vi	2
vf	10
del	0,5

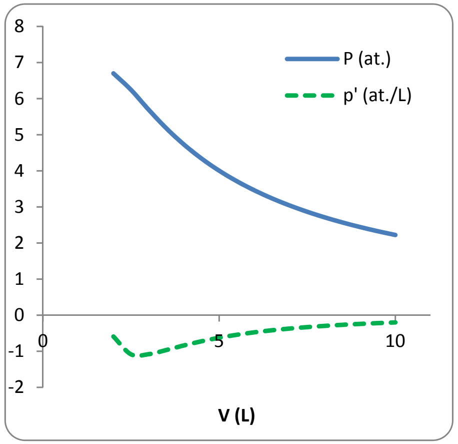
P	2,5
T	298
R	0,082

a
381

$$P = \frac{RT}{v} - \frac{a}{v^2\sqrt{T}}$$

$$P' = -\frac{RT}{v^2} + \frac{2a}{v^3\sqrt{T}}$$

v	P (at.)	p' (at./L)
2	6,700316	-0,59132
2,5	6,243082	-1,08471
3	5,693029	-1,08024
3,5	5,180021	-0,96524
4	4,729579	-0,83754
4,5	4,340309	-0,72231
5	4,004371	-0,62431
5,5	3,713298	-0,54249
6	3,459591	-0,47442
6,5	3,237	-0,41763
7	3,040434	-0,37
7,5	2,865765	-0,32979
8	2,709645	-0,2956
8,5	2,569346	-0,26634
9	2,442633	-0,24113
9,5	2,327659	-0,21927
10	2,222893	-0,20022



W =	30,51 at. L/ K. mol

$$v = v + \frac{RT}{v} - \frac{a}{v^2\sqrt{T}} - P$$

v	g(v)
9,77	9,54
9,54	9,36
9,36	9,22
9,22	9,11
9,11	9,03
9,03	8,96
8,96	8,91
8,91	8,88
8,88	8,85
8,85	8,83
8,83	8,81
8,81	8,80
8,80	8,79
8,79	8,79
8,79	8,78
8,78	8,78
8,78	8,78
8,78	8,77
8,77	8,77
8,77	8,77

v (L) =	8,77

$$Q(v) = \frac{RT}{v} - \frac{a}{v^2\sqrt{T}} - P = 0.$$

$$Q'(v) = -\frac{RT}{v^2} + \frac{2a}{v^3\sqrt{T}}$$

v	Q	Q'	del
9,7744	-0,23101	-0,2085	-1,10797
8,66643	0,025758	-0,25753	0,100019
8,766449	0,000256	-0,25245	0,001013
8,767461	2,57E-08	-0,2524	1,02E-07
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0
8,767461	0	-0,2524	0

v (L) =	8,77

$$v = \frac{RT}{P + \frac{a}{v^2\sqrt{T}}}$$

v	g(v)
9,77	8,95
8,95	8,80
8,80	8,77
8,77	8,77
8,77	8,77
8,77	8,77

Emplea MATHEMATICA para resolver los siguientes apartados:

1. (4 puntos) Calcula el pH de una disolución 0.05M de la sal cálcica CaA2, siendo HA un ácido débil monoprótico con constante de acidez Ka=1.5·10^-5.

2. (3 puntos) Se dispone de una disolución 0.03M de un ácido monoprótico desconocido HX. Para valorar 30 mL de esta disolución se han necesitado 40 mL de amoniaco 0.01M (Kb(NH3)=[NH4+][OH-]/[NH3]=1.8·10^-5). Calculad el pH correspondiente a este volumen de equivalencia si kHX=2.32819·10^-5.

3. (3 puntos) Se dispone de una disolución 0.03M de un ácido monoprótico desconocido HX. Para valorar 30 mL de esta disolución se han necesitado 40 mL de amoniaco 0.01M (Kb(NH3)=[NH4+][OH-]/[NH3]=1.8·10^-5). El pH correspondiente a este volumen de equivalencia resultó ser de 4.54. Determina la constante de acidez KHX del ácido HX.

```
ClearAll["Global`*"]
```

