2 The presentation of physical quantities with their inaccuracies

This chapter is about the *presentation* of experimental results. When the value of a physical quantity is reported, the uncertainty in the value must be properly reported too, and it must be clear to the reader what kind of uncertainty is meant and how it has been estimated. Given the uncertainty, the value must be reported with the proper number of digits. But the quantity also has a unit that must be reported according to international standards. Thus this chapter is about reporting your results: this is the last thing you do, but we'll make it the first chapter before more serious matters require attention.

2.1 How to report a series of measurements

In most cases you derive a result on the basis of a series of (similar) measurements. In general you do not report all individual outcomes of the measurements, but you report the best estimates of the quantity you wish to "measure," based on the experimental data and on the model you use to derive the required quantity from the data. In fact, you use a *data reduction method*. In a publication you are *required* to be explicit about the method used to derive the end result from the data. However, in certain cases you may also choose to report details of the data themselves (preferably in an appendix or deposited as "additional material"); this enables the reader to check your results or apply alternative data reduction methods.

List all data, a histogram or percentiles

The fullest report of your experimental data is a list or table of all data. Almost[1] equivalent is the report of a *cumulative distribution* of the data (see Section 5.1 on page 54). Somewhat less complete is reporting a *histogram* after collecting data in a limited number of intervals, called *bins*. Much less

[1] Not quite, because one loses information on possible sequential correlation between data points.

Table 2.1 *Thirty observations, numbered in increasing order.*

1	6.61	6	7.70	11	8.35	16	8.67	21	9.17	26	9.75
2	7.19	7	7.78	12	8.49	17	9.00	22	9.38	27	10.06
3	7.22	8	7.79	13	8.61	18	9.08	23	9.64	28	10.09
4	7.29	9	8.10	14	8.62	19	9.15	24	9.70	29	11.28
5	7.55	10	8.19	15	8.65	20	9.16	25	9.72	30	11.39

complete is to report certain *percentiles* of the cumulative distribution, usually the 0, 25%, 50%, 75% and 100% values (i.e., the full range, the median and the first and third quartiles). This is done in a *box-and-whisker* display. See the example below.

List properties of the data set

The methods above are *rank-based* reports: they follow from ranking the data in a sequence. You can also report *properties* of the set of data, such as the number of observations, their average, the mean squared deviation from the average or the root of that number, the correlation between successive observations, possible outliers, etc. Note that we do not use the names *mean, variance, standard deviation*, which we reserve for properties of probability distributions, not data sets. Use of these terms may cause confusion; for example, the *best estimate* for the variance of the parent probability distribution – of which the data set is supposed to be a random sample – is not equal to the mean squared deviation from the average, but slightly larger ($n/(n-1)\times$). See Section 5.3 on page 58.

Example: 30 observations

Suppose you measure a quantity x and you have observed 30 samples with the results as given in Table 2.1. Figure 2.1 shows the cumulative distribution function of these data and Fig. 2.2 shows the same, but plotted on a "probability scale" which should produce a straight line for normal-distributed data. A histogram using six equidistant bins is shown in Fig. 2.3. It is clear that this sampling is rather unevenly distributed.

These numbers and cumulative distributions were generated with **Python code** 2.1 on page 171

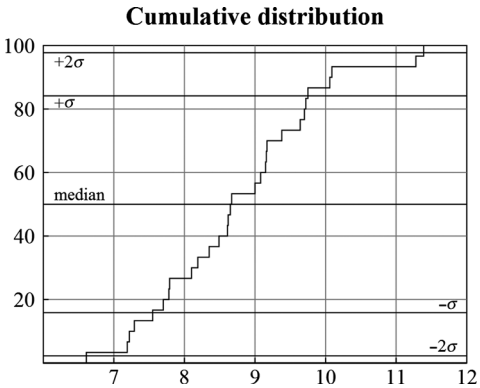

Figure 2.1 The cumulative distribution function of thirty observations. The vertical scale represents the cumulative percentage of the total.

