Appendix

A.1 The Atomic Weights

Periodic Table of the Elements

Legend: IUPAC ←group number→ CAS; period; atomic number / element symbol / atomic weight (IUPAC, 2007, with up to 5 significant figures) / name

period	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 H 1.0079 hydrogen																	2 He 4.0026 helium
2	3 Li 6.941 lithium	4 Be 9.0122 beryllium											5 B 10.811 boron	6 C 12.011 carbon	7 N 14.007 nitrogen	8 O 15.999 oxygen	9 F 18.998 fluor	10 Ne 20.180 neon
3	11 Na 22.990 sodium	12 Mg 24.305 magnesium											13 Al 26.982 aluminium	14 Si 28.086 silicon	15 P 30.974 phosphorus	16 S 32.065 sulfur	17 Cl 35.453 chlorine	18 Ar 39.948 argon
4	19 K 39.098 potassium	20 Ca 40.078 calcium	21 Sc 44.956 scandium	22 Ti 47.867 titanium	23 V 50.942 vanadium	24 Cr 51.996 chromium	25 Mn 54.938 manganese	26 Fe 55.845 iron	27 Co 58.933 cobalt	28 Ni 58.693 nickel	29 Cu 63.546 copper	30 Zn 65.38 zinc	31 Ga 69.723 gallium	32 Ge 72.61 germanium	33 As 74.922 arsenic	34 Se 78.96 selenium	35 Br 79.904 bromine	36 Kr 83.80 krypton
5	37 Rb 85.468 rubidium	38 Sr 87.62 strontium	39 Y 88.906 yttrium	40 Zr 91.224 zirconium	41 Nb 92.906 niobium	42 Mo 95.96 molybdenum	43 Tc (98) technetium	44 Ru 101.07 ruthenium	45 Rh 102.91 rhodium	46 Pd 106.42 palladium	47 Ag 107.87 silver	48 Cd 112.41 cadmium	49 In 114.82 indium	50 Sn 118.71 tin	51 Sb 121.76 antimony	52 Te 127.60 tellurium	53 I 126.90 iodine	54 Xe 131.29 xenon
6	55 Cs 132.91 cesium	56 Ba 137.33 barium	57 La† 138.91 lanthanum	72 Hf 178.49 hafnium	73 Ta 180.95 tantalum	74 W 183.84 tungsten	75 Re 186.21 rhenium	76 Os 190.23 osmium	77 Ir 192.22 iridium	78 Pt 195.08 platinum	79 Au 196.97 gold	80 Hg 200.59 mercury	81 Tl 204.38 thallium	82 Pb 207.2 lead	83 Bi 208.98 bismuth	84 Po (209) polonium	85 At (210) astatine	86 Rn (222) radon
7	87 Fr (223) francium	88 Ra (226) radium	89 Ac‡ (227) actinium	104 Rf (267) rutherfordium	105 Db (268) dubnium	106 Sg (271) seaborgium	107 Bh (272) bohrium	108 Hs (270) hassium	109 Mt (276) meitnerium	110 Ds (281) darmstadtium	111 Rg (280) roentgenium							

† lanthanoids	58 Ce 140.12 cerium	59 Pr 140.91 praseodymium	60 Nd 144.24 neodymium	61 Pm (145) promethium	62 Sm 150.36 samarium	63 Eu 151.96 europium	64 Gd 157.25 gadolinium	65 Tb 158.93 terbium	66 Dy 162.50 dysprosium	67 Ho 164.93 holmium	68 Er 167.26 erbium	69 Tm 168.93 thulium	70 Yb 173.04 ytterbium	71 Lu 174.97 lutetium
‡ actinoids	90 Th* 232.04 thorium	91 Pa* 231.04 protactinium	92 U* 238.03 uranium	93 Np (237) neptunium	94 Pu (244) plutonium	95 Am (243) americium	96 Cm (247) curium	97 Bk (247) berkelium	98 Cf (251) californium	99 Es (252) einsteinium	100 Fm (257) fermium	101 Md (258) mendelevium	102 No (259) nobelium	103 Lr (262) lawrencium

* The atomic weight cannot be given for the elements have no stable nuclides. For these elements, the value enclosed in parentheses indicates the mass number of the longest-lived isotope of the element. However, there are three exceptions (Th, Pa and U) because they have characteristic composition in the crust of Earth so their atomic weights can be given.

