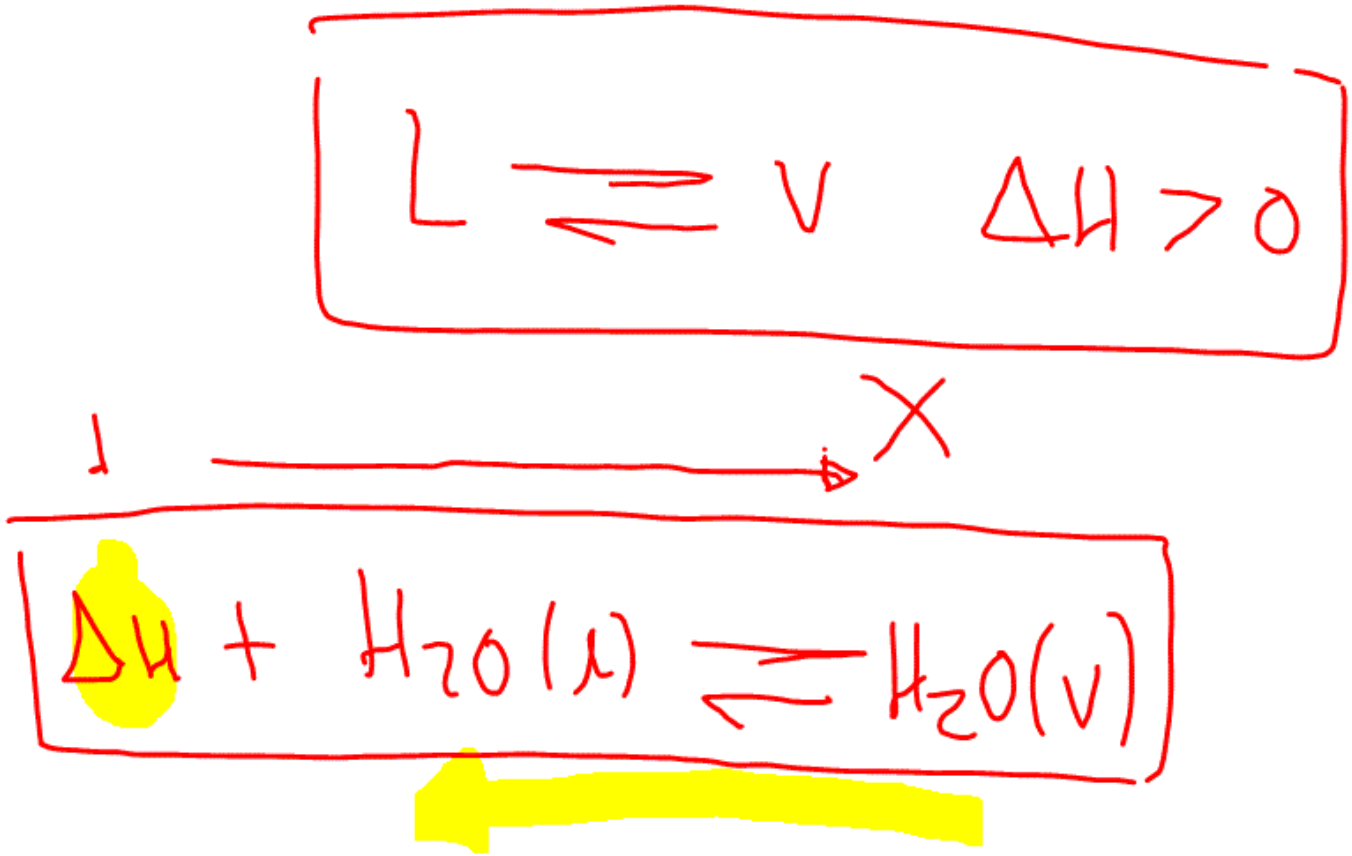


http://biomodel.uah.es/Jmol/plots/phase-diagrams/inicio.htm


L ⇌ V ΔH > 0
I
X
ΔH + H2O(l) ⇌ H2O(v)

ΔH_V y TNE (H_2O)

