

## UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Kedua  
Sidang Akademik 1997/98

Februari 1998

KTE 211- Teori Kumpulan dan Spektroskopi

Masa : [2 jam]

Jawab sebarang EMPAT soalan.

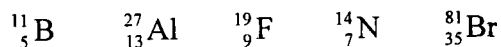
Hanya EMPAT jawapan yang pertama sahaja akan diperiksa.

Jawab tiap-tiap soalan pada muka surat yang baru.

Kertas ini mengandungi LIMA soalan semuanya dan lampiran (17 muka surat)

1. Molekul berikatan enam,  $\text{Ni(en)}_2\text{Cl}_2$  mempunyai dua struktur yang mungkin.
  - (i) Lukiskan kedua-dua struktur tersebut dan berikan kumpulan titik bagi setiap struktur.
  - (ii) Dapatkan perwakilan terturunkan dan perwakilan takterturunkan bagi setiap struktur di atas dengan menggunakan ikatan Ni-Cl sebagai fungsi dasar.
  - (iii) Bagaimanakah simetri molekul membezakan di antara kedua-dua struktur tersebut? Jelaskan jawapan anda.

(25 markah)
  
2. (a) Ramalkan nombor kuantum spin I (sifar, setengah integer atau penuh) bagi setiap isotop berikut :-



(5 markah)

- (b) Apakah yang dimaksudkan dengan pengkupelan spin-spin dalam resonans magnet nukleus?

(5 markah)

- (c) Beberapa peralihan putaran bagi  $H^{79}Br$  diperhatikan pada nombor gelombang 138.57, 155.26 dan 188.53  $cm^{-1}$  dengan kedua-dua yang pertama itu muncul sebagai garisan berturutan.

Terbitkan suatu ungkapan yang umum bagi tenaga peralihan putaran termasuk pemalar-pemalar putaran B dan erutan mengempar D.

Kiralah nilai B dan D bagi  $H^{79}Br$  dari data tersebut di atas.

(15 markah)

3. (a) Terangkan dengan jelas tiap-tiap istilah berikut :

- (i) Paksi putaran wajar,  $C_n$ .
- (ii) Paksi putaran-pemantulan,  $S_n$ .
- (iii) Perwakilan terturunkan.
- (iv) Jadual Karakter.

(10 markah)

- (b) Di dalam kajian RMN, Hukum Taburan Boltzmann digunakan untuk menghitung bilangan nukleus pada paras tenaga yang berlainan. Bincangkan dengan menggunakan persamaan yang sesuai.

(5 markah)

- (c) Kedudukan jalur spektrum penyerapan mikrogelombang bagi molekul  $\text{H}^{55}\text{Cl}$  pada suhu 300 K adalah seperti berikut :

| <u><math>\nu/\text{cm}^{-1}</math></u> | <u>Keamatan</u> |
|--|-----------------|
| 104.10                                 | Lemah           |
| 124.30                                 | Sederhana       |
| 145.03                                 | Sederhana       |
| 165.51                                 | Kuat            |
| 185.86                                 | Sederhana       |

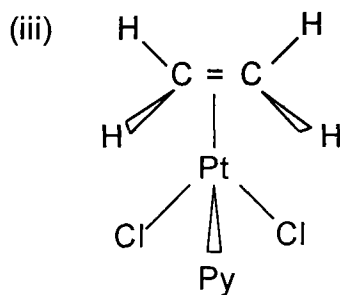
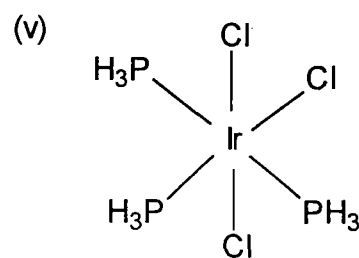
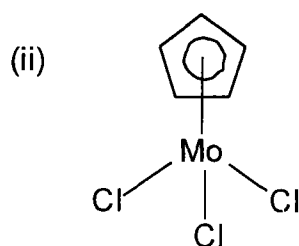
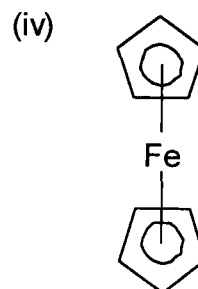
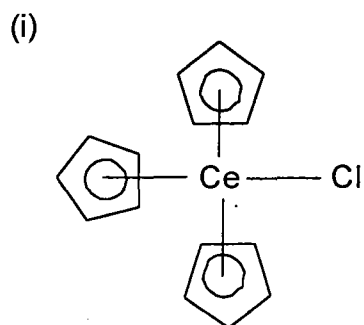
- (i) Tentukan peralihan  $J \longrightarrow J'$  yang memberikan tiap-tiap jalur di atas.

(5 markah)

- (ii) Terangkan perubahan jarak antara jalur dalam spektrum tersebut.