A.2 Fundamental Constants for the Calculations

Symbol	Value	Quantity
$c^{\ominus}$	1 M	standard concentration
F	96485 C/mol	Faraday's constant
p_0 $p^{\ominus}$	101325 Pa	1 atm pressure expressed in SI unit (it is the standard pressure, as well)
R	$8.314\,\frac{\mathrm{J}}{\mathrm{mol\,K}}$	gas constant
T_0	–273.15 °C	absolute zero degree

A.3 Temperature and Concentration Dependence of the Potential of the Calomel Reference Electrode

The potential of calomel electrode (E_{cal}) can be calculated with ±0.1 mV accuracy in the 0–70 °C temperature range and at different KCl concentrations with the

$$\boxed{E_{cal} = E^{25\,°C} - \sum_{i=1}^{3} a_i \cdot (t - 25\,°C)^i} \qquad (A.1)$$

expression where t is the temperature expressed in °C, furthermore empirical constants $E^{25\,°C}$, a_1, a_2 and a_3 are the followings:

[KCl]/M	lg([KCl]/M)	$E^{25\,°C}$/V	a_1/(V/°C)	a_2/(V/°C)	a_3/(V/°C)
0.1	−1	0.3337	8.75×10^{-5}	3.00×10^{-6}	0
1.0	0	0.2801	2.75×10^{-4}	2.50×10^{-6}	4×10^{-9}
3.5	0.5441	0.2500	4.00×10^{-4}	0	0
5.15*	0.7114	0.2412	6.61×10^{-4}	1.75×10^{-6}	9×10^{-10}

*It is the concentration of the saturated KCl solution at 25 °C.

For other concentration of KCl solution, the values of the four empirical constants must be interpolated as functions of the logarithm of the concentration. E.g., in case of [KCl]=0.5 M, the 10-based logarithm of the concentration is −0.3010 so the

$$\frac{-0.301-(-1)}{0-(-1)} = \frac{E^{25\,°C}-0.3337}{0.2801-0.3337} = \frac{a_1-8.75\times10^{-5}}{2.75\times10^{-4}-8.75\times10^{-5}} = \frac{a_2-3\times10^{-6}}{2.5\times10^{-6}-3\times10^{-6}} = \frac{a_3-0}{4\times10^{-9}-0}$$

equations are to be solved to get the appropriate values of $E^{25\,°C}$, a_1, a_2 and a_3 in order to use (A.1).

A.4 Specific Conductivity Values of KCl Solutions at DifferenT Temperatures and Concentrations

t/ °C	18	19	20	21	22	23	24
0.01 M KCl	0.001225	0.001251	0.001278	0.001305	0.001332	0.001359	0.001386
0.1 M KCl	0.01119	0.01143	0.01167	0.01191	0.01215	0.01239	0.01264
1.0 M KCl	0.09822	0.10014	0.10207	0.10400	0.10554	0.10789	0.10984
t/ °C	25	26	27	28	29	30	
0.01 M KCl	0.001413	0.001441	0.001468	0.001496	0.001524	0.001552	
0.1 M KCl	0.01288	0.01313	0.01337	0.01362	0.01387	0.01412	
1.0 M KCl	0.11180	0.11377	0.11524	–	–	–	

The specific conductivity values are given in $\Omega^{-1}\mathrm{cm}^{-1}$ unit in this table.

A.5 Temperature Dependence of the Density of Water

The density of water can be calculated with five digits accuracy after the decimal point by the help of the

$$\boxed{\varrho_v(t) = 1.00026 - 5.08692\times10^{-6}\cdot t^2} \tag{A.2}$$

empirical formula in the range of 15 °C≤t≤35 °C. The result is given in g/cm^3 unit at t temperature (expressed in °C).

If either different temperature range or higher accuracy is needed then the next (more complicated) empirical formula should be used:

$$\boxed{\varrho_v(t) = a_0 + \sum_{i=1}^{n} a_i\cdot t^i}, \tag{A.3}$$

where the next values must be substituted as empirical coefficients:

range	0–55 °C	0–31 °C	0–55 °C	0–100 °C
number of precise digits	4	6	5	5
n	3	5	5	10
a_0	0.99987	0.9998406403	0.9998419163	0.99984014
a_1	5.291×10^{-05}	6.801284×10^{-05}	6.694929×10^{-05}	6.8755×10^{-05}
a_2	-7.47×10^{-06}	-9.11644×10^{-06}	-8.91382×10^{-06}	-9.3732×10^{-06}
a_3	3.36×10^{-08}	1.02356×10^{-07}	8.77509×10^{-08}	1.38951×10^{-07}
a_4	–	-1.22323×10^{-09}	-7.80638×10^{-10}	-3.87034×10^{-09}
a_5	–	8.11007×10^{-12}	3.35582×10^{-12}	1.152421×10^{-10}
a_6	–	–	–	-2.552887×10^{-12}
a_7	–	–	–	3.700248×10^{-14}
a_8	–	–	–	-3.290154×10^{-16}
a_9	–	–	–	1.623754×10^{-18}
a_{10}	–	–	–	-3.3993×10^{-21}

For example, if the density of the water is required with the precision of four digits, the

$$\varrho_v(t) = 0.99987 + 5.291\times10^{-05}\cdot54 - 7.47\times10^{-06}\cdot54^2 + 3.36\times10^{-08}\cdot54^3 = 0.9862\,\mathrm{g/cm^3}$$

equation is suitable to calculate it.

