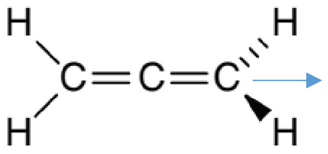
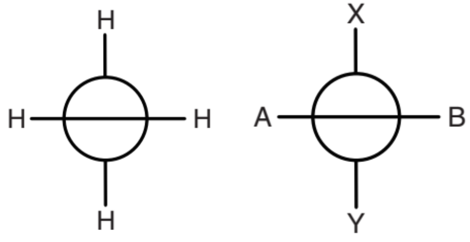
Symmetry & Bonding

Answers to the Questions1,3bc, 4egi

1. Allene, C_3H_4.



$S_4 || C_2$



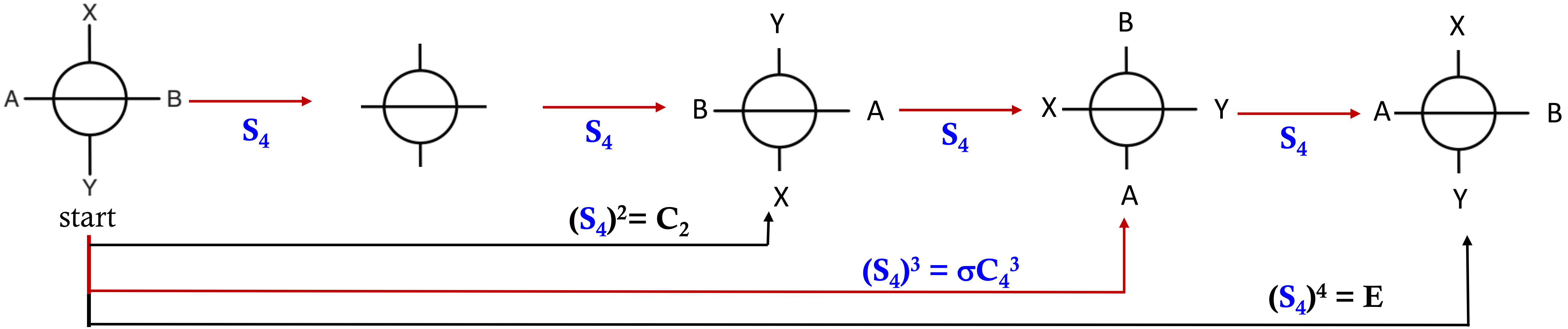
view down long axis　　labelling

纽曼投影图

（a） Draw diagrams, similar to those in Fig. 2.1 on page 11, to show the effect of all the operations generated by this four-fold improper axis i.e. S_4, $(S_4)^2$ …

（b）Shown that $(S_4)^2 \equiv C_2$ (where the two-fold axis is also along the long axis) and that $(S_4)^4 \equiv E$

（c）Hence identify the *distinct* symmetry operations generated by this four-fold axis of improper rotation.

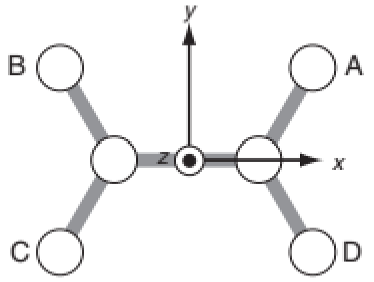


（b）上图图示证明了$(S_4)^2 \equiv C_2$ ，$(S_4)^4 \equiv E$; 亦可由公式证明：$S_4 = \sigma_h C_4 \rightarrow (S_4)^2 = (\sigma_h)^2 (C_4)^2 = C_2$

（c）由上图可判断S_4映转轴所产生的独特操作有：S_4，$(S_4)^3$ (或写成 S_4^3)。 & $(S_4)^4 = (\sigma_h)^4 (C_4)^4 = E$

3. (b) Are the three mirror planes in C_2H_4 in the same class? Give reasons for your answer.
(c) XeF_4 has a planar structure in which the fluorine atoms are at the corners of a square and the xenon atom is in the middle. It has a four-fold axis of symmetry, two mirror planes which pass through fluorine atoms at opposite corners of the square, two mirror planes which pass through the mid points on opposite sides of the square, and a mirror plane in the plane of the molecule. Group the mirror planes into classes, giving your reasons.