(5 markah)

4. (a) Nyatakan kumpulan titik bagi tiap-tiap molekul berikut :

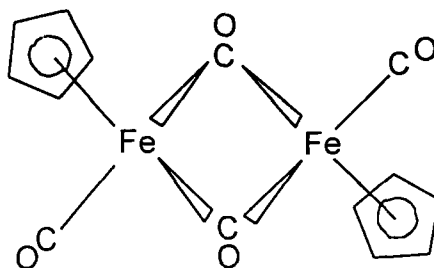


(10 markah)

(b) Berpandukan molekul yang sesuai, dapatkan perwakilan-perwakilan  $\Gamma_{p_x}$ ,  $\Gamma_{p_y}$  dan  $\Gamma_{p_z}$  bagi kumpulan titik  $C_{2h}$ .

(10 markah)

(c) Bagi sebatian berikut :



Huraikan secara ringkas cara penentuan kumpulan titik bagi sebatian tersebut.

Dapatkan perwakilan terturunkan bagi sebatian tersebut.

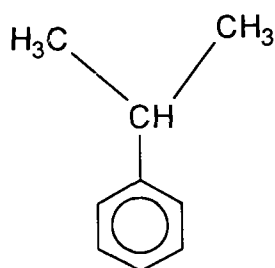
(5 markah)

5. (a) Terangkan istilah-istilah berikut :

- (i) Proses persantiaan spin-spin.
- (ii) Anjakan kimia,  $\delta$ .
- (iii) Kesan perlindungan (shielding) dan pendelindungan (deshielding).

(10 markah)

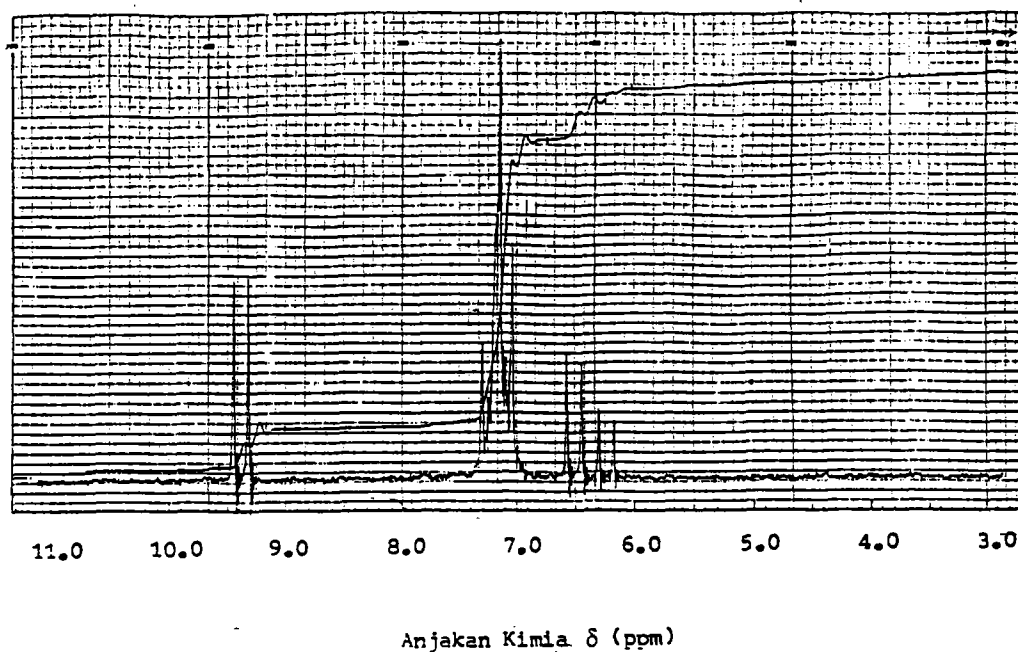
(b) Ramalkan corak spektrum RMN  $^1\text{H}$  dan julat anjakan kimia ( $\delta$ ) bagi puncak-puncak yang paling mungkin untuk sebatian berikut :



(5 markah)

- (c) Spektrum RMN  $^1\text{H}$  bagi sebatian ditunjukkan dalam Rajah 1. Cadangkan satu struktur molekul yang sesuai bagi sebatian  $\text{C}_9\text{H}_8\text{O}$  tersebut dengan memberikan sebab yang munasabah.

(10 markah)



Rajah 1 : Spektrum RMN  $^1\text{H}$  bagi sebatian  $\text{C}_9\text{H}_8\text{O}$

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LAMPIRAN

# Character Tables

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## THE NONAXIAL GROUPS

|       |     |            |                 |                             |
|-------|-----|------------|-----------------|-----------------------------|
| $C_1$ | $E$ |            |                 |                             |
| $A$   | 1   |            |                 |                             |
| $C_2$ | $E$ | $\sigma_h$ |                 |                             |
| $A'$  | 1   | 1          | $x, y, R_z$     | $x^2, y^2, z^2, xy$         |
| $A''$ | 1   | -1         | $z, R_x, R_y$   | $yz, xz$                    |
| $C_3$ | $E$ |            | $i$             |                             |
| $A_g$ | 1   | 1          | $R_x, R_y, R_z$ | $x^2, y^2, z^2, xy, xz, yz$ |
| $A_u$ | 1   | -1         | $x, y, z$       |                             |

