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atomic units

The units designed to simplify the form of the fundamental equations of quantum mechanics by eliminating from them fundamental constants. The atomic unit of length is the Bohr radius, $a_o = \frac{h^2}{4\pi^2 m e^2} = 5.291\,77249 \times 10^{-11}$ m (0.529177249 Å). Energy is measured in hartrees, where 1 hartree $= \frac{e^2}{a_o} = 4.359\,7482 \times 10^{-18}$ J. Masses are specified in terms of atomic mass unit, amu $= 1.6605402 \times 10^{-27}$ kg and of the electron mass unit, $m_e = 0.910953 \times 10^{-30}$ kg. The advantage of atomic units is that if all calculations are directly expressed in such units, the results do not vary with any revision of the numerical values of the fundamental constants.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1924