A.6 Temperature and Ionic Strength Dependence of the Ionic Product of Water

The negative logarithm of the ionic product of water is given with two digits accuracy after the decimal point at a given temperature t (expressed in °C) and at ionic strength I (expressed in molar concentration) by the

$$\boxed{pK_v = 13.99 - 1.02\cdot\sqrt{I} - 0.0343\cdot(t-25)} \tag{A.4}$$

empirical formula in the range of 15 °C≤t≤30 °C and at ionic strength values less than 0,05 M.

A.7 Preparation of Starch Solution

For the preparation of 100 cm^3, ~0.5 % starch solution, 0.1 g salicylic acid is solved in about 100 cm^3 boiling water in a ~250 cm^3 Erlenmeyer flask. ~0.5 g starch (made from potato) is shaken with about 10 cm^3 distilled water in a test tube, and this solution is infused into the boiling salicylic acid solution. This mixture is boiled until it is getting lose its translucency and the solution becomes opalescent (no more than two minutes). This solution must be cooled and filtered through cotton wad. This starch solution can be used in about two months if it is stored in fridge. If starch is made from corn then the starch solution can be used only within two weeks. If the starch solution is to be used soon (within 4–5 days) then the salicylic acid can be omitted from the above procedure and everything else remains the same.

A.8 Standard Deviation of Data

It frequently happens during the laboratory exercises that the same value is determined more times from more measurements (e.g., a pseudo-first-order rate coefficient can be calculated from any point of a kinetic curve). These values do not equal to each other completely because of experimental and other uncertainties. Assume that a value is measured m times and let denote the jth data with z_j. In this case, the final (more precisely the most probable) value is regarded as the mean of the individual values, and the value ($\bar{z}$) and its standard deviation ($\sigma_{\bar{z}}$) can be given with the following formulas:

$$\boxed{\bar{z} = \frac{\sum_{j=1}^{m} z_j}{m}} \quad \text{és} \quad \boxed{\sigma_{\bar{z}} = \sqrt{\frac{\sum_{j=1}^{m}(z_j-\bar{z})^2}{m-1}}} = \sqrt{\frac{m\cdot\sum_{j=1}^{m} z_i^2 - \left(\sum_{j=1}^{m} z_i\right)^2}{m\cdot(m-1)}}. \tag{A.5}$$

It should be emphasized that the statistical error is not the same as the standard deviation. Their relation is the

$$\text{standard deviation} = \sqrt{\text{degree of freedom}}\cdot\text{error}\,,[1]$$

formula where the degree of freedom=m−1. Many computer program calculates the errors only and the above formula is needed to calculate the standard deviation.

A.9 Calculation of the Error Propagation

The calculation of the error propagation (more precisely, the standard deviation propagation) is a frequent task when measured data are evaluated. The most simple approximate rule is well known: the absolute values of the deviations are to be added in cases of addition and subtraction, and the relative values of the deviation are to be added in cases of multiplication and division. This procedure, however, always overestimates the deviation of the result, moreover, it cannot be applied even to the most common function transformations (e.g., square root, logarithm). This section gives those formulas by the help of which the calculation of the deviations can be done correctly.

We assume that there are two data and their deviations are known: $X\pm\sigma_X$ and $Y\pm\sigma_Y$. A result (Z) must be calculated by using one or both of them, and the deviation of Z (σ_Z) is also to be known. Table A.1 summarizes the formulas applicable for the basic arithmetic operations and also for the most common function transformations to get the deviation of the result. If the wanted result requires the use of more operation and/or transformations then these formulas can be used one after another to get the final result. For example:

$$\begin{aligned}\ln(2.0\pm0.1)+(0.4\pm0.02)^{0.5} &= \left(\ln 2\pm\frac{0.1}{2}\right)+\left(0.4^{0.5}\pm(|0.5\cdot0.02\cdot0.4^{-0.5}|)\right)\\ &= (0.693\pm0.050)+(0.632\pm0.016)\\ &= (0.693\pm0.632)+\left(\sqrt{0.05^2\pm0.016^2}\right)\\ &= \underline{\underline{1.34\pm0.05\ (\text{or } 1.336\pm0.052)}}\end{aligned}$$