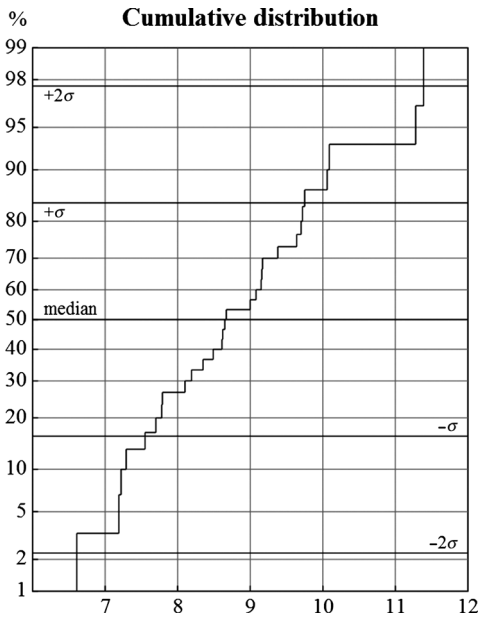

Figure 2.2 The cumulative distribution function of thirty observations. The vertical scale represents the cumulative percentage of the total on a probability scale, designed to produce straight lines for normal distributions.

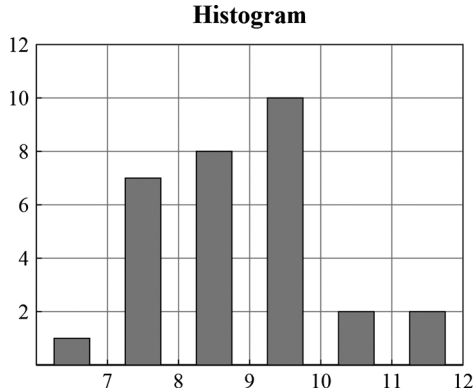

Figure 2.3 A histogram of thirty observations. The data have been gathered in six equidistant bins. The vertical scale gives the number of observations in each bin.

The histogram of Fig. 2.3 was generated with **Python code** 2.2 on page 171

The *properties* of the data set you can report are:

(i) *number of observations*: $n = 30$
(ii) *average*: $m = 8.78$
(iii) *mean squared deviation from average*: msd $= 1.28$
(iv) *root-mean-square deviation from average*: rmsd $= 1.13$

The properties are available as array methods or functions. See **Python code** 2.3 on page 171

Other rank-based properties of the data set are values that exceed a given fraction of the data, such as the *median* (at 50%), the first and third *quartile* (at 25 and 75%) or the p-th *percentile*. The latter is a value x_p such that $p\%$ of the data has a value $\leq x_p$ and $(100 - p)\%$ has a value $> x_p$.[2] The total *range* is the interval between the minimum and maximum values. Figure 2.4 shows the data as a box-and-whisker display of the total range (the whisker) and the quartiles (the box).

A simple program to determine a series of percentiles is **Python code** 2.4 on page 172

[2] There may be an ambiguity here. The p-th percentile may be exactly one of the data values, e.g. the median equals the 5th value out of a set of 9. In general, the percentile will fall in a range between two values, e.g. the median lies between the 5th and the 6th value out of a set of 10 values. In that case linear interpolation is used.

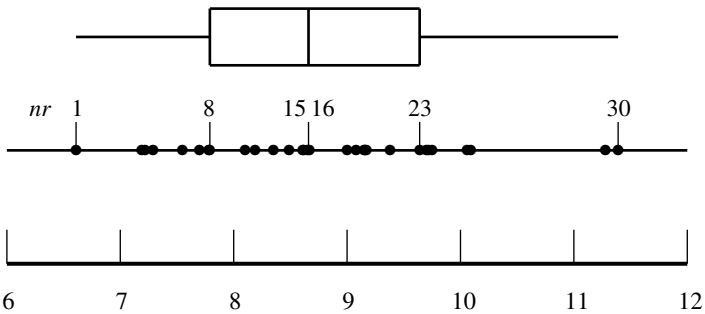

Figure 2.4 A *box-and-whisker* display of the total range, the median and the first and third quartile of thirty observations. Note that the median falls between nr 15 and nr 16 (15 observations on both sides); the average between the two values is taken.

2.2 How to represent numbers

Decimal separator: comma or period?

In the English language and in all "computer languages" (and among others also in China, Israel and Switzerland) the decimal *point* is used as separator between the integer and fractional parts of a real decimal number. In many other languages (all other European languages, Russian and related languages) the decimal *comma* is used instead. Be consistent and adhere to what your language requires! In order to avoid confusion, scientists are strongly advised *not* to use periods or commas to divide long numbers into groups of three digits, like 300,000 (English) or 300.000 (e.g. French). Instead, use a *space* (or even better, if your text editor allows it, a *thin space*) to separate groups of three digits: 300 000.[3]

Significant figures

The end result of a measurement must be presented with as many digits as are compatible with the accuracy of the result. Also when a number ends with zeros! These are the *significant figures* of the result. However, intermediate results in a calculation should be expressed with a higher precision in order to prevent accumulation of rounding errors. Always indicate the accuracy of the end result! If the accuracy is not explicitly given, it is assumed that the error in the last digit is ± 0.5.

