New definitions of the kilogram

and the mole

- Discussion -

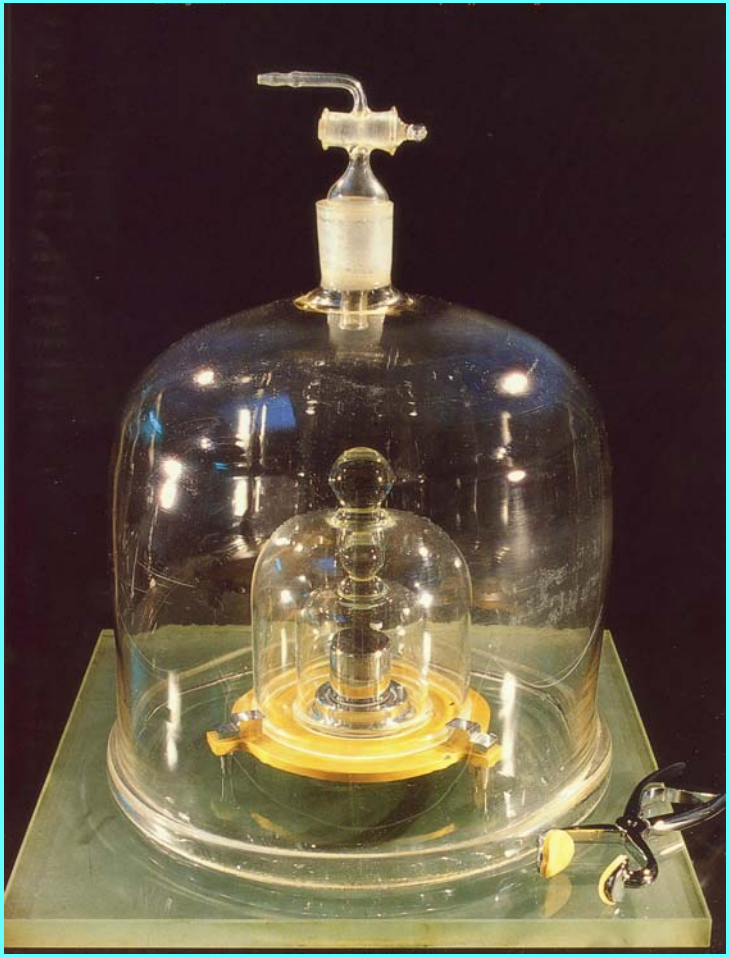
Michael Gläser, PTB, Germany

Definition of the kilogram

The kilogram is the unit of mass;
it is equal to the mass of the
international prototype of the kilogram

(1st CGPM 1889 and 3rd CGPM 1901)

International Prototype of the kilogram



Current results of the experiments

Experiment	Fundamental constant	Relative uncertainty	Institutes
Silicon experiment (2003)	N_A	3.4×10^{-7}	PTB, NIST, IMGC, NMIJ/AIST, CSIRO, IRMM
watt balance (2005)	h	3.6×10^{-8}	NIST, NPL, OFMET, BNM

but:

$$\frac{h(\mathrm{Si}) - h(\mathrm{WB})}{h} \approx 1 \cdot 10^{-6}$$

where:

$$h = \frac{c\alpha^2}{2R_\infty} m_e = \frac{c\alpha^2}{2R_\infty} \frac{A_\mathrm{r}(e) M_\mathrm{u}}{N_\mathrm{A}}$$

New definitions under discussion (1)

PTB

1. **The kilogram is the mass of a body whose Compton frequency is 1.356392… $\times$ 10^{50} hertz exactly.**

Bordé, Ch.J.: Base Units of the SI, Fundamental Constants and Modern Quantum Physics, Trans. Roy. Soc. A 363 (2005), 2177 ff

2. **The kilogram is the mass of a body whose equivalent energy is equal to that of a number of photons whose frequencies sum to exactly [299 792 458^2/(662 606 93 $\times$ 10^{41})] hertz .**