A.10 Slope, Intercept and their Statistics of Fitted Lines

During the laboratory exercises, the calculation of the slope and/or intercept of a fitted line is the most frequent method to get the result. This section summarizes the formulas (without deduction) necessary to get the parameters of a fitted line and their deviations even with a single calculator. Before these formulas, however, there are two important remarks:

[1] There is an important fact that many programs (more versions of EXCEL are among them) use the degree of freedom incorrectly, it is simply replaced by the number of data in many functions. It causes negotiable change in the numerical values of the deviation if there are numerous data, otherwise this change can even be 20 %. During the laboratory practices, it is acceptable to calculate the deviation values from the error values given by the EXCEL functions.

Table A.1: Calculation of the standard deviation during the basic arithmetic operations and applying the most important functions. a denotes the constant, deviationless values in the following formulas. For the trigonometric functions, the values of the angles and their deviations should be given in radian. The other abbreviations are exlained in the text.

operation or function	result and deviation ($Z\pm\sigma_Z$)	example
multiply with a	$(a\cdot X)\pm(\lvert a\cdot\sigma_X\rvert)$	$3\cdot(1,2\pm0,3)=\quad(3\cdot1,2)\pm(3\cdot0,3)=\underline{\underline{3,6\pm0,9}}$
addition	$(X+Y)\pm\left(\sqrt{\sigma_X^2+\sigma_Y^2}\right)$	$(2,2\pm0,3)+(8,4\pm0,5)=$ $(2.2+8.4)\pm\left(\sqrt{0.3^2+0.5^2}\right)=\underline{\underline{10.6\pm0.6}}$
subtraction	$(X-Y)\pm\left(\sqrt{\sigma_X^2+\sigma_Y^2}\right)$	$(3.2\pm0.3)-(2.4\pm0.5)=$ $(3.2-2.4)\pm\left(\sqrt{0.3^2+0.5^2}\right)=\underline{\underline{0.8\pm0.6}}$
multiplication	$(X\cdot Y)\pm\left(\sqrt{Y^2\cdot\sigma_X^2+X^2\cdot\sigma_Y^2}\right)$	$(2.2\pm0.2)\cdot(8.4\pm1.0)=$ $(2.2\cdot8.4)\pm\left(\sqrt{8.4^2\cdot0.2^2+2.2^2\cdot1.0^2}\right)=\underline{\underline{18.5\pm2.8}}$
division	$\left(\frac{X}{Y}\right)\pm\left(\sqrt{\frac{Y^2\cdot\sigma_X^2+X^2\cdot\sigma_Y^2}{Y^4}}\right)$	$(22.0\pm2.0)/(8.4\pm1.0)=$ $\left(\frac{22.0}{8.4}\right)\pm\left(\sqrt{\frac{8.4^2\cdot2.0^2+22.0^2\cdot1.0^2}{8.4^4}}\right)=\underline{\underline{2.6\pm0.4}}$
reciprocal	$\left(\frac{1}{X}\right)\pm\left(\frac{\sigma_X}{X^2}\right)$	$\frac{1}{(0.44\pm0.12)}=\quad\left(\frac{1}{0.44}\right)\pm\left(\frac{0.12}{0.44^2}\right)=\underline{\underline{2.3\pm0.6}}$
raising to a power	$(X^a)\pm(\lvert a\cdot\sigma_X\cdot X^{a-1}\rvert)$	$(3.0\pm0.5)^{1.2}=$ $\left(3.0^{1.2}\right)\pm\left(\lvert1.2\cdot0.5\cdot3.0^{1.2-1}\rvert\right)=\underline{\underline{3.7\pm0.7}}$
exponential functions	$(e^X)\pm(\sigma_X\cdot e^X)$ $(10^X)\pm(\ln(10)\cdot\sigma_X\cdot10^X)$	$e^{(2.0\pm0.5)}=\quad\left(e^{2.0}\right)\pm\left(0.5\cdot e^{2.0}\right)=\underline{\underline{7.4\pm3.7}}$ $10^{(1.3\pm0.1)}=\quad\left(10^{1.3}\right)\pm\left(2.3\cdot0.1\cdot10^{1.3}\right)=\underline{\underline{20\pm5}}$
logarithmic functions	$(\ln X)\pm(\sigma_X/X)$ $(\lg X)\pm\left(\frac{\sigma_X}{\ln(10)\cdot X}\right)$	$\ln(2.0\pm0.1)=\quad(\ln(2.0))\pm(0.1/2.0)=\underline{\underline{0.69\pm0.05}}$ $\lg(20\pm10)=\quad(\lg(20))\pm(10/(2.3\cdot20))=\underline{\underline{1.3\pm0.2}}$
trigono-metric functions	$(\sin X)\pm(\lvert\cos X\rvert\cdot\sigma_X)$ $(\cos X)\pm(\lvert\sin X\rvert\cdot\sigma_X)$ $(\tan X)\pm\left(\frac{\sigma_X}{(\cos X)^2}\right)$	$\sin(60°\pm5°)=\quad\left(\sin\frac{\pi}{3}\right)\pm\left(\left\lvert\cos\frac{\pi}{3}\right\rvert\cdot\frac{5\cdot\pi}{180}\right)=\underline{\underline{0.87\pm0.04}}$ $\cos(60°\pm5°)=\quad\left(\cos\frac{\pi}{3}\right)\pm\left(\left\lvert\sin\frac{\pi}{3}\right\rvert\cdot\frac{5\cdot\pi}{180}\right)=\underline{\underline{0.5\pm0.08}}$ $\tan(45°\pm5°)=\left(\tan\frac{\pi}{4}\right)\pm\left(\frac{5\cdot\pi}{180}\Big/\left(\cos\frac{\pi}{4}\right)^2\right)=\underline{\underline{1.0\pm0.2}}$
inverse trigonomet-ric functions	$(\arcsin X)\pm\left(\frac{\sigma_X}{\sqrt{1-X^2}}\right)$ $(\arccos X)\pm\left(\frac{\sigma_X}{\sqrt{1-X^2}}\right)$ $(\arctan X)\pm\left(\frac{\sigma_X}{1+X^2}\right)$	$\arcsin(0.87\pm0.08)=$ $\left(\arcsin(0.87)\pm\left(\frac{0.08}{\sqrt{1-0.87^2}}\right)\right)\cdot\frac{180}{\pi}=\underline{\underline{60°\pm9°}}$ $\arccos(0.5\pm0.08)=$ $\left(\arccos(0.5)\pm\left(\frac{0.08}{\sqrt{1-0.5^2}}\right)\right)\cdot\frac{180}{\pi}=\underline{\underline{60°\pm5°}}$ $\arctan(1.0\pm0.2)=$ $\left(\arctan(1.0)\pm\left(\frac{0.2}{1+1.0^2}\right)\right)\cdot\frac{180}{\pi}=\underline{\underline{45°\pm6°}}$