## THE AXIAL GROUPS

### ► The $C_n$ Groups

|       |  |    |                                |   |
|-------|--|----|--------------------------------|---|
| $C_2$ | $E$  |    | $C_2$                          |   |
| $A$   | 1  | 1  | $z, R_z$                       | $x^2, y^2, z^2, xy$                             |
| $B$   | 1  | -1 | $x, y, R_x, R_y$               | $yz, xz$  |
| $C_3$ | $E$  |    | $C_3$                          |   |
|       |  |    | $C_3^2$                        |   |
|       |  |    | $\varepsilon = \exp(2\pi i/3)$ |   |
| $A$   | 1  | 1  | 1                              | $z, R_z$  |
| $E$   | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$ |    | $(x, y), (R_x, R_y)$           | $x^2 + y^2, z^2$<br>$(x^2 - y^2, xy), (yz, xz)$ |

| $C_4$ | $E$  | $C_4$ | $C_2$ | $C_4^3$ |          |                      |
|-------|--|-------|-------|---------|----------|----------------------|
| A     | 1  | 1     | 1     | 1       | $z, R_z$ | $x^2 + y^2, z^2$     |
| B     | 1  | -1    | 1     | -1      |          | $x^2 - y^2, xy$      |
| E     | $\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$ |       |       |         |          | $(x, y), (R_x, R_y)$ |

| $C_5$ | $E$  | $C_5$ | $C_5^2$ | $C_5^3$ | $C_5^4$ | $\varepsilon = \exp(2\pi i/5)$ |                      |                   |
|-------|--|-------|---------|---------|---------|--------------------------------|----------------------|-------------------|
| A     | 1  | 1     | 1       | 1       | 1       | $z, R_z$                       | $x^2 + y^2, z^2$     |                   |
| $E_1$ | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon \end{Bmatrix}$ |       |         |         |         |                                | $(x, y), (R_x, R_y)$ | $(yz, xz)$        |
| $E_2$ | $\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 \end{Bmatrix}$ |       |         |         |         |                                |                      | $(x^2 - y^2, xy)$ |

| $C_6$ | $E$  | $C_6$ | $C_3$ | $C_2$ | $C_3^2$ | $C_6^5$ | $\varepsilon = \exp(2\pi i/6)$ |                      |            |
|-------|--|-------|-------|-------|---------|---------|--------------------------------|----------------------|------------|
| A     | 1  | 1     | 1     | 1     | 1       | 1       | $z, R_z$                       | $x^2 + y^2, z^2$     |            |
| B     | 1  | -1    | 1     | -1    | 1       | -1      |                                |                      |            |
| $E_1$ | $\begin{Bmatrix} 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon \end{Bmatrix}$   |       |       |       |         |         |                                | $(x, y), (R_x, R_y)$ | $(xz, yz)$ |
| $E_2$ | $\begin{Bmatrix} 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon \\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* \end{Bmatrix}$ |       |       |       |         |         |                                | $(x^2 - y^2, xy)$    |            |

| $C_7$ | $E$  | $C_7$ | $C_7^2$ | $C_7^3$ | $C_7^4$ | $C_7^5$ | $C_7^6$ | $\varepsilon = \exp(2\pi i/7)$ |                      |                   |
|-------|--|-------|---------|---------|---------|---------|---------|--------------------------------|----------------------|-------------------|
| A     | 1  | 1     | 1       | 1       | 1       | 1       | 1       | $z, R_z$                       | $x^2 + y^2, z^2$     |                   |
| $E_1$ | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^3 & \varepsilon^{3*} & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^{3*} & \varepsilon^3 & \varepsilon^2 & \varepsilon \end{Bmatrix}$ |       |         |         |         |         |         |                                | $(x, y), (R_x, R_y)$ | $(xz, yz)$        |
| $E_2$ | $\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^{3*} & \varepsilon^* & \varepsilon & \varepsilon^3 & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon^3 & \varepsilon & \varepsilon^* & \varepsilon^{3*} & \varepsilon^2 \end{Bmatrix}$ |       |         |         |         |         |         |                                |                      | $(x^2 - y^2, xy)$ |
| $E_3$ | $\begin{Bmatrix} 1 & \varepsilon^3 & \varepsilon^* & \varepsilon^2 & \varepsilon^{2*} & \varepsilon & \varepsilon^{3*} \\ 1 & \varepsilon^{3*} & \varepsilon & \varepsilon^{2*} & \varepsilon^2 & \varepsilon^* & \varepsilon^3 \end{Bmatrix}$ |       |         |         |         |         |         |                                |                      |                   |