3. **The kilogram is the mass of a body whose de Broglie-Compton frequency is equal to exactly [299 792 458^2/(6.626 0693 $\times$ 10^{-34})] hertz.**

Mills, J.M., Mohr, P.J., Quinn, T.J., Taylor, B.N., Williams, E.R.: Redefinition of the kilogram, ampere, kelvin and mole: a proposed approach to implementing CIPM recommendation 1 (CI-2005), Metrologia 43 (2006), 227-246

Louis de Broglie

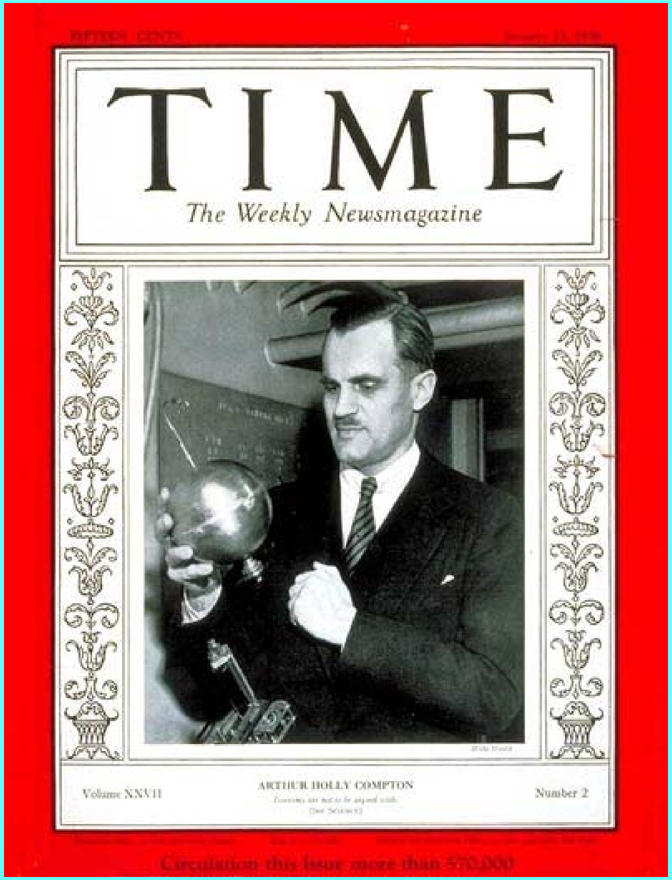
Wave property of a massive particle (1924), confirmed by electron diffraction on a crystal

$$\lambda = \frac{c}{\nu} = \frac{h}{m_0 \gamma v}$$

$$h\nu = m_0 \gamma c v$$

Arthur Compton

PTB



Scattering photon – electron (1923)

$$\frac{h\nu'}{h\nu} = \frac{1}{1 + \dfrac{\nu}{\nu_{\mathrm{C}}}\left(1 - \cos\vartheta_{\gamma}\right)}$$

$$\frac{h\nu'}{h\nu} = \frac{1}{1 + \dfrac{h\nu}{m_{\mathrm{e}}c^{2}}\left(1 - \cos\vartheta_{\gamma}\right)}$$

$$h\nu_{\mathrm{C}} = m_{\mathrm{e}}c^{2}$$

or: $$h\nu_{\mathrm{C}} = m_{\mathrm{e}0}\gamma c^{2}$$

„de Broglie-Compton frequency“

PTB

$$m_{\text{kg}} = \frac{h\nu_{\text{g}}\nu_{\text{m}}}{4gv} \quad \text{WB} \qquad \qquad \nu_{\text{c,kg}} = \frac{c^2}{4}\frac{\nu_{\text{g}}\nu_{\text{m}}}{gv} ?$$

- **Neither the de Broglie frequency nor the Compton frequency are directly measured with the watt balance.**

- **Compton frequency: mass of elementary or atomic particles**

  Compton frequency of *m* = 1 kg ?