1. At the first look, the formulas may seem rather complicated, their usage, however, is more simple in the practice. The reader can ascertain this statement by solving

the problem given in Table A.2 (page A.7) with a single calculator. Moreover, the most scientific calculator can calculate statistical functions and automatically store the partial results making the calculations even faster.

2. Many special and general programs (e.g. spreadsheets) are able to calculate the parameters of a fitted line so their use is rapidly spreading. Most of these programs, however, give the errors as statistical parameters, not deviations! Some manuals mention deviations but the error is the really calculated value. The relation between the deviation and the error is given by the

$$\text{standard deviation} = \sqrt{\text{degree of freedom}} \cdot \text{error}\,,$$ [1]

formula. Assume that n data pairs is used for fitting. The degree of freedom equals to $(n-2)$ if both the slop and the intercept are fitted. The degree of freedom equals to $(n-1)$ if only the slope is fitted and the intercept is supposed to be zero.

The following abbreviations are used in the formulas:

- n is the number of fitted data pairs,
- x_i is the value of the *independent* variable in the i^{th} data pair ($i = 1\ldots n$),
- y_i is the value of the *dependent* variable in the i^{th} data pair ($i = 1\ldots n$),
- a the slope of the fitted line ($y=a\cdot x+b$ vagy $y=a\cdot x$),
- b the intercept of the fitted line ($y=a\cdot x+b$),
- σ_a the standard deviation of the slope and
- σ_b the standard deviation of the intercept.