Pvap (mmHg)	T°C
17.54	20
23.76	25
31.82	30
55.32	40
233.7	70
355.1	80

$$\ln\left(\frac{P_2}{P_1}\right) = \frac{\overline{\Delta H_v}}{R}\left[\frac{1}{T_{NE}} - \frac{1}{T_2}\right]$$

$$\ln p = \frac{\overline{\Delta H_v}}{RT_{NE}} - \frac{\overline{\Delta H_v}}{RT_2}$$

$$y = b - mx \qquad x = \frac{1}{T}$$

$$m = -\frac{\overline{\Delta H_v}}{R}$$

$$m = k$$

$$\frac{cal/mol}{cal/molK}$$

acomodar la tabla y realizar regresión lineal

P (mmHg)	T(°C)	P(atm)	T(K)	ln P	$\frac{1}{T}$
17.54	20	0.02307	293.15	-3.7692	3.41×10^{-3}
23.76	25	0.03126	298.15	-3.4654	3.354×10^{-3}
31.82	30	0.04186	303.15	-3.1734	3.298×10^{-3}
55.32	40	0.07278	313.15	-2.6202	3.193×10^{-3}
233.7	70	0.3045	343.15	-1.1793	2.914×10^{-3}
355.1	80	0.4672	353.15	-0.7609	2.8316×10^{-3}

$y = mx + b$ $m = -5202.49\ K$

$b = 13.9631$ adimensional

Obtención de la Entalpía de vaporización de una sustancia pura

Insertar en las celdas de color amarillo los valores corrspondientes

Temperatura			Presion		
[°C]	[K]	1/T	mmHg	atm	ln p
20	293.15	0.00341122	17.54	0.02307895	-3.76883445
25	298.15	0.00335402	23.76	0.03126316	-3.46531494
30	303.15	0.0032987	31.82	0.04186842	-3.17322341
70	343.15	0.00291418	233.7	0.3075	-1.17928019
80	353.15	0.00283166	355.1	0.46723684	-0.76091899

R(cal/molK)	1.9889

ΔH exp	10319.5187	[cal/mol]
ΔH teorico	9720.00	[cal/mol]
TNE	372.300783	K

m	-5188.55586
b	13.9364624
r	-0.99999336

Modelo

$$\ln p = -\frac{\Delta Hv}{R}\left[\frac{1}{T}\right] + C$$

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Temperatura			Presion		
[°C]	[K]	1/T	mmHg	atm	ln p
20	293.15	0.00341122	17.54	0.02307895	-3.76883445
25	298.15	0.00335402	23.76	0.03126316	-3.46531494
30	303.15	0.0032987	31.82	0.04186842	-3.17322341
40	313.15	0.00319336	55.32	0.07278947	-2.62018393
80	353.15	0.00283166	355.1	0.46723684	-0.76091899

R(cal/molK)	1.9889

ΔH exp	10309.1535	[cal/mol]
ΔH teorico	9720.00	[cal/mol]
TNE	372.334041	K

m	-5183.34432
b	13.9212206
r	-0.99999683

Modelo

$$\ln p = -\frac{\Delta Hv}{R}\left[\frac{1}{T}\right] + C$$

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Obtención de la Entalpía de vaporización de una sustancia pura

Insertar en las celdas de color amarillo los valores corrspondientes

Temperatura			Presion		
[°C]	[K]	1/T	mmHg	atm	ln p
25	298.15	0.00335402	23.76	0.03126316	-3.46531494
30	298.15	0.00335402	31.82	0.04186842	-3.17322341
40	303.15	0.0032987	55.32	0.07278947	-2.62018393
70	313.15	0.00319336	233.7	0.3075	-1.17928019
80	353.15	0.00283166	355.1	0.46723684	-0.76091899

R(cal/molK)	1.9889

m	-4783.73399
b	13.098537
r	-0.99291239

ΔH exp	9514.3685	[cal/mol]
ΔH teorico	9720.00	[cal/mol]
TNE	365.21132	K

Modelo

$$\ln p = -\frac{\Delta Hv}{R}\left[\frac{1}{T}\right] + C$$

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Obtención de la Entalpía de vaporización de una sustancia pura

