Calculate the following in the MKS unit system.

    A. One atomic unit of energy (Hartree = 2 Rydbergs)

Soln: The Hartree is equivalent to twice the binding energy of the hydrogen atom or 2 Rydbergs.

1 Hartree = 27.2 eV = 4.37×10^{-18} Joules

To convert from eV to Joules one multiplies by the charge on an electron, 1.602×10^{-19} C

    B. One atomic unit of dipole moment (Electron-Bohrs)

The MKS unit of dipole moment is the Coulomb-meter.

1 Cm = $(1.602 \times 10^{-19}$ C$)(0.52977 \times 10^{-10}$ m$) = 8.486 \times 10^{-30}$ Cm

1 Debye = 3.33×10^{-30} Cma. Thus, 1 Electron-Bohr = 2.5 Debye

    C. One atomic unit of electric field (Hartree per Electron-Bohr)

Taking information from the above calculations and keeping mind that V/m is a unit in the MKS system. We find 1 Hartree/Electron-Bohr = $(4.37 \times 10^{-18}$ Joules$)/(8.486 \times 10^{-30}$ Cm$) = 5.15 \times 10^{11}$ V/m.

1