The formulas are more simple by introducing the following abbreviations: S_x and S_y are the sums of x_i and y_i; S_{xy} is the sum of of the products of x_i and y_i data; S_{xx} is the sum of x_i data and S_Δ is the sum of the squares of deviations between the measured data (y_i) and their calculated corresponding data ($a\cdot x_i+b$), respectively:

$$\boxed{S_x=\sum_{i=1}^{n} x_i,\ S_y=\sum_{i=1}^{n} y_i,\ S_{xy}=\sum_{i=1}^{n} x_i\cdot y_i,\ S_{xx}=\sum_{i=1}^{n} x_i^2 \text{ and } S_\Delta=\sum_{i=1}^{n}(y_i-a\cdot x_i-b)^2}\,.$$

The slope (a) and its standard deviation (σ_a) of the fitted line in case of *no intercept* ($b=0$):

$$\boxed{a=\frac{S_{xy}}{S_{xx}}} = \left(\sum_{i=1}^{n} x_i\cdot y_i\right)\Big/\left(\sum_{i=1}^{n} x_i^2\right) \tag{A.6a}$$

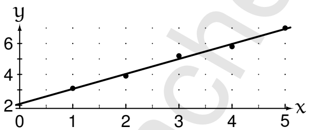
$$\boxed{\sigma_a=\sqrt{\frac{n^2}{n-1}\cdot\frac{S_\Delta}{n\cdot S_{xx}-(S_x)^2}}} = \sqrt{\frac{n^2}{n-1}\cdot\frac{\sum_{i=1}^{n}(y_i-a\cdot x_i)^2}{n\cdot\sum_{i=1}^{n}x_i^2-\left(\sum_{i=1}^{n}x_i\right)^2}} \tag{A.6b}$$

The slope (a) and its standard deviation (σ_a) of the fitted line in case of *fitted intercept* ($b\neq 0$):

Table A.2: A detailed example how to calculate the a and b parameters, as well as their standard deviations of a fitted $y=a\cdot x+b$ equation. The abbreviations defined from page A.7 are used in the followings.

Data:

i:	1	2	3	4	5
x_i:	1.0	2.0	3.0	4.0	5.0
y_i:	3.1	3.9	5.2	5.8	7.0



Partial results:

$$\begin{aligned} S_x &= 1.0+2.0+3.0+4.0+5.0=\underline{15.0}\\ S_y &= 3.1+3.9+5.2+5.8+7.0=\underline{25.0}\\ S_{xy} &= 1.0\cdot 3.1+2.0\cdot 3.9+3.0\cdot 5.2+4.0\cdot 5.8+5.0\cdot 7.0=\underline{84.7}\\ S_{xx} &= 1.0^2+2.0^2+3.0^2+4.0^2+5.0^2=\underline{55.0}\\ n\cdot S_{xx}-(S_x)^2 &= 5\cdot 55.0-15.0^2=\underline{50.0}\end{aligned}$$

The slope from (A.7a) and the intercept from (A.8a):

$$\underline{\underline{a}}=\frac{5\cdot 84.7-15.0\cdot 25.0}{50.0}=\underline{\underline{0.97}} \qquad \underline{\underline{b}}=\frac{55.0\cdot 25.0-15.0\cdot 84.7}{50.0}=\underline{\underline{2.09}}$$

Partial result:

$$\begin{aligned} S_\Delta = {} & (3.1-0.97\cdot 1.0-2.09)^2+(3.9-0.97\cdot 2.0-2.09)^2+\\ & (5.2-0.97\cdot 3.0-2.09)^2+(5.8-0.97\cdot 4.0-2.09)^2+\\ & (5.9-0.97\cdot 5.0-2.09)^2 = \underline{0.091}\end{aligned}$$

The standard deviation of the slope and the intercept from (A.7b) and (A.8b), respectively:

$$\underline{\underline{\sigma_a}}=\sqrt{\frac{5^2}{5-2}\cdot\frac{0.091}{50.0}}=\underline{\underline{0.12}} \qquad \underline{\underline{\sigma_b}}=\sqrt{\frac{5\cdot 55.0}{5-2}\cdot\frac{0.091}{50.0}}=\underline{\underline{0.41}}$$

Remark: Many programs (including EXCEL) calculate slightly different values for the deviations: σ_a=0.095 és σ_b=0.32. The reason is that these programs apply simplified expressions for calculating the errors and deviations, particularly only n is used instead of $n-1$ and $n-2$ in the denominators of equations (A.6b), (A.7b) and (A.8b).

$$\boxed{a=\frac{n\cdot S_{xy}-S_x\cdot S_y}{n\cdot S_{xx}-(S_x)^2}} = \frac{n\cdot\sum_{i=1}^{n}x_i\cdot y_i-\left(\sum_{i=1}^{n}x_i\right)\cdot\left(\sum_{i=1}^{n}y_i\right)}{n\cdot\sum_{i=1}^{n}x_i^2-\left(\sum_{i=1}^{n}x_i\right)^2} \tag{A.7a}$$

$$\boxed{\sigma_a=\sqrt{\frac{n^2}{n-2}\cdot\frac{S_\Delta}{n\cdot S_{xx}-(S_x)^2}}} = \sqrt{\frac{n^2}{n-2}\cdot\frac{\sum_{i=1}^{n}(y_i-a\cdot x_i-b)^2}{n\cdot\sum_{i=1}^{n}x_i^2-\left(\sum_{i=1}^{n}x_i\right)^2}} \tag{A.7b}$$