| $C_8$ | $E$  | $C_8$ | $C_4$ | $C_2$ | $C_4^3$ | $C_8^3$ | $C_8^5$ | $C_8^7$ | $\varepsilon = \exp(2\pi i/8)$ |                      |            |
|-------|--|-------|-------|-------|---------|---------|---------|---------|--------------------------------|----------------------|------------|
| A     | 1  | 1     | 1     | 1     | 1       | 1       | 1       | 1       | $z, R_z$                       | $x^2 + y^2, z^2$     |            |
| B     | 1  | -1    | 1     | 1     | 1       | -1      | -1      | -1      |                                |                      |            |
| $E_1$ | $\begin{Bmatrix} 1 & \varepsilon & i & -1 & -i & -\varepsilon^* & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -i & -1 & i & -\varepsilon & -\varepsilon^* & \varepsilon \end{Bmatrix}$ |       |       |       |         |         |         |         |                                | $(x, y), (R_x, R_y)$ | $(xz, yz)$ |
| $E_2$ | $\begin{Bmatrix} 1 & i & -1 & 1 & -1 & -i & i & -i \\ 1 & -i & -1 & 1 & -1 & i & -i & i \end{Bmatrix}$   |       |       |       |         |         |         |         |                                | $(x^2 - y^2, xy)$    |            |
| $E_3$ | $\begin{Bmatrix} 1 & -\varepsilon & i & -1 & -i & \varepsilon^* & \varepsilon & -\varepsilon^* \\ 1 & -\varepsilon^* & -i & -1 & i & \varepsilon & \varepsilon^* & -\varepsilon \end{Bmatrix}$ |       |       |       |         |         |         |         |                                |                      |            |



► The  $S_n$  Groups

| $S_4$ | $E$  | $S_4$ | $C_2$ | $S_4^2$ |                      |                  |
|-------|--|-------|-------|---------|----------------------|------------------|
| $A$   | 1  | 1     | 1     | 1       | $R_z$                | $x^2 + y^2, z^2$ |
| $B$   | 1  | -1    | 1     | -1      | $z$                  | $x^2 - y^2, xy$  |
| $E$   | $\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$ |       |       |         | $(x, y), (R_x, R_y)$ | $(xz, yz)$       |

| $S_6$ | $E$  | $C_3$ | $C_3^2$ | $i$ | $S_6^2$ | $S_6$ | $\varepsilon = \exp(2\pi i/3)$ |                                  |
|-------|--|-------|---------|-----|---------|-------|--------------------------------|----------------------------------|
| $A_2$ | 1  | 1     | 1       | 1   | 1       | 1     | $R_z$                          | $x^2 + y^2, z^2$                 |
| $E_g$ | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon & 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$       |       |         |     |         |       | $(R_x, R_y)$                   | $(x^2 - y^2, xy),$<br>$(xy, yz)$ |
| $A_u$ | 1  | 1     | 1       | -1  | -1      | -1    | $z$                            |                                  |
| $E_u$ | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & -1 & -\varepsilon & -\varepsilon^* \\ 1 & \varepsilon^* & \varepsilon & -1 & -\varepsilon^* & -\varepsilon \end{Bmatrix}$ |       |         |     |         |       | $(x, y)$                       |                                  |

| $S_8$ | $E$  | $S_8$ | $C_4$ | $S_8^2$ | $C_2$ | $S_8^3$ | $C_4^2$ | $S_8^4$ | $\varepsilon = \exp(2\pi i/8)$ |                   |
|-------|--|-------|-------|---------|-------|---------|---------|---------|--------------------------------|-------------------|
| $A$   | 1  | 1     | 1     | 1       | 1     | 1       | 1       | 1       | $R_z$                          | $x^2 + y^2, z^2$  |
| $B$   | 1  | -1    | 1     | -1      | 1     | -1      | 1       | -1      | $z$                            |                   |
| $E_1$ | $\begin{Bmatrix} 1 & \varepsilon & i & -\varepsilon^* & -1 & -\varepsilon & -i & \varepsilon^* \\ 1 & \varepsilon^* & -i & -\varepsilon & -1 & -\varepsilon^* & i & \varepsilon \end{Bmatrix}$ |       |       |         |       |         |         |         | $(x, y),$<br>$(R_x, R_y)$      |                   |
| $E_2$ | $\begin{Bmatrix} 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & -i & -1 & i & 1 & -i & -1 & i \end{Bmatrix}$   |       |       |         |       |         |         |         |                                | $(x^2 - y^2, xy)$ |
| $E_3$ | $\begin{Bmatrix} 1 & -\varepsilon^* & -i & \varepsilon & -1 & \varepsilon^* & i & -\varepsilon \\ 1 & -\varepsilon & i & \varepsilon^* & -1 & \varepsilon & -i & -\varepsilon^* \end{Bmatrix}$ |       |       |         |       |         |         |         |                                | $(xz, yz)$        |

