

The System of Units

We define a new time unit T such that a wave number $\tilde{\nu}$ has the same numerical value as the corresponding angular wave frequency $\omega = \tilde{\nu}2\pi c$ (c is the speed of light).

	SI	New
$\tilde{\nu}$	1 cm ⁻¹	1cm ⁻¹
ω	$1.8836515673088531 \times 10^{11}$ s ⁻¹	1T ⁻¹
Time Unit(SI)	1 s	$1.8836515673088531 \times 10^{11}$ T
Time Unit(New)	$5.308837458876145 \times 10^{12}$ s	1T

Table 1: The Defining Relationship: $\omega = 2\pi c\nu$. $c = 2.997\,924\,58 \times 10^{10}$ cm s⁻¹.

With the time unit defined, we further define a new energy unit E such that Planck's constant \hbar is 1E T. Planck's constant in SI is $1.054\,571\,817 \times 10^{-34}$ J s. Once E is defined, for $\tilde{\nu} = 1$ cm, we will have the corresponding angular frequency $\omega = 1\text{cm}^{-1}$ and the energy $\mathcal{E} = \hbar\omega = 1\text{E T} \times 1\text{T}^{-1} = 1\text{E}$.

	SI	New
\hbar	$1.054571817 \times 10^{-34}$ J s	1E · T
Time Unit(SI)	1 s	$1.8836515673088531 \times 10^{10}$ T
Time Unit(New)	$5.308\,837\,458\,876\,145 \times 10^{-12}$ s	1T
Energy Unit(SI)	1 J	$5.0341165706272096 \times 10^{22}$ E
Energy Unit(New)	$1.986445855931795 \times 10^{-23}$ J	1E

Table 2: The Defining Relationship: $\hbar = 1.054571817 \times 10^{-34}$ J s = 1ET.

With the two units defined, we calculate the value of Boltzmann's constant in this system of units.

	SI	New
Energy Unit(SI)	1 J	$5.0341165706272096 \times 10^{22}$ E
Energy Unit(New)	$1.986445855931795 \times 10^{-23}$ J	1E
k_B	1.380649×10^{23} J K ⁻¹	0.6950348009119888 E K ⁻¹

Table 3: The Defining Relationship: $k_B = 1.380\,649 \times 10^{-23}$ J K⁻¹ = $1.380\,649 \times 10^{-23}$ J K⁻¹ \times $15.034\,116\,570\,627\,209\,6 \times 10^{22} \frac{\text{E}}{\text{J}}$ = $0.695\,034\,800\,911\,988\,8$ E K⁻¹.

Now we list the necessary unit conversion coefficients from atomic units to this new set of units

	a.u.	New
Mass	1 a.u.	$1.627096855727954 \times 10^{11}$ M
Mass	$6.145915631756325 \times 10^{-12}$ a.u.	1 M
Length	1 a.u.	$5.29177210903 \times 10^{-9}$ cm
Energy	1 a.u.	2.1947463068×10^5 E

Table 4: The Defining Relationship: .