  $\nu_{\text{c,kg}} = 1.356 \times 10^{50}$ Hz ? (ν(Ar-laser) = 10^{15} Hz, $\nu_{\text{C,p}} = 10^{23}$ Hz)

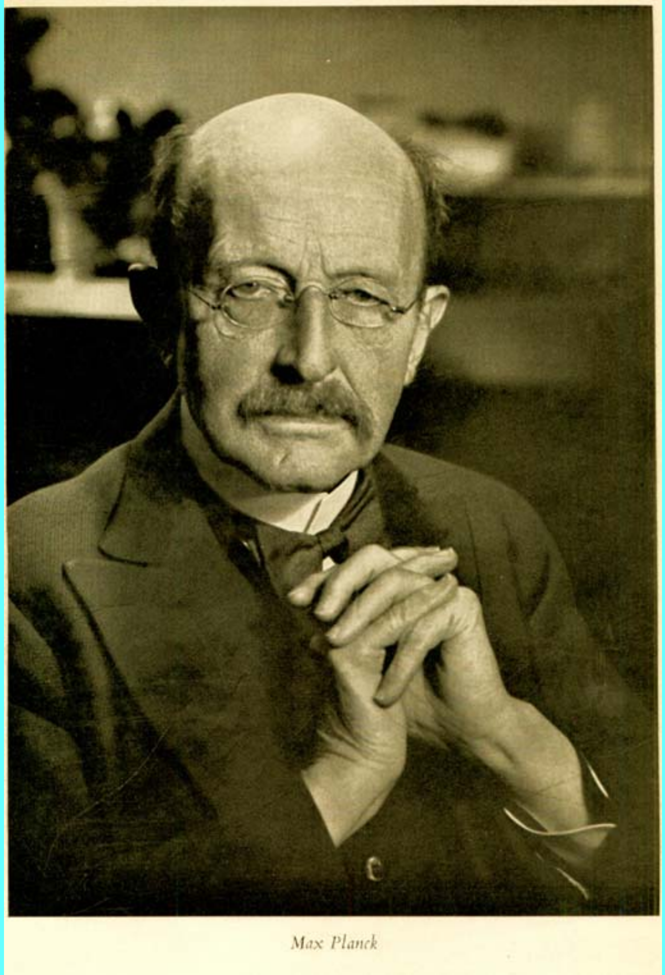
- **Can the kilogram be specified in the wave model rather than in the particle model of physics (in the definition)?**

New definitions under discussion (2)

4. The kilogram, the unit of mass, is such that the Planck constant is exactly 6.626 0693 $\times$ 10^{-34} Joule second.

Mills, J.M., Mohr, P.J., Quinn, T.J., Taylor, B.N., Williams, E.R.: Redefinition of the kilogram, ampere, kelvin and mole: a proposed approach to implementing CIPM recommendation 1 (CI-2005), Metrologia 43 (2006), 227-246

Max Planck



Black body radiation (1900)

$$E = h\nu = kT$$

The Planck constant, watt balance

PTB

$$m_{\mathrm{kg}}g = I\frac{\partial \Phi}{\partial z} = \frac{U_{\mathrm{g}}}{R}\frac{\partial \Phi}{\partial z} = \frac{\nu_{\mathrm{g}} e}{2}\frac{\partial \Phi}{\partial z}$$

Gravitational mode

$$\infty \quad U_{\mathrm{m}} = \frac{\nu_{\mathrm{m}} h}{2e} = v\frac{\partial \Phi}{\partial z}$$

Moving coil mode

$$\Rightarrow m_{\mathrm{kg}} = \frac{h\nu_{\mathrm{g}}\nu_{\mathrm{m}}}{4gv}$$

Energy of a Cooper pair: $2eU = h\nu$

- **The watt balance establishes an indirect, artificial link between the Planck constant and a macroscopic mass like the kilogram.**
- **With the watt balance the Planck constant relies on the Compton frequency of the electron.**

The Planck constant contd.