► The  $C_{nv}$  Groups

| $C_{2v}$ | $E$ | $C_2$ | $\sigma_v(xz)$ | $\sigma'_v(yz)$ |          |                 |
|----------|-----|-------|----------------|-----------------|----------|-----------------|
| $A_1$    | 1   | 1     | 1              | 1               | $z$      | $x^2, y^2, z^2$ |
| $A_2$    | 1   | 1     | -1             | -1              | $R_z$    | $xy$            |
| $B_1$    | 1   | -1    | 1              | -1              | $x, R_y$ | $xz$            |
| $B_2$    | 1   | -1    | -1             | 1               | $y, R_x$ | $yz$            |

| $C_{3v}$ | $E$ | $2C_3$ | $3\sigma_v$ |                      |                             |
|----------|-----|--------|-------------|----------------------|-----------------------------|
| $A_1$    | 1   | 1      | 1           | $z$                  | $x^2 + y^2, z^2$            |
| $A_2$    | 1   | 1      | -1          | $R_z$                |                             |
| $E$      | 2   | -1     | 0           | $(x, y), (R_x, R_y)$ | $(x^2 - y^2, xy), (xz, yz)$ |

## C-4

## APPENDIX C

| $C_{4v}$ | $E$ | $2C_4$ | $C_2$ | $2\sigma_v$ | $2\sigma_d$ |                      |                  |
|----------|-----|--------|-------|-------------|-------------|----------------------|------------------|
| $A_1$    | 1   | 1      | 1     | 1           | 1           | $z$                  | $x^2 + y^2, z^2$ |
| $A_2$    | 1   | 1      | 1     | -1          | -1          | $R_z$                |                  |
| $B_1$    | 1   | -1     | 1     | 1           | -1          |                      | $x^2 - y^2$      |
| $B_2$    | 1   | -1     | 1     | -1          | 1           |                      | $xy$             |
| $E$      | 2   | 0      | -2    | 0           | 0           | $(x, y), (R_x, R_y)$ | $(xz, yz)$       |

| $C_{3v}$ | $E$ | $2C_3$             | $2C_2$             | $3\sigma_v$ |                      |                   |
|----------|-----|--------------------|--------------------|-------------|----------------------|-------------------|
| $A_1$    | 1   | 1                  | 1                  | 1           | $z$                  | $x^2 + y^2, z^2$  |
| $A_2$    | 1   | 1                  | 1                  | -1          | $R_z$                |                   |
| $E_1$    | 2   | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0           | $(x, y), (R_x, R_y)$ | $(xz, yz)$        |
| $E_2$    | 2   | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0           |                      | $(x^2 - y^2, xy)$ |

| $C_{6v}$ | $E$ | $2C_6$ | $2C_3$ | $C_2$ | $3\sigma_v$ | $3\sigma_d$ |                      |
|----------|-----|--------|--------|-------|-------------|-------------|----------------------|
| $A_1$    | 1   | 1      | 1      | 1     | 1           | 1           | $z$                  |
| $A_2$    | 1   | 1      | 1      | 1     | -1          | -1          | $R_z$                |
| $B_1$    | 1   | -1     | 1      | -1    | 1           | -1          |                      |
| $B_2$    | 1   | -1     | 1      | -1    | -1          | 1           |                      |
| $E_1$    | 2   | 1      | -1     | -2    | 0           | 0           | $(x, y), (R_x, R_y)$ |
| $E_2$    | 2   | -1     | -1     | 2     | 0           | 0           |                      |

► The  $C_{nh}$  Groups

| $C_{2h}$ | $E$ | $C_2$ | $i$ | $\sigma_h$ |            |                     |
|----------|-----|-------|-----|------------|------------|---------------------|
| $A_g$    | 1   | 1     | 1   | 1          | $R_z$      | $x^2, y^2, z^2, xy$ |
| $B_g$    | 1   | -1    | 1   | -1         | $R_x, R_y$ | $xz, yz$            |
| $A_u$    | 1   | 1     | -1  | -1         | $z$        |                     |
| $B_u$    | 1   | -1    | -1  | 1          | $x, y$     |                     |

| $C_{3h}$ | $E$  | $C_3$  | $C_3^2$  | $\sigma_h$   | $S_3$  | $S_3^2$  | $\varepsilon = \exp(2\pi i/3)$ |
|----------|--|--|--|--|--|--|--------------------------------|
| $A'$     | 1  | 1  | 1  | 1  | 1  | 1  | $R_z$                          |
| $E'$     | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$ | $\begin{Bmatrix} \varepsilon & 1 \\ \varepsilon^* & 1 \end{Bmatrix}$ | $\begin{Bmatrix} \varepsilon^* & \varepsilon \\ \varepsilon & \varepsilon^* \end{Bmatrix}$ | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$   | $\begin{Bmatrix} \varepsilon & \varepsilon^* \\ \varepsilon^* & \varepsilon \end{Bmatrix}$     | $\begin{Bmatrix} \varepsilon^* & \varepsilon \\ \varepsilon & \varepsilon^* \end{Bmatrix}$     | $(x, y)$                       |
| $A''$    | 1  | 1  | 1  | -1   | -1   | -1   | $z$                            |
| $E''$    | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$ | $\begin{Bmatrix} \varepsilon & 1 \\ \varepsilon^* & 1 \end{Bmatrix}$ | $\begin{Bmatrix} \varepsilon^* & \varepsilon \\ \varepsilon & \varepsilon^* \end{Bmatrix}$ | $\begin{Bmatrix} -1 & \varepsilon & \varepsilon^* \\ -1 & \varepsilon^* & \varepsilon \end{Bmatrix}$ | $\begin{Bmatrix} -\varepsilon & -\varepsilon^* \\ -\varepsilon^* & -\varepsilon \end{Bmatrix}$ | $\begin{Bmatrix} -\varepsilon^* & -\varepsilon \\ -\varepsilon & -\varepsilon^* \end{Bmatrix}$ | $(R_x, R_y)$                   |