[3] This is the IUPAC recommendation, see http://old.iupac.org/reports/provisional/guidelines.html#printing

Examples, for the English language

(i) 1.65 ± 0.05
(ii) 2.500 ± 0.003
(iii) $35\,600 \pm 200$: better as $(3.56 \pm 0.02) \times 10^4$
(iv) 5.627 ± 0.036 is allowed, but makes sense only when the inaccuracy itself is known with sufficient accuracy. If not, this value should be written as 5.63 ± 0.04.
(v) Avogadro's number is known as $(6.022\,141\,79 \pm 0.000\,000\,30) \times 10^{23}$ mol^{-1} (CODATA 2006). The notation $6.022\,141\,79(30) \times 10^{23}$ mol^{-1} is a commonly accepted abbreviation.
(vi) 2.5 means 2.50 ± 0.05
(vii) 2.50 means 2.500 ± 0.005
(viii) In older literature one sometimes finds a subscript $_5$, indicating an inaccuracy of about one quarter in the last decimal: $2.3_5 = 2.35 \pm 0.03$, but this is not recommended.

When inaccuracies must be rounded, then do this in a conservative manner: when in doubt, round up rather than down. For example, if a statistical calculation yields an inaccuracy of 0.2476, then round this to 0.3 rather than 0.2, unless the statistics of your measurement warrants the expression in two decimals (0.25). See Section 5.5 on page 60. Be aware of the fact that calculators know nothing about statistics and generally suggest a totally unrealistic precision.

2.3 How to express inaccuracies

There are many ways to express the (in)accuracy of a result. When you report an inaccuracy it must be absolutely clear which kind of inaccuracy you mean. In general, when no further indication is given, it is assumed that the quoted number represents the *standard deviation* or *root-mean-square error* of the estimated probability distribution.

Absolute and relative errors

You can indicate inaccuracies as *absolute*, with the same dimension as the reported quantity, or as a dimensionless *relative* value. Absolute inaccuracies are often given as numbers in parentheses, relating to the last decimal(s) of the quantity itself.

Examples

(i) 2.52 ± 0.02
(ii) $2.52 \pm 1\%$
(iii) 2.52(2)
(iv) $N_A = 6.022\,141\,79(30) \times 10^{23}$ mol^{-1}

Using probability distributions

If the degree of knowledge you have about the reported quantity θ can be expressed as a *probability distribution* of that quantity, you can report one or more *confidence intervals*. This is usually the case if a Bayesian analysis has been made (see Chapter 8). In cases where the estimated probability distribution deviates significantly from a Gaussian shape and the variance or standard deviation may be a meaningless or uninformative quantity, a confidence interval is the best way to report the accuracy of a quantity. One then gives the *Bayesian estimate* for the quantity as the expectation (mean) over the distribution, with e.g. a 90 percent confidence interval. That interval is given by two values; the probability that the quantity is less than the lower boundary is 0.05 and the probability that it exceeds the higher boundary is also 0.05. For the reader's information it is advised to also give the number n of independent experiments on which the estimate is based.

There are several possibilities to express the *estimated value* $\hat{\theta}$:

(i) the *mean* or expectation over the probability distribution $E[\theta] = \int \theta\, p(\theta)\, d\theta$,
(ii) the *median*, i.e., the value for which the cumulative distribution (see Section 4.2 on page 29) reaches 50 percent. The probability that the real value is smaller than the median equals the probability that it is larger,
(iii) the *mode* or *most probable value*, which marks the maximum of the probability distribution.

These estimates are similar and in general their difference is insignificant, being much less than the standard deviation. For symmetric distributions they are all equal. In any case be explicit as to the kind of estimate you report.