PTB

- The kilogram mass is a classical, macroscopic quantity, whereas Compton frequency and Planck constant describe quantum mechanical effects of point-like, structureless particles (e.g. the electron).
- How the mass of a macroscopic body is related to quantum mechanics is not clarified or experimentally proved.

- Moreover, the quantities h or ν_C are a not of the same kind as mass (Js, Hz - kg).

New definitions under discussion (3)

5. **The kilogram is $(6.022\,1415 \times 10^{23}/0.012)$ times the rest mass of the ^{12}C atom in the ground state.**

6. **The kilogram is $(6.022\,1415 \times 10^{23}/0.012)$ times the rest mass of a particle whose creation energy equals that of a photon whose frequency is $[(0.012/6.022\,1415 \times 10^{23}) \times 299\,792\,458^2/(6.626\,0693 \times 10^{-34})]$ Hz.**

Becker, P., de Bièvre, P. Fujii, K., Gläser, M., Inglis, B., Luebbig, H., Mana, G.: Considerations on future redefinitions of the kilogram, the mole and of other units, Metrologia 44 (2007), 1-14

Amadeo Avogadro

Same number of molecules (1811)

$$\frac{pV}{kT} = \mathrm{const} = nN_\mathrm{A}$$

The Avogadro Constant

- **Defining the kilogram (def.5) by the mass of a number of atomic particles, like ^{12}C (or the electron), by fixing N_A, is quite obvious and understandable and refers to a classical relation.**

$$m_{\mathrm{kg}} = \{N_{\mathrm{A}}\}\frac{m\left({}^{12}\mathrm{C}\right)}{0.012}$$

The ^{12}C atom has an internal structure and thus can exist in various excited states with slightly different mass values.

A kilogram definition based on the mass of the electron may therefore be more reliable, but its realization requires the knowledge of the ratio $A_r(e)/A_r(X)$, where X is an atom that forms solid bodies.

N_A/0.012, h and creation frequency

- Definition 6 defines the kilogram by the mass of a **fixed number** of (virtual) particles, that are specified by their **fixed creation frequency**.

$$1\ \text{kg} = \overline{\left\{\frac{N_\text{A}}{0.012}\right\}} m_\text{X} \qquad \nu_\text{X} = m_\text{X}\frac{c^2}{h} = \overline{\left\{\frac{0.012}{N_\text{A}}\frac{c^2}{h}\right\}}\text{Hz}$$

- The combination of the two numbers (top-lined) gives *h* as a fixed value and:

$$1\ \text{kg} = \overline{\left\{\frac{N_\text{A}}{0,012}\right\}}\,\overline{\nu_\text{X}}\,\frac{\bar{h}}{c^2}$$

Definition 6

- In contrast to definitions 1, 2 and 3,
  definition 6 addresses the creation (Compton) frequency of an atomic particle like ^{12}C rather than that of a body of 1 kg,

  which is physically more realistic.

- In addition, definition 6 gives the number of massive particles that constitute 1 kg,

  a statement that makes the definition understandable for the general public, at least to some extent.

Molar mass factor (1)

The particle is - strictly speaking - not ^{12}C, but its mass is very close to ^{12}C.

If the second were defined by the creation frequency of ^{12}C, then the particle is ^{12}C and $m_X = m(^{12}C)$ or $\nu_X = \nu_{12C}$.

Because the second is not defined like this, we may define a correction factor, called ‚molar mass factor':

$$1+\kappa = \frac{m\left(^{12}\mathrm{C}\right)}{m(\mathrm{X})} = \frac{\nu_{12\mathrm{C}}}{\nu_{\mathrm{X}}}$$

If N_A will be fixed by a new definition of the mole, we have to apply the molar mass factor for example in:

$$m_{\mathrm{u}} = \left(10^{-3}\,\frac{\mathrm{kg}}{\mathrm{mol}}\right)(1+\kappa)\frac{1}{N_{\mathrm{A}}}$$

and in:

$$M(\mathrm{S}) = \left(10^{-3}\,\frac{\mathrm{kg}}{\mathrm{mol}}\right)(1+\kappa)A_{\mathrm{r}}(\mathrm{S})$$