| $C_{4h}$ | $E$  | $C_4$ | $C_2$ | $C_2^3$ | $i$ | $S_4^3$ | $\sigma_h$ | $S_4$ |          |                  |
|----------|--|-------|-------|---------|-----|---------|------------|-------|----------|------------------|
| $A_g$    | 1  | 1     | 1     | 1       | 1   | 1       | 1          | 1     | $R_z$    | $x^2 + y^2, z^2$ |
| $B_g$    | 1  | -1    | 1     | -1      | 1   | -1      | 1          | -1    |          |                  |
| $E_g$    | $\begin{Bmatrix} 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & -i & -1 & i & 1 & -i & -1 & i \end{Bmatrix}$ |       |       |         |     |         |            |       | $z$      | $(xz, yz)$       |
| $A_u$    | 1  | 1     | 1     | 1       | -1  | -1      | -1         | -1    |          |                  |
| $B_u$    | 1  | -1    | 1     | -1      | -1  | 1       | -1         | 1     | $(x, y)$ |                  |
| $E_u$    | $\begin{Bmatrix} 1 & i & -1 & -i & -1 & -i & 1 & i \\ 1 & -i & -1 & i & -1 & i & 1 & -i \end{Bmatrix}$ |       |       |         |     |         |            |       |          |                  |

| $C_{5h}$ | $E$  | $C_5$ | $C_5^2$ | $C_5^3$ | $C_5^4$ | $\sigma_h$ | $S_5$ | $S_5^2$ | $S_5^3$ | $S_5^4$ | $\varepsilon = \exp(2\pi i/5)$ |                   |
|----------|--|-------|---------|---------|---------|------------|-------|---------|---------|---------|--------------------------------|-------------------|
| $A'$     | 1  | 1     | 1       | 1       | 1       | 1          | 1     | 1       | 1       | 1       | $R_z$                          | $x^2 + y^2, z^2$  |
| $E_1'$   | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* & 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon & 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon & \varepsilon^* \end{Bmatrix}$ |       |         |         |         |            |       |         |         |         |                                |                   |
| $E_2'$   | $\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} & 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 & 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 \end{Bmatrix}$                 |       |         |         |         |            |       |         |         |         | $z$                            | $(x^2 - y^2, xy)$ |
| $A''$    | 1  | 1     | 1       | 1       | 1       | -1         | -1    | -1      | -1      | -1      |                                |                   |
| $E_1''$  | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* & -1 & -\varepsilon & -\varepsilon^2 & -\varepsilon^{2*} & -\varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon & -1 & -\varepsilon^* & -\varepsilon^{2*} & -\varepsilon^2 & -\varepsilon \end{Bmatrix}$       |       |         |         |         |            |       |         |         |         |                                |                   |
| $E_2''$  | $\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} & -1 & -\varepsilon^2 & -\varepsilon^* & -\varepsilon & -\varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 & -1 & -\varepsilon^{2*} & -\varepsilon & -\varepsilon^* & -\varepsilon^2 \end{Bmatrix}$       |       |         |         |         |            |       |         |         |         |                                |                   |

| $C_{6h}$ | $E$  | $C_6$ | $C_3$ | $C_2$ | $C_3^2$ | $C_6^5$ | $i$ | $S_6^5$ | $S_6^4$ | $\sigma_h$ | $S_6$ | $S_6^3$ | $\varepsilon = \exp(2\pi i/6)$ |                   |
|----------|--|-------|-------|-------|---------|---------|-----|---------|---------|------------|-------|---------|--------------------------------|-------------------|
| $A_g$    | 1  | 1     | 1     | 1     | 1       | 1       | 1   | 1       | 1       | 1          | 1     | 1       | $R_z$                          | $x^2 + y^2, z^2$  |
| $B_g$    | 1  | -1    | 1     | -1    | 1       | -1      | 1   | -1      | 1       | -1         | 1     | -1      |                                |                   |
| $E_{1g}$ | $\begin{Bmatrix} 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* & 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon & 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon \end{Bmatrix}$     |       |       |       |         |         |     |         |         |            |       |         | $z$                            | $(x^2 - y^2, xy)$ |
| $E_{2g}$ | $\begin{Bmatrix} 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon \\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* \end{Bmatrix}$ |       |       |       |         |         |     |         |         |            |       |         |                                |                   |
| $A_u$    | 1  | 1     | 1     | 1     | 1       | 1       | -1  | -1      | -1      | -1         | -1    | -1      | $(x, y)$                       |                   |
| $B_u$    | 1  | -1    | 1     | -1    | 1       | -1      | -1  | 1       | -1      | 1          | -1    | 1       |                                |                   |
| $E_{1u}$ | $\begin{Bmatrix} 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* & -1 & -\varepsilon & \varepsilon^* & 1 & \varepsilon & -\varepsilon^* \\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon & -1 & -\varepsilon^* & \varepsilon & 1 & \varepsilon^* & -\varepsilon \end{Bmatrix}$     |       |       |       |         |         |     |         |         |            |       |         |                                |                   |
| $E_{2u}$ | $\begin{Bmatrix} 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon & -1 & \varepsilon^* & \varepsilon & -1 & \varepsilon^* & \varepsilon \\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* & -1 & \varepsilon & \varepsilon^* & -1 & \varepsilon & \varepsilon^* \end{Bmatrix}$     |       |       |       |         |         |     |         |         |            |       |         |                                |                   |