APARTADO A

```
eq1 = Eliminate[{kw == h * oh, ka == h * a / ha, 2 * cs == ha + a, 2 * cs + h == oh + a}, {oh, a, ha}]
```

$$(h + ka)\, kw == h^2\, (2\, cs + h + ka)$$

```
dat1 = {kw → 10^-14, ka → 1.5 * 10^-5, cs → 0.05}; sol1 = Solve[eq1 /. dat1, h]
```

$$\{\{h \to -0.100015\}, \{h \to -1.2246 \times 10^{-9}\}, \{h \to 1.2247 \times 10^{-9}\}\}$$

```
ph = -Log[10, sol1[[3, 1, 2]]]
```

8.91197

APARTADO B

```
ClearAll["Global`*"]
```

```
eq3 = Eliminate[{kw == h * oh, ka == h * x / hx, kb == nh4 * oh / nh3,
   ca == hx + x, cb == nh3 + nh4, nh4 + h == oh + x}, {oh, x, hx, nh3, nh4}]
```

$$-h^4\, kb + ca\, h^2\, ka\, kb - h^3\, ka\, kb - h^3\, kw + ca\, h\, ka\, kw - h^2\, ka\, kw + h^2\, kb\, kw + h\, ka\, kb\, kw + h\, kw^2 + ka\, kw^2 == cb\, h^2\, (h + ka)\, kb$$

```
sol3 = Solve[
  eq3 //. {ca → ca0 * va / (va + vb), cb → cb0 * vb / (va + vb), kw -> 10^-14, kb -> 1.8 * 10^-5,
    ca0 -> 0.03, va -> 30, cb0 -> 0.01, vb -> 40, ka -> 2.32819 * 10^-5}, h]
```

$$\{\{h \to -0.00576641\}, \{h \to -1.00059 \times 10^{-9}\}, \{h \to -7.77294 \times 10^{-13}\}, \{h \to 0.0000288403\}\}$$

```
Print["pH = ", -Log[10, sol3[[4, 1, 2]]]]
```

pH = 4.54

APARTADO C

```
eq2 = Eliminate[{kw == h * oh, khx == h * x / hx, kb == nh4 * oh / nh3,
   ca == hx + x, cb == nh3 + nh4, nh4 + h == oh + x}, {oh, x, hx, nh3, nh4}]
```

$$-h^4\, kb + ca\, h^2\, kb\, khx - h^3\, kb\, khx - h^3\, kw + h^2\, kb\, kw + ca\, h\, khx\, kw - h^2\, khx\, kw + h\, kb\, khx\, kw + h\, kw^2 + khx\, kw^2 == cb\, h^2\, kb\, (h + khx)$$

```
sol2 = Solve[eq2, khx]
```

$$\left\{\left\{khx \to \frac{cb\, h^3\, kb + h^4\, kb + h^3\, kw - h^2\, kb\, kw - h\, kw^2}{ca\, h^2\, kb - cb\, h^2\, kb - h^3\, kb + ca\, h\, kw - h^2\, kw + h\, kb\, kw + kw^2}\right\}\right\}$$

```
(sol2[[1, 1, 2]] /. {ca → ca0 * va / (va + vb), cb → cb0 * vb / (va + vb)}) /.
 {kw → 10^-14, kb → 1.8 * 10^-5, ca0 → 0.03, va → 30, cb0 → 0.01, vb → 40, h → 10^-4.54}
```

0.0000232819

t	2,78

Conc (x)	Abs. (y)	x^2	y_c	$I(y_c)$	y_s	y_i
0	0	0	0	0	0	0
1	0,11	1	0,0983333	0,003736	0,102069	0,094598
2	0,19	4	0,1966667	0,007471	0,204138	0,189196
3	0,3	9	0,295	0,011207	0,306207	0,283793
4	0,39	16	0,3933333	0,014942	0,408275	0,378391
	$<x^2>$	6				