The intercept (b) and its standard deviation (σ_b) of the fitted line:

$$\boxed{b=\frac{S_{xx}\cdot S_y - S_x\cdot S_{xy}}{n\cdot S_{xx}-(S_x)^2}} = \frac{\left(\sum\limits_{i=1}^{n} x_i^2\right)\cdot\left(\sum\limits_{i=1}^{n} y_i\right)-\left(\sum\limits_{i=1}^{n} x_i\right)\cdot\left(\sum\limits_{i=1}^{n} x_i\cdot y_i\right)}{n\cdot\sum\limits_{i=1}^{n} x_i^2-\left(\sum\limits_{i=1}^{n} x_i\right)^2} \tag{A.8a}$$

$$\boxed{\sigma_b=\sqrt{\frac{n\cdot S_{xx}}{n-2}\cdot\frac{S_\Delta}{n\cdot S_{xx}-(S_x)^2}}} = \sqrt{\frac{n\cdot\sum\limits_{i=1}^{n} x_i^2}{n-2}\cdot\frac{\sum\limits_{i=1}^{n}(y_i-a\cdot x_i-b)^2}{n\cdot\sum\limits_{i=1}^{n} x_i^2-\left(\sum\limits_{i=1}^{n} x_i\right)^2}} \tag{A.8b}$$

A.11 Creating Scientific Figures

The requirements are the same both for a hand-made figure created on a graph paper and for a figure created by a computer program:

- If there is no specific reason for the omission of some data then all measured data (or their derived quantities) should be indicated on the figure.
- There must be appropriate titles for both the axes (also including the unit if it is necessary) and for the whole figure. The titles must be correct from both professional and grammatical points of view. There should be student's name and date on the figure, preferably.
- Such divisions, ticks and labels should be chosen for the axes which make possible easy back-reading, fast plotting of data (for hand-made figures) and minimizing the useless areas. This principle should always be applied to the actual task. For example, in case of fitting a straight line, sometimes it is advisable to show the intercept, even it is outside of the range of data.
- In case of curve-fitting, the figure must show both the fitted and the omitted data (with different symbol!), as well as, the fitted curve together with the value(s) of the fitted parameter(s).
- If a figure contains more curves and/or data series then they have to be distinguished clearly.

There can be more expectations depending on the concrete task. In rare cases, one or more requirements cannot be fulfilled completely. For example, if the value of an erroneous point differs from the others by orders of magnitude, it would fully distort the figure. However, accepting the above principles is enough for perfect figures in the vast majority of the cases.

It may be clear from the above considerations that sloppy knowledge about the used graphing program is not enough in many times. *A figure created by the default options of a program cannot be accepted usually as the final one. The user must be able to handle the used program in such level which makes possible to fulfill the above detailed requirements!* This statement is to be emphasized even sharply in scientific life since most commercial graphing programs (also including the spreadsheet programs)

set up their default options to serve economic and presentation purposes and not scientific requirements, like precision.

Hereinafter those typical errors are demonstrated through an example which are more frequent during creating figures with a computer program. Both figures A.1 and A.2 illustrate straight line fitting for the same data series. Figure A.1 fully comply the above detailed expectations while Figure A.2 show the more frequent errors (according to the experience). If a program is used with care and knowledge, these errors can be avoided easily. The rest of this section in this appendix compares the two figures to help how to sidestep the following typical errors and imperfections:

Automatically connected points. By default, almost all programs denote the data with a symbol and also connect them, usually with lines. These lines do not carry additional information just lead on the eyes through the tendency of the points, the economic figures look nicer. Lines usually denote fitted or calculated curves on scientific figures so connecting the measured data may be misleading. Furthermore, it can result unintelligible figure if the order of the x-values is not strictly increasing or decreasing. For example, a single point deviating from the strict order gives an unwanted line on Figure A.2.

Unsuitable range(s) for the axes. A few programs automatically indicate the origin of the coordinate system. Depending on the range of the points to be plotted, it can result that all points jostle into a tiny part of the figure and their structure becomes unclear.

Inexact division of the axes can be the outcome if a program calculates the minimum and maximum values of the axes from the minimum and maximum values of the data series to be plotted. On Figure A.2, the division of the y-axis is wrong because the range of 13–120 cannot be divided well into ten parts. Additionally, the labels of the main ticks are incorrect since they are rounded to the nearest integer. Therefore the back-reading is wrong, different values can be read from ranges with the same length (e.g., 120–109≠109–99)! It must be known how to set up the minimum and maximum values of the axes, the density of the division and the displayed form of the labels.