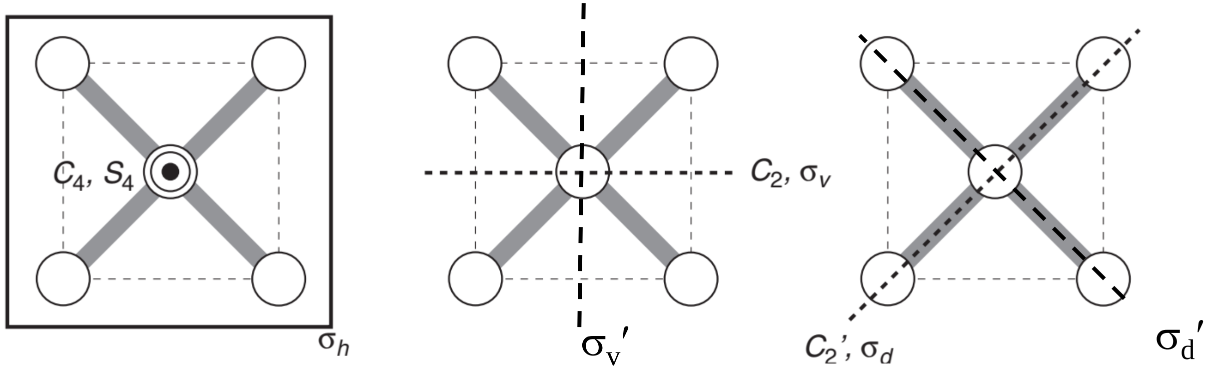
A: (b) The three mirror planes in C_2H_4 are not in the same class, because they can not be related to each other by any of the allowed symmetry operations of this molecule.



σ_{xy}, σ_{xz}, σ_{yz} , **i**

$C_{2(y)}$, $C_{2(z)}$, $C_{2(x)}$, E

(c) The 5 mirror planes in XeF_4 fall into three classes, i.e., σ_h, (σ_v, σ_v'), (σ_d, σ_d').



The two mirror planes, σ_v and σ_v', can be related by either a C_4 operation or a C_2' operation.

The two mirror planes, σ_d and σ_d', can be related by either a C_4 operation or a C_2 operation.

4. For each of the following molecules identify the key elements of symmetry and hence determine the point group. Having identified the point group verify that all of the symmetry elements whose presence is indicated in the relevant character table are indeed present. Make *clear*, *labelled* sketches showing the positions of all of the symmetry elements present. If you are uncertain about the structures of any of the molecules mentioned, look them up in a reliable source.

(e) biphenyl, Ph–Ph, where the angle between the plane of the two benzene rings is: (i) 0◦; (ii) 90◦; (iii) some angle greater than 0◦ but less that 90◦.

(g) SF_5Cl; H_2O_2; O_3; N_2O; SF_6; $POCl_3$

(i) ferrocene with the two five-membered rings (i) eclipsed, (ii) staggered.

A: (e) Ph-Ph: (i) α = 0◦, symmetry elements ~ E, $3C_2$, $2\sigma_v$, σ_h, i; D_{2h}, h = 8;

(ii) α = 90◦, symmetry elements ~ E, $3C_2$, $2\sigma_d$, S_4; D_{2d}, h= 8;

(iii) 0◦ < α <90◦, symmetry elements ~ E, $3C_2$; D_2, h= 4;

(须画出结构来，这里略去！）

(g) SF_5Cl: E, C_4, $2\sigma_v$, $2\sigma_v'$; C_{4v}, h = 8。 H_2O_2: E, C_2； C_2, h = 2。

O_3: E, C_2, $2\sigma_v$; C_2, h = 2。 N_2O: E, C_∞, $\infty\sigma_v$; $C_{\infty v}$, h = ∞。

$POCl_3$: E, C_3, $3\sigma_v$; C_{3v}, h = 6。

SF_6: E(1), $3C_4$(9), $4C_3$(8) , $3S_4$(6), $4S_6$(8), *i*(1), $3\sigma_h$(3), $6C_2$, $6\sigma_d$； O_h, h = 48;

(i) ferrocene: (i) eclipsed ~ E, C_5, $5C_2$, S_5, σ_h, $5\sigma_v$； D_{5h}, h = 20;

(ii) staggered ~ E, C_5, $5C_2$, S_{10}, i, $5\sigma_d$； D_{5d}, h = 20;