b	0,098
Sb	0,001
I(b)	0,004

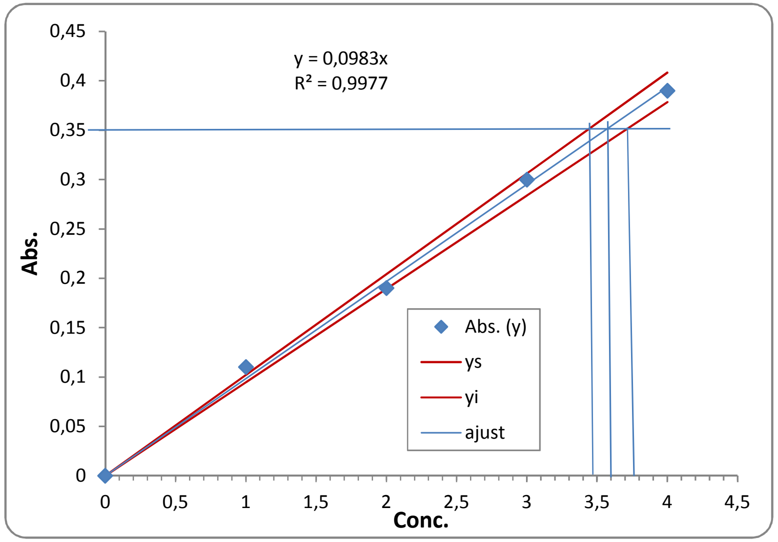
b	a	0,098333	0
Sb	Sa	0,001344	#N/A
R2	Sreg	0,999254	0,00736
F	graus llib.	5355,385	4
D2y	D2reg	0,290083	0,000217

binf	0,095
bsup	0,102

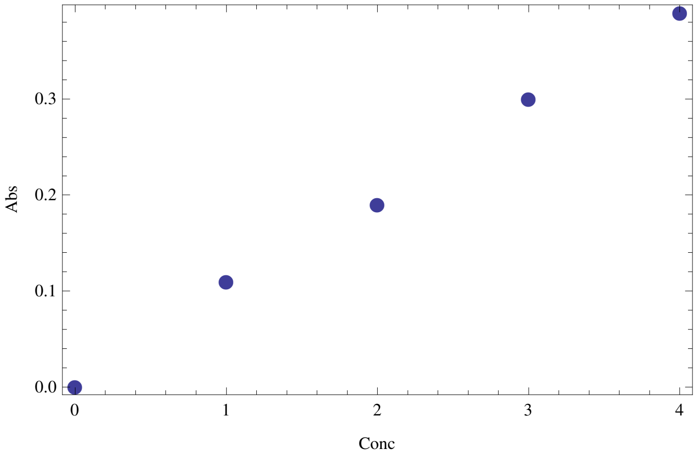
$$S^2_{y_i^c} = x_i^2 \frac{S^2_{reg}}{N\ \overline{x^2}}$$

conc = abs/b

Abs (y)	***Con.(x)***	***Conc (m)***	***Conc (M)***
0,16	1,63	1,69	1,57
0,35	3,56	3,70	3,43
0,1	1,017	1,06	0,98



```
ClearAll["Global`*"]

dades = {{0, 0}, {1, 0.11}, {2, 0.19}, {3, 0.3}, {4, 0.39}};

f1 = ListPlot[dades, PlotMarkers → {Automatic, Medium},
  Frame → True, FrameLabel → {"Conc", "Abs"}]
```




```
sol = NonlinearModelFit[dades, a * x, a, x]
```

FittedModel[0.0983333 x]

```
sol["Properties"];

sol["MeanPredictionConfidenceIntervalTable"]
```

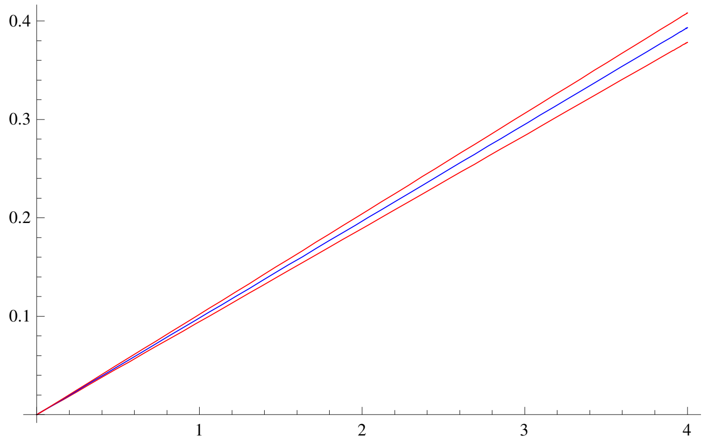
Observed	Predicted	Standard Error	Confidence Interval
0	0.	0.	{0., 0.}
0.11	0.0983333	0.00134371	{0.0946026, 0.102064}
0.19	0.196667	0.00268742	{0.189205, 0.204128}
0.3	0.295	0.00403113	{0.283808, 0.306192}
0.39	0.393333	0.00537484	{0.37841, 0.408256}

```
b = sol["ParameterConfidenceIntervalTable"]
```