Molar mass factor (2)

- **At the time of the redefinition, the molar mass factor will be exactly 1, but its uncertainty does not vanish, which is that of ν_{12C}.**
- **For any particle Y, we can write:**

$$\nu_{\mathrm{12C}} = \nu_{\mathrm{Y}} \frac{m\left({}^{12}\mathrm{C}\right)}{m(\mathrm{Y})} = \nu_{Y} \frac{A_r\left({}^{12}\mathrm{C}\right)}{A_r(\mathrm{Y})}$$

preferred: $$\nu_{\mathrm{Y}} = \nu_{\mathrm{e}} = \frac{2cR_{\infty}}{\alpha^2}$$

Because ν_{e} and $A_{\mathrm{r}}(\mathrm{e})$ have the smallest relative uncertainties at present with 1.5×10^{-9} and 4.4×10^{-10}, respectively, they may be taken over.
The uncertainty of $1 + \kappa$ then is negligibly small for most applications, at least in chemistry.

Molar mass factor (3)

$$1+\kappa = \frac{m(^{12}\mathrm{C})}{m(\mathrm{X})} = \frac{\nu_{12\mathrm{C}}}{\nu_{\mathrm{X}}}$$

Becker et al. Metrologia 44 (2007)

$$\nu_{12\mathrm{C}} = \nu_{\mathrm{e}} \frac{A_{\mathrm{r}}(^{12}\mathrm{C})}{A_{\mathrm{r}}(\mathrm{e})} = \frac{2cR_{\infty}}{\alpha^2} \frac{A_{\mathrm{r}}(^{12}C)}{A_{\mathrm{r}}(\mathrm{e})}$$

$$\nu_{\mathrm{X}} = \overline{\left\{\frac{0.012}{N_{\mathrm{A}}} \frac{c^2}{h}\right\}}\mathrm{Hz} = \overline{\left[\frac{12M_{\mathrm{u}}}{N_{\mathrm{A}}}\right]} \frac{c^2}{\overline{h}}$$

$$1+\kappa = \frac{2R_{\infty}\overline{h}}{c\alpha^2} \frac{A_{\mathrm{r}}(^{12}\mathrm{C})}{A_{\mathrm{r}}(e)} \overline{\left[\frac{N_{\mathrm{A}}}{12M_{\mathrm{u}}}\right]}$$

$$1+\kappa = \frac{2R_{\infty}\overline{N_{\mathrm{A}}}h}{c\alpha^2 A_{\mathrm{r}}(\mathrm{e})M_{\mathrm{u}}}$$

Mills et al. Metrologia 43 (2006)

New electrical units

Kilogram	fixed value	electrical unit	fixed value
• Def. 1 – 4	h	ampere	e
• Def. 5	N_A	volt	h/e
• Def. 6	h	ampere	e

- **If *h* and *e* are independently fixed, then volt, ohm and ampere are SI units, when realized by Josephson and Quantum Hall effects.**

- **If the ratio *h*/*e* is fixed, then the volt is a SI unit, when realized by the Josephson effect.**

  The uncertainty of the Quantum Hall resistance is limited by *h* and *e* with a relative uncertainty of about 1.5×10^{-9}

  as well as the uncertainty of the ampere realization.