Insertar en las celdas de color amarillo los valores corrspondientes

Temperatura			Presion		
[°C]	[K]	1/T	mmHg	atm	ln p
60	333.15	0.00300165	149.4	0.19657895	-1.62669116
70	343.15	0.00291418	233.7	0.3075	-1.17928019
80	353.15	0.00283166	355.1	0.46723684	-0.76091899
90	363.15	0.00275368	525.28	0.69115789	-0.36938698
100	373.15	0.00267989	760	1	0

R(cal/molK)	1.9889

m	-5054.45736
b	13.5482539
r	-0.99999153

ΔH exp	10052.8102	[cal/mol]
ΔH teorico	9720.00	[cal/mol]
TNE	373.070758	K

Modelo

$$\ln p = -\frac{\Delta Hv}{R}\left[\frac{1}{T}\right] + C$$

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$$m = -5202.49\,K$$

$$-5202.49\,K = -\frac{\overline{\Delta H_v}}{R}$$

$$5202.49\,K = \frac{\overline{\Delta H_v}}{R}$$

$$\overline{\Delta H_v} = \left(5202.49\,K\right)\left(1.9889\,\frac{cal}{mol\,K}\right)$$

$$= 10347.23\,\frac{cal}{mol}$$

$$TNE =$$

$$b = \frac{\overline{\Delta H_v}}{RTNE} = 13.9351 \; \frac{\frac{cal}{mol}}{\frac{cal}{molK} \; K}$$

$$= \text{adimensional.}$$

$$13.9631 = \frac{\overline{\Delta H_v}}{RTNE}$$

$$TNE = \frac{\overline{\Delta H_v}}{R \; 13.9631} = \frac{5202.49}{13.9631} = \boxed{372.53K}$$

$$\ln p = \frac{\Delta \bar{H}_v}{RTNE} - \frac{\Delta \bar{H}_v}{RT_2}$$

$$\ln p = A - \frac{B}{T} \quad \text{ec. Antoine}$$

$$\ln p = A - \frac{B}{T+C} \qquad T = K$$

$$\ln p = A - \frac{B}{t+C} \qquad t = °C$$

$$\log_p = A - \frac{B}{T+C}$$

$$\log p = A - \frac{B}{t+C}$$

$p = p_{vap}$.

p_{vap} → vaporización

p_{vap} → sublimación

Ecuación de Antoine

Insertar en las celdas de color amarillo los valores correspondientes

Constantes de Antoine			
A	B [K]	C [K ó °C]	
18.30360	3816.4400	-46.13	Modelo 1
7.94897	1657.7000	227.03	Modelo 2

Obtención de temperatura de ebullición y presión de vapor

p [mm Hg]	585.00
T [K]	365.98
T [°C]	92.83

Modelo 1

$$\ln p = A - \frac{B}{T+C} \quad \therefore \quad T = \frac{B}{A - \ln p} - C$$

$$p = e^{\left[A - \frac{B}{T+C}\right]}$$

T [K]	365.979
T [°C]	92.829

p [mmHg]	584.99

Modelo 2

$$\log p = A - \frac{B}{t+C} \quad \therefore \quad t = \frac{B}{A - \log p} - C$$

$$p = 10^{\left[A - \frac{B}{t+C}\right]}$$

T [K]	366.027
T [°C]	92.877

p [mmHg]	585.00

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Con apoyo del programa UNAM-DGAPA-PAPIME PE-200419

Constantes de Antoine			
A	B [K]	C [K ó °C]	
18.30360	3816.4400	-46.13	Modelo 1
7.94897	1657.7000	227.03	Modelo 2

$\log 2 = 0.3010 \quad \ln 2 = 0.6931$

$$\frac{0.6931}{0.3010} = 2.303$$

$$A = \frac{18.30360}{2.303} = 7.9477 \qquad B = \frac{3816.44}{2.303} = 1657.16$$

$$C = -46.13 + 273.15 = 227.02$$