Examples

(i) In a simulation you "observe" the occurrence of a certain event (e.g. a conformational change of a protein molecule) that is irreversible on the attainable time scale. Your theory predicts that the event occurs with constant probability $k\Delta t$ in any small time interval Δt. You observe seven such events (occurring at $t_1, t_2, \ldots, t_7$) and apply a Bayesian analysis (see Chapter 8, page 120) to derive a probability distribution for k. The expectation of the rate constant is $E[k] = 7/(t_1 + t_2 + \cdots t_7) = 1.0\ \mathrm{ns}^{-1}$. This distribution $p(k)$, with cumulative distribution $P(k)$ (see Fig. 2.5) has the following properties (given in too many decimals):
- The *mean* equals 1.00; this is the best estimate $\hat{k}$.
- The *median* equals 0.95.
- The *mode* is 0.86.

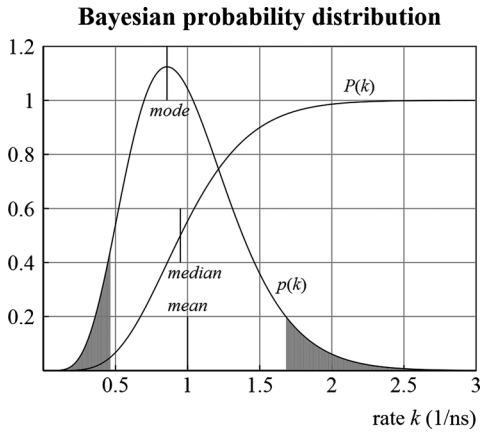

Figure 2.5 The Bayesian probability distribution for the rate k of an exponential decay process, based on seven lifetime observations.

- The *standard deviation*, i.e., the square root of the expectation of the squared deviation from the mean: $\hat{\sigma} = \sqrt{E[(k-\hat{k})^2]} = 0.38$. Just to see how well the standard deviation describes the width of the distribution: for a normal distribution 68% of the cumulative probability lies in the interval $(\hat{k}-\hat{\sigma}, \hat{k}+\hat{\sigma})$; for the Bayesian distribution of this example 69% is in the range $(1-0.38, 1+0.38)$. So the central region of the distribution is much like normal and the use of the standard deviation really makes sense in that range. But the tails are quite different!
- 90% confidence levels: $k(P=0.05) = 0.47$; $k(P=0.95) = 1.69$. This means that there is a 90% probability that the value of k lies between 0.5 and 1.7.

In this case you can report all "experimental" values $t_1, t_2, \ldots, t_7$, allowing the reader to draw her/his own conclusions. The result can be reported in various ways. The simplest is $\hat{k} = 1.0 \pm 0.4$, but that says nothing about the kind of distribution. It is better to give in addition a confidence interval and the number of observations, e.g.:

90% Bayes confidence interval $= (0.5, 1.7); n = 7$.

If you wish to be exhaustive, give the full probability distribution as in Fig. 2.5.

(ii) You measure the velocity of particles in a particle beam by time-of-flight determinations of 100 individual particles. Each velocity value is a sample from an unknown distribution. You want to determine two properties of the beam: the *mean* and the *standard deviation* of the one-dimensional

(forward) velocity distribution of all particles in the beam. This kind of problem is treated in Section 5.2 on page 57. Your set of 100 measurements is characterized by an average $\langle v \rangle$ of 1053 m/s and a mean square deviation from the average $\langle (\Delta v)^2 \rangle$ of 2530 m^2/s^2. Here, $\Delta v = v - \langle v \rangle$. For each property you wish to give the best estimate and its standard error. You may report:

- mean velocity: 1053 ± 5 m/s,
- s.d. of velocity distribution: 50 ± 4 m/s.
  Realizing that you do not know beforehand what the variance of the distribution is, you may apply Student's t-distribution (see Section 5.4 on page 59) and report:
- mean velocity: 1053 m/s; 90% t-distr. confidence interval = (1045, 1061) m/s, $\nu = 99$.

In this case with a large number of degrees of freedom, reporting a t-distribution confidence interval is hardly meaningful, as the difference with a normal distribution is negligible. Reporting the standard error is much better.

2.4 Reporting units

SI units

Physical quantities not only have a numerical value with inaccuracy, but also a *unit*. *Always include the proper unit in the correct notation when you report a physical quantity.* There are international agreements on units and notation. The agreed system of units is the "Système International d'Unités" (SI).[4] The SI units are derived from the *SI base units* m, kg, s, A, K, mol, cd (see data sheet UNITS on page 215). You should make it a habit to adhere strictly to these units, even if you are often confronted with non-SI units in the literature (dominantly originating from the USA). So, kJ/mol and not kcal/mol, nm (or pm) and not Å, N and not kgf, Pa and not psi.