## THE DIHEDRAL GROUPS

### ► The $D_n$ Groups

| $D_2$ | $E$ | $C_2(z)$ | $C_2(y)$ | $C_2(x)$ |          |                 |
|-------|-----|----------|----------|----------|----------|-----------------|
| $A$   | 1   | 1        | 1        | 1        |          | $x^2, y^2, z^2$ |
| $B_1$ | 1   | 1        | -1       | -1       | $z, R_z$ | $xy$            |
| $B_2$ | 1   | -1       | 1        | -1       | $y, R_y$ | $xz$            |
| $B_3$ | 1   | -1       | -1       | 1        | $x, R_x$ | $yz$            |

| $D_3$ | $E$ | $2C_3$ | $3C_2$ | (x axis is coincident with $C_2$ ) |  |                             |
|-------|-----|--------|--------|------------------------------------|--|-----------------------------|
| $A_1$ | 1   | 1      | 1      |                                    |  | $x^2 + y^2, z^2$            |
| $A_2$ | 1   | 1      | -1     | $z, R_z$                           |  |                             |
| $E$   | 2   | -1     | 0      | $(x, y), (R_x, R_y)$               |  | $(x^2 - y^2, xy), (xz, yz)$ |

| $D_4$ | $E$ | $2C_4$ | $C_2(=C_2^2)$ | $2C_2'$ | $2C_2''$ | (x axis coincident with $C_2'$ ) |                  |
|-------|-----|--------|---------------|---------|----------|----------------------------------|------------------|
| $A_1$ | 1   | 1      | 1             | 1       | 1        |                                  | $x^2 + y^2, z^2$ |
| $A_2$ | 1   | 1      | 1             | -1      | -1       | $z, R_z$                         |                  |
| $B_1$ | 1   | -1     | 1             | 1       | -1       |                                  | $x^2 - y^2$      |
| $B_2$ | 1   | -1     | 1             | -1      | 1        |                                  | $xy$             |
| $E$   | 2   | 0      | -2            | 0       | 0        | $(x, y), (R_x, R_y)$             | $(xz, yz)$       |

| $D_5$ | $E$ | $2C_5$             | $2C_5^2$           | $5C_2$ | (x axis coincident with $C_2$ ) |                   |
|-------|-----|--------------------|--------------------|--------|---------------------------------|-------------------|
| $A_1$ | 1   | 1                  | 1                  | 1      |                                 | $x^2 + y^2, z^2$  |
| $A_2$ | 1   | 1                  | 1                  | -1     | $z, R_z$                        |                   |
| $E_1$ | 2   | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0      | $(x, y), (R_x, R_y)$            | $(xz, yz)$        |
| $E_2$ | 2   | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0      |                                 | $(x^2 - y^2, xy)$ |

| $D_6$ | $E$ | $2C_6$ | $2C_3$ | $C_2$ | $3C_2'$ | $3C_2''$ | (x axis coincident with $C_2'$ ) |                   |
|-------|-----|--------|--------|-------|---------|----------|----------------------------------|-------------------|
| $A_1$ | 1   | 1      | 1      | 1     | 1       | 1        |                                  | $x^2 + y^2, z^2$  |
| $A_2$ | 1   | 1      | 1      | 1     | -1      | -1       | $z, R_z$                         |                   |
| $B_1$ | 1   | -1     | 1      | -1    | 1       | -1       |                                  |                   |
| $B_2$ | 1   | -1     | 1      | -1    | -1      | 1        |                                  |                   |
| $E_1$ | 2   | 1      | -1     | -2    | 0       | 0        | $(x, y), (R_x, R_y)$             | $(xz, yz)$        |
| $E_2$ | 2   | -1     | -1     | 2     | 0       | 0        |                                  | $(x^2 - y^2, xy)$ |

