Quantum Chemistry by Levine

LuMg

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1 Chapter 12 Molecular Symmetry

12.1
(a) False
(b) False
(c) True

12.2
(a) H_2S: C2, σ
(b) NH_3: $C3$, σ
(c) CHF_3: $C3$, σ
(d) $HOCl$: σ
(e) $C3, \sigma, S3$
(f) $C2, \sigma$
(g) no symmetry element

12.3
(a) $E, \sigma_a, \sigma_b, C_2$
(b) $E, C_3, C_3^2, \sigma_a, \sigma_b, \sigma_c$
(c) $E, C_3, C_3^2, \sigma_a, \sigma_b, \sigma_c$
(d) E, σ
(e) $E, C_3, S_3 \ldots$
(f) $E, C_2, \sigma_a, \sigma_b$
(g) E

12.4
No, the structure is changed

12.5
(a) E

(b) σ
(c) C_2
(d) C_2
(e) C_2
(f) S_2
(g) C_4
(h) i

12.6
$C_2(x)C_4(z)! = C_4(z)C_2(x)$

12.7
(a) T
(b) F
(c) T
(d) T
(e) T

12.8
(a) T
(b) T
(c) T
(d) T
(e) F
(f) T
(g) T

12.9
(a) False, $o - o$ is rotating
(b) not optically active

12.10
(a) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
(b) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
(c) $\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

(d) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
(e) $\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
(f) $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$

12.11
$C_2(x) =$
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\sigma_{xy} =$
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\sigma_{xz} =$
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

12.12
(a)$\hat{O}_{C4}^4 = E$
So eigenvalue $1, -1, i, -i$
(b) its eigenvalue is imaginary, so not Hermitian

12.13
(a)$\hat{O}_{C2}^2 = E$
so the eigenvalue is $1, -1$
it is Hermitian

12.14
(a)$2p_z$
(b)$2p_x$

12.16
(a)T
(b)F
(c)T

12.17
True

12.18
True