Non-SI units

Some non-SI units are allowed, such as the minute (min), hour (h), day (d), degree (°), minute angle (′), second angle (″), liter (L = dm^3), metric ton (t = 1000 kg)) and astronomical unit (ua = $1.495\,978\,70 \times 10^{11}$ m). Chemists use the liter a lot: note that its symbol is upper case L, *not* (as is still quite common) lower case l.[5] Thus a milliliter is mL, not ml. The concentration unit mol/L is allowed next to the SI unit mol/m^3, but the symbol M for *molar*

[4] The SI system was established in 1960 by the CGPM (Conférence Générale des Poids et Measures), an intergovernmental treaty organization.

[5] This is the CGPM recommendation since 1979.

(= mol/L) is now obsolete. Note that mol is written with lower case m and without an e as in *mole*. A *mole* is the English name for the quantity that has the unit mol. Some other non-SI units are not officially allowed, but often used within restricted contexts, such as the nautical mile (= 1852 m), knot (nautical mile/h), are (100 m^2), hectare (10^4 m^2), ångström (Å = 10^{-10} m), barn ($b = 10^{-28}$ m^2) and bar (10^5 Pa). Use only official notations; not sec but s, not gr but g, not micron but μm. Use the *prefixes* as tabulated in the data sheet DATA:UNITS on page 215, preferably as powers that are multiples of 3. Be careful with capitalization: not m for Mega, not g for Giga. Finally, do not use confusing notations for more complex units, such as two slashes: not kg/m/s or kg/m s, but kg m^{-1} s^{-1}.

Typographical conventions

There are also agreed *typographical conventions*, which should be adhered to not only in scientific manuscripts, but even in informal reports. With modern text editors there is no excuse not to use roman, italic or bold type when required. The rules are simple:

- italic type for scalar quantities and variables,
- roman type for units and prefixes (mind capitalization),
- italic boldface for a vector or matrix quantity,
- sans-serif bold italic for tensors,
- roman type for chemical elements and other descriptive terms, including mathematical constants, functions and operators.

Examples

(i) The input voltage $V_{\mathrm{in}} = 25.2$ mV,
(ii) The molar volume $V_{\mathrm{m}} = 22.4$ L/mol,
(iii) The force on the i-th particle $F_i = 15.5$ pN,
(iv) The symbol for nitrogen is N, the nitrogen molecule is N_2,
(v) A nitrogen oxide mixture NO_x with $x = 1.8$,
(vi) $\mathrm{e} = 2.718\ldots$; $\pi = 3.14\ldots$,
(vii) $F = ma = -\,\mathbf{grad}\, V$,
(viii) The surviving fraction of the k-th species, $f_k^{\mathrm{surv}}(t) = \exp(-t/\tau_k)$.

2.5 Graphical presentation of experimental data

Experimental results are often presented in graphical form. The expectation or mean is given as the position (x, y) of (the center of) a symbol in a plot. The usual representation of inaccuracies in x and/or y is an *error bar* with a total length of twice the standard error. While both x and y values may be subject to experimental errors, very often one of the values (usually x)

Table 2.2 *Concentration of a reactant as a function of time. The inaccuracy is given as the estimated standard error.*

time t/s	conc. c/mmol L^{-1} ± s.d.
20	75 ± 4
40	43 ± 3
60	26 ± 3
80	16 ± 3
100	10 ± 2
120	5 ± 2
140	3.5 ± 1.0
160	1.8 ± 1.0
180	1.6 ± 1.0

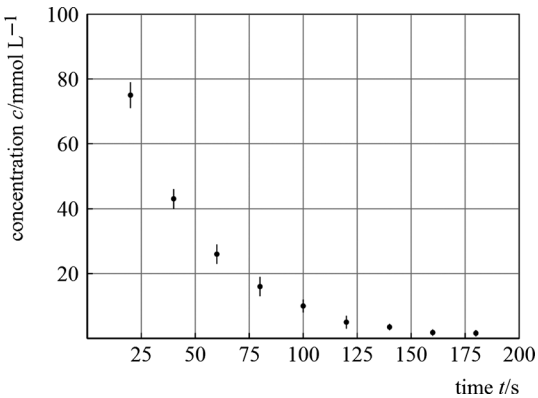

Figure 2.6 A linear plot of concentration of a reactant versus time, with error bars representing ± the standard error. The data are given in Table 2.2.

is so accurate that it makes no sense to plot an error bar. Figures 2.6 and 2.7 give examples of such a graphical representation, using the data given in Table 2.2. The reason to use a logarithmic scale for the concentration is that an expected exponential decay with time would show up as a straight line.