- **μ_0 is no more fixed and must be measured with uncertainty.**

Fundamental constants, rel. uncertainties in 10^{-8}

PTB

Constant	CODATA 2002	N_A and e fixed	N_A and h/e fixed	h, N_A and e fixed
N_A	17	0	0	0
h/e	8.5	0.15	0	0
h	17	0.15	0.15	0
$N_A h$	0.67	0.15	0.15	0
e	8.5	0	0.15	0
m_u	17	0	0	0.15
m_e	18	0.044	0.044	0.14
m_p	17	0.013	0.013	0.15
F	8.6	0	0.15	0
R_K	0.33	0.15	0.15	0
K_J	8.5	0.15	0	0
μ_B	8.6	0.15	0.21	0.14
γ_p	8.6	1.0	1.0	1.0
$\{m_u c_0^2/e\}$	8.6	0	0.15	0.15
$1+\kappa$	-	-	-	0.15
μ_0	0	0.16	0.08	0.07
defining:		kg, ampere, mole	kg, volt, mole	kg, ampere, mole

Understanding

The kilogram

defined as the mass of a number of atoms or particles

is much easier understood than

defined by the frequency of a number photons

or defined by the de Broglie-Compton frequency

or defined just by the numerical value of the Planck constant

We should consider, that the definitions of the kilogram, the meter and the second, are part of the general education of students.

„Any new definition of the kilogram should, if possible, be easily understood by the general public“ (Rec. Q1 CCQM, 2005)

The Mole

- **Students and scietists often are confused by understanding the mole among the other SI units.**

  For chemical reactions, number ratios are the information chemists need, e.g. that H_2O consists of two atoms H and one atom O, no matter which mass their samples have.

  The mole and the Avogadro constant should therefore be numbers, e.g. „Avogadro number“. Also, the mole should be defined without referring to the kilogram.

Proposed definition:

„The mole is the unit of amount-of-substance. It is equal to 6.022 1415 $\times$ 10^{23} specified identical entities. The entities may be atoms, ions, molecules or other particles.“

N_A: „Avogadro number“

People understand easier:

$$n = \frac{\text{number of molecules in a sample}}{6.022... \times 10^{23}}$$

$$m_u = \frac{10^{-3}}{N_A}\,\text{kg} \qquad \text{or:} \qquad m_u = (1+\kappa)\frac{10^{-3}}{N_A}\,\text{kg}$$

than:

$$n = \frac{\text{number of molecules in a sample}}{6.022... \times 10^{23}\ \text{mol}^{-1}}$$

$$m_u = \frac{10^{-3}}{N_A}\frac{\text{kg}}{\text{mol}} \qquad \text{or:} \qquad m_u = (1+\kappa)\frac{10^{-3}}{N_A}\frac{\text{kg}}{\text{mol}}$$

„mol“ is just another name for a ratio of numbers.

Proposals: kg, V or kg, A

PTB

Proposal 1:

(kg-N_A) **"The kilogram is (6.022 141 5 × 10^{23} / 0.012) times the rest mass of the ^{12}C atom in the ground state."**

(kg-N_e) **"The kilogram is 1.097 769 24 × 10^{30} times the rest mass of the electron".**

(V-K_J) **"The volt is equal to the difference between two electrical potentials within which the energy of a pair of electrons equals that of a photon whose frequency is 4.835 978 79 × 10^{14} Hz."**

Proposal 2:

(kg-N_C,h) **"The kilogram is (6.022 141 5 × 10^{23} / 0.012) times the rest mass of a particle whose creation energy equals that of a photon whose frequency is [(0.012 / 6.022 141 5 ×10^{23}) × 299 792 4582 / (6.626 0693 × 10^{-34})] Hz."**

(kg-N_e,h) **"The kilogram is [6.022 141 5 × 10^{23} / (5.485 799 0945 × 10^{-7})] times the rest mass of a particle whose creation energy is that of a photon whose frequency is [(5.485 799 0945 × 10^{-7} / 6.022 141 5 × 10^{23}) × 299 792 4582 / (6.626 0693 × 10^{-34})] Hz."**

(A-e) **"The ampere is the electric current in the direction of the flow of 6.241 509 48 × 10^{18} elementary charges per second"**

Proposal: mol

(mol-N_A) **The mole is the unit of amount of substance. It is equal to $6.022\,141\,5 \times 10^{23}$ specified identical entities.**

The entities may be atoms, ions, molecules or other particles".

Thank you for your attention