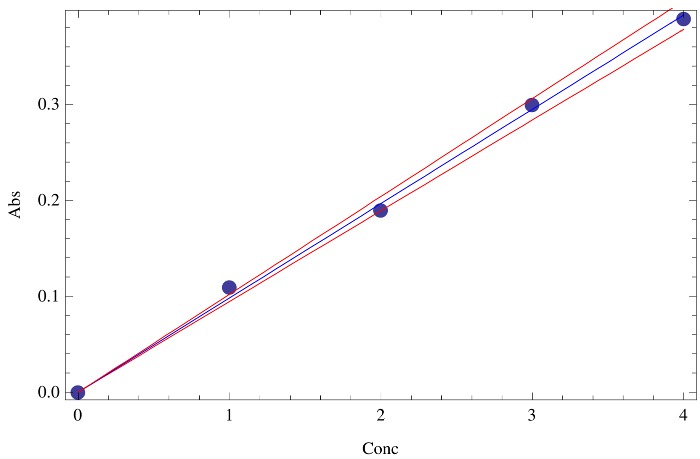
	Estimate	Standard Error	Confidence Interval
a	0.0983333	0.00134371	{0.0946026, 0.102064}

```
b[[1, 1, 2]]

{a, 0.0983333, 0.00134371, {0.0946026, 0.102064}}

inf = b[[1, 1, 2, 4, 1]];
sup = b[[1, 1, 2, 4, 2]];
cent = b[[1, 1, 2, 2]];
```

```
f2 = Plot[{inf x, cent x, sup x}, {x, 0, 4},
  PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 0, 1], RGBColor[1, 0, 0]}]
```




```
Show[f1, f2]
```




```
abs = {0.16, 0.35, 0.1}; conc = {{"Abs", "conc", "conc(min)", "conc(max)"}};
For[i = 1, i ≤ 3, i++,
  AppendTo[conc, {abs[[i]], abs[[i]] / cent, abs[[i]] / sup, abs[[i]] / inf}]
 ];
conc // TableForm
```

Abs	conc	conc(min)	conc(max)
0.16	1.62712	1.56764	1.69129
0.35	3.55932	3.42922	3.69969
0.1	1.01695	0.979777	1.05705

```
(*-------------------------------------------------------------*)



(*-------------------------------------------------------------*)

(* alternativament si volem controlar els decimals farem: *)
```

```
abs = {0.16, 0.35, 0.1}; conc = {{"Abs", "conc", "conc(min)", "conc(max)"}};
For[i = 1, i ≤ 3, i++,
  un = NumberForm[abs[[i]], 3];
  dos = NumberForm[abs[[i]] / cent, 3];
  tres = NumberForm[abs[[i]] / sup, 3];
  quatre = NumberForm[abs[[i]] / inf, 3];
  AppendTo[conc, {un, dos, tres, quatre}]
 ];
conc // TableForm
```

Abs	conc	conc(min)	conc(max)
0.16	1.63	1.57	1.69
0.35	3.56	3.43	3.7
0.1	1.02	0.98	1.06

```
(*--------alternativament si volem representar les llistes-----------*)

sol2 = sol["MeanPredictionConfidenceIntervalTable"];
calc = {}; lower = {}; upper = {};
For[i = 1, i ≤ Length[dades], i++,
  calc = AppendTo[calc, {dades[[i, 1]], sol2[[1, 1, i + 1, 2]]}];
  lower = AppendTo[lower, {dades[[i, 1]], sol2[[1, 1, i + 1, 4, 1]]}];
  upper = AppendTo[upper, {dades[[i, 1]], sol2[[1, 1, i + 1, 4, 2]]}];];
ListPlot[{dades, calc, lower, upper},
 AxesLabel → {"[S]", "V"}, Joined -> {False, True, True, True},
 PlotMarkers → {{"●", Medium}, "", "", ""},
 PlotStyle → {RGBColor[0, 0, 1], RGBColor[0, 0, 1], RGBColor[1, 0, 0], RGBColor[1, 0, 0]}]
```