The linear plot can hardly show the small standard deviations of the last three points; on the logarithmic plot the s.d. on the small values show as much

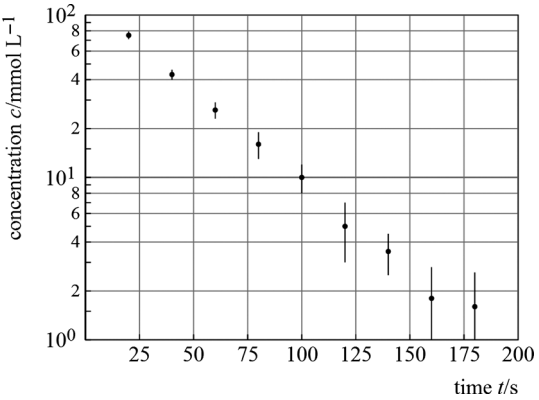

Figure 2.7 A logarithmic plot of the same data.

larger and asymmetric error bars. Note that the error bars on the last two points extend below the lower limit (1 mmol/L) of the logarithmic scale and therefore appear too short on the graph. Negative ordinate values (which may occur as a result of random errors) cannot be shown at all on a logarithmic scale.

Some authors use "whiskers" marking the ends of the error bars in order to make them more visible, but this does not add any useful information to the whiskerless error bars.

A scientifically acceptable graph should indicate *which* variables are plotted on the horizontal and vertical axes and *what units* the numbers represent. It is acceptable is to put the units in parentheses: time t (s), but it is advisable to use the notation time t/s as in Figs. 2.6 and 2.7; this notation indicates a dimensionless quantity represented by the numbers along the axes. Both notations are acceptable as long as the notation is consistent throughout a publication. Don't use more than one forward slash: $E_{\mathrm{pot}}/\mathrm{kJ\,mol^{-1}}$ is OK, but $E_{\mathrm{pot}}/\mathrm{kJ/mol}$ is not!

Of course there are several plotting programs to realize fancy graphics on a computer, but in many cases a quick sketch by hand on graph paper suffices to get a crude idea of a functional relationship and the importance of inaccuracies.

See **Python code** 2.5 on page 172 to produce Fig. 2.7 with a logarithmic scale.

Summary *In this chapter you have seen how experimental results are properly presented in a report or publication. A proper presentation gives numerical values with as many*

significant digits as is warranted by the precision of the value, it includes an unequivocal report of the (in)accuracy of the value, it includes the proper unit in which the result is expressed and it uses the conventional typography for variables, numbers, units and prefixes. Experimental results are always presented with an error estimate and it must be made explicit what the reported inaccuracy means and how the error estimate has been obtained.

Exercises

2.1 Correct the following notations:
(a) $l = 3128 \pm 20$ cm,
(b) $c = 0.01532$ mol/L ± 0.1 mmol/L,
(c) $\kappa = 2.52 \times 10^2$ A m^{-2}/V m^{-1},
(d) k/L mol^{-1}/s $= 3571 \pm 2\%$,
(e) $g = 2 \pm 0.03$.

2.2 Convert the following quantities to SI units or units allowed within the SI system (see data sheet UNITS on page 215):
(a) a pressure of 1.30 mm Hg,
(b) a pressure of 33.5 psi,
(c) a concentration of 2.3 mM (millimolar),
(d) an interatomic distance of 1.45 Å,
(e) an activation energy of 5.73 kcal/mol,
(f) a daily energy requirement of 2000 calories,
(g) a force of 125 lbf,
(h) an (absorbed) radiation dose of 20 mrad,
(i) a fuel consumption of 3.4 (US) gallon per 100 mile,
(j) a dipole moment of 1.85 debye,
(k) a polarizability of 1.440 Å^3. Note that polarizability α in rationalized SI units is the ratio of induced dipole moment (in Cm) and electric field (in V/m). In unrationalized units the polarizability is $\alpha' = \alpha/(4\pi\varepsilon_0)$, expressed in units of volume.