

Solutions to Exercises, Chapter 2

2.1 (a) 109.5° (b) 120° (c) 180°

2.2 Ethane: sp^3 hybrid AOs of C and 1s AO of H.

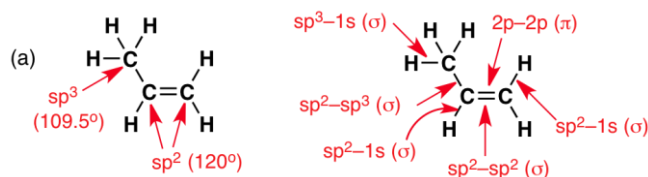
CCl_4 : sp^3 hybrid AOs of C and 3p AO of Cl.

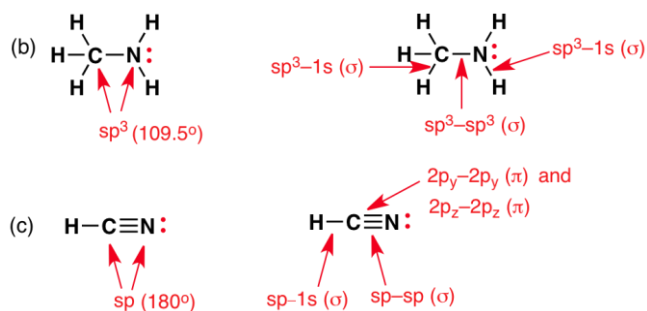
2.3 The C–C bond in ethane is formed by end-to-end interactions between sp^3 AOs on the two C atoms, and the resulting MOs are circularly symmetrical about the C–C bond axis.

2.4 The carbon atom of methanal is sp^2 hybridized and trigonal planar. If the 2s and two 2p orbitals of O are sp^2 hybridized with an unpaired electron initially in one of these and another in the unhybridized 2p orbital, we have lone pairs in the other two sp^2 orbitals. The C=O double bond is formed by (i) end-on overlap of the sp^2 orbitals (σ bond), and (ii) side-on overlap of the unhybridized 2p orbitals (π bond) of the C and the O. The C also forms σ bonds using its other two sp^2 AOs and the 1s AO of two H atoms.

2.5 The σ orbitals are derived from the two sp hybrid AOs of the C and one sp^2 hybrid of each of the two O atoms; one π orbital is formed by combination of the $2p_y$ AOs of the C and one O, and the other π orbital is from the $2p_z$ AOs of the C and the other O; the planes of the two π orbitals are perpendicular to each other (orthogonal), and each O atom has two hybrid sp^2 orbitals left over to accommodate lone pairs.

2.6

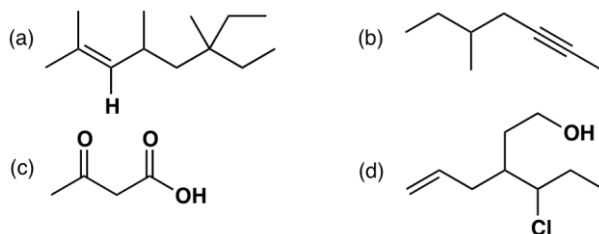




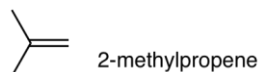
2.7

- (a) $(CH_3)_3CCH_2CH=CH_2$ (b) $CH_3CH_2CH(OH)CH_3$ (c) $(CH_3)_2CHCONH_2$ (d) $CH_3CH_2CH_2OCH_3$

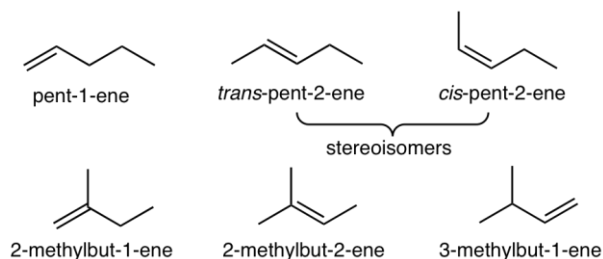
2.8



2.9



2.10 *trans*- and *cis*-pent-2-enes are stereoisomers, and others are constitutional isomers.



2.11

- (a) $-CH(CH_3)_2 > -CH_2CH(CH_3)_2$ (b) $-F < -Cl$ (c) $-OCH_3 > -N(CH_3)_2$
 (d) $-Cl > -SCH_3$ (e) $-CH=CH_2 < -C(CH_3)_3$

2.12

- (a) *Z* (groups of higher priority: Cl and OCH₃)
- (b) *E* (groups of higher priority: CH₃ and CHO)