

USEFUL CONVERSIONS

Energy Conversions	1 cm ⁻¹	1 = X cm ⁻¹
kJ/mol	0.0120	83.3
THz	0.030	33
Hartree (E _h)	4.556 x 10 ⁻⁶	219475
kcal/mol	0.00286	350
meV	0.1240	8.07
kJ	1.99 x 10 ⁻²³	5.03 x 10 ²²

1 atomic unit of	in MKS units
time	24 x 10 ⁻¹⁸ s
distance	0.529 x 10 ⁻¹⁰ m
mass	9.11 x 10 ⁻³¹ kg
energy	4.36 x 10 ⁻¹⁸ J
temperature	3.16 x 10 ⁵ K

Constants	in atomic units	in MKS units	energy in cm ⁻¹
h-bar	1	1.05 x 10 ⁻³⁴ J s	5.29 x 10 ⁻¹² cm ⁻¹ s
k _B	3.17 x 10 ⁻⁶	1.38 x 10 ⁻²³ J K ⁻¹	0.695 cm ⁻¹ K ⁻¹
m _e	1	9.11 x 10 ⁻³¹ kg	---
c	137	3.00 x 10 ⁸ m s ⁻¹	---
atomic mass unit	1822	1.66 x 10 ⁻²⁷ kg	---