

# *Units*

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A number of different sets of units are used throughout this volume. Conversions to SI units are as follows:

Energy: 1 a.u. (hartree) = 4.359 828 aJ  $\equiv$  2625.47 kJ mol<sup>-1</sup>

1 eV = 0.160 210 aJ  $\equiv$  96.4868 kJ mol<sup>-1</sup>

1 cm<sup>-1</sup> = 1.986 31  $\times$  10<sup>-23</sup> J  $\equiv$  11.9626 J mol<sup>-1</sup>

Length: 1 a.u. (bohr) = 0.529 177  $\times$  10<sup>-10</sup> m

1 Å (ångström) = 10<sup>-10</sup> m

Dipole moment: 1 D (debye) = 3.335 64  $\times$  10<sup>-30</sup> C m

Magnetic moment: 1  $\mu_B$  (Bohr magneton) = 9.2732  $\times$  10<sup>-24</sup> J T<sup>-1</sup>