Automatic axis setup may lead to wrong division, meaningless or missing titles and/or labels along the axes. On Figure A.2, the labels of the ticks are missing along the x-axis, the meaningless automatic axes titles may come from the used filenames and column numbers, the limiting data just hang at the edges of the figure.

Inexpressive main title may make the understanding more difficult mainly if lots of time pass between the creation and the reading of the figure. Several programs default the main title to the name of the file containing the data and/or the graphical settings.

Missing name, title or date may also be an annoying information loss. In the example, the date is missing from the wrong figure.

Wrong positioning in any part of the figure is just funny in lucky cases but it may lead to information loss in worse cases. The position of the legend box is wrong on Figure A.2 so the half of it is hidden.

Automatic legend block is meaningless very often. Either it should be omitted completely or it should be filled with precise information.This block has a definite role if more curves are included in a figure and short notes are necessary to distinguish them.

Grid is not essential part of figures but if there is any it should be adjusted appropriately. Too dense grid does not help to read the figure since it may disturb the recognition of the curves. Too sparse grid is also imperfect since it makes difficult to back-read data from the figures. Several times, the figure is more clear if there is not any grid. What is certainly wrong that either only the horizontal or only the vertical grids are indicated as illustrated on the wrong figure in our example.

Inappropriate font type and/or font size may lead to ugly and funny titles and remarks in a better case but it may cause misinterpretation in a worse case. The name indicated on Figure A.2 is unnecessary tawdry. Usually it is worth to use sans serif font types (e.g., Swiss, Arial, Helvetica, Tahoma, Verdana, Calibri, etc.) and the boldface variants often look better.

Points omitted from fitting are either removed or their symbol is identical with that of the fitted points frequently. If the omitted points are not indicated on the figure then information is lost about both the real precision of measurement and the reason(s) of omitting points. If the fitted and omitted points are denoted by the same symbol then the reproducibility of the fitting procedure becomes almost impossible.

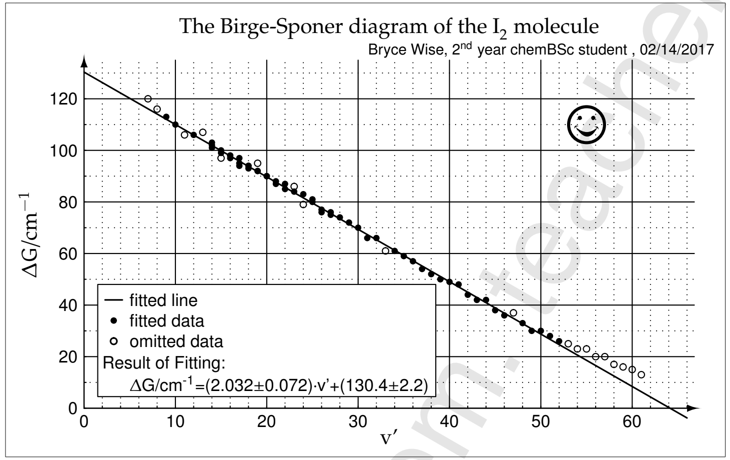


Figure A.1: A perfect figure made on a computer.

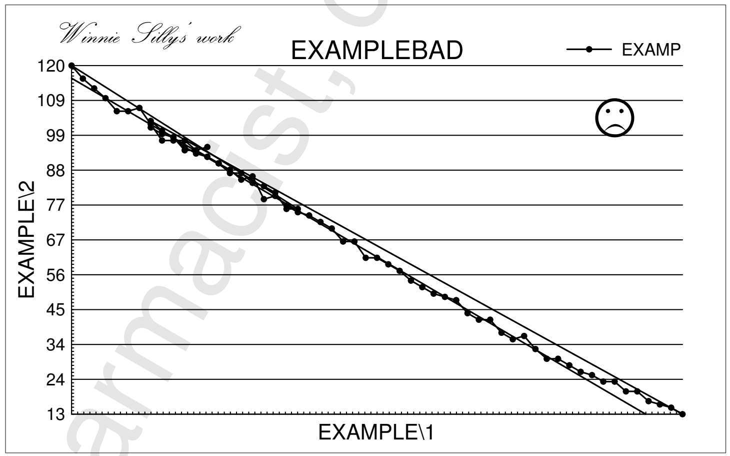


Figure A.2: A figure made on a computer to show the typical errors.

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