► The  $D_{nh}$  Groups

| $D_{2h}$ | E | $C_2(z)$ | $C_2(y)$ | $C_2(x)$ | $i$ | $\sigma(xy)$ | $\sigma(xz)$ | $\sigma(yz)$ |       |                 |
|----------|---|----------|----------|----------|-----|--------------|--------------|--------------|-------|-----------------|
| $A_g$    | 1 | 1        | 1        | 1        | 1   | 1            | 1            | 1            |       | $x^2, y^2, z^2$ |
| $B_{1g}$ | 1 | 1        | -1       | -1       | 1   | 1            | -1           | -1           | $R_z$ | $xy$            |
| $B_{2g}$ | 1 | -1       | 1        | -1       | 1   | -1           | 1            | -1           | $R_y$ | $xz$            |
| $B_{3g}$ | 1 | -1       | -1       | 1        | 1   | -1           | -1           | 1            | $R_x$ | $yz$            |
| $A_u$    | 1 | 1        | 1        | 1        | -1  | -1           | -1           | -1           |       |                 |
| $B_{1u}$ | 1 | 1        | -1       | -1       | -1  | -1           | 1            | 1            | $z$   |                 |
| $B_{2u}$ | 1 | -1       | 1        | -1       | -1  | 1            | -1           | 1            | $y$   |                 |
| $B_{3u}$ | 1 | -1       | -1       | 1        | -1  | 1            | 1            | -1           | $x$   |                 |

| $D_{3h}$ | E | $2C_3$ | $3C_2$ | $\sigma_h$ | $2S_6$ | $3\sigma_v$ | (x axis coincident with $C_2$ ) |                   |
|----------|---|--------|--------|------------|--------|-------------|---------------------------------|-------------------|
| $A_1'$   | 1 | 1      | 1      | 1          | 1      | 1           |                                 | $x^2 + y^2, z^2$  |
| $A_2'$   | 1 | 1      | -1     | 1          | 1      | -1          | $R_z$                           |                   |
| $E'$     | 2 | -1     | 0      | 2          | -1     | 0           | (x, y)                          | $(x^2 - y^2, xy)$ |
| $A_1''$  | 1 | 1      | 1      | -1         | -1     | -1          |                                 |                   |
| $A_2''$  | 1 | 1      | -1     | -1         | -1     | 1           | $z$                             |                   |
| $E''$    | 2 | -1     | 0      | -2         | 1      | 0           | ( $R_x, R_y$ )                  | $(xz, yz)$        |

| $D_{4h}$ | E | $2C_4$ | $C_2$ | $2C_2'$ | $2C_2''$ | $i$ | $2S_4$ | $\sigma_h$ | $2\sigma_v$ | $2\sigma_d$ | (x axis coincident with $C_2'$ ) |                  |
|----------|---|--------|-------|---------|----------|-----|--------|------------|-------------|-------------|----------------------------------|------------------|
| $A_{1g}$ | 1 | 1      | 1     | 1       | 1        | 1   | 1      | 1          | 1           | 1           |                                  | $x^2 + y^2, z^2$ |
| $A_{2g}$ | 1 | 1      | 1     | -1      | -1       | 1   | 1      | 1          | -1          | -1          | $R_z$                            |                  |
| $B_{1g}$ | 1 | -1     | 1     | 1       | -1       | 1   | -1     | 1          | 1           | -1          |                                  | $x^2 - y^2$      |
| $B_{2g}$ | 1 | -1     | 1     | -1      | 1        | 1   | -1     | 1          | -1          | 1           |                                  | $xy$             |
| $E_g$    | 2 | 0      | -2    | 0       | 0        | 2   | 0      | -2         | 0           | 0           | ( $R_x, R_y$ )                   | $(xz, yz)$       |
| $A_{1u}$ | 1 | 1      | 1     | 1       | 1        | -1  | -1     | -1         | -1          | -1          |                                  |                  |
| $A_{2u}$ | 1 | 1      | 1     | -1      | -1       | -1  | -1     | -1         | 1           | 1           | $z$                              |                  |
| $B_{1u}$ | 1 | -1     | 1     | 1       | -1       | -1  | 1      | -1         | -1          | 1           |                                  |                  |
| $B_{2u}$ | 1 | -1     | 1     | -1      | 1        | -1  | 1      | -1         | 1           | -1          |                                  |                  |
| $E_u$    | 2 | 0      | -2    | 0       | 0        | -2  | 0      | 2          | 0           | 0           | (x, y)                           |                  |

| $D_{5h}$ | E | $2C_5$             | $2C_5^2$           | $5C_2$ | $\sigma_h$ | $2S_5$              | $2S_5^3$            | $5\sigma_v$ | (x axis coincident with $C_2$ ) |                   |
|----------|---|--------------------|--------------------|--------|------------|---------------------|---------------------|-------------|---------------------------------|-------------------|
| $A_1'$   | 1 | 1                  | 1                  | 1      | 1          | 1                   | 1                   | 1           |                                 | $x^2 + y^2, z^2$  |
| $A_2'$   | 1 | 1                  | 1                  | -1     | 1          | 1                   | 1                   | -1          | $R_z$                           |                   |
| $E_1'$   | 2 | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0      | 2          | $2 \cos 72^\circ$   | $2 \cos 144^\circ$  | 0           | (x, y)                          |                   |
| $E_2'$   | 2 | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0      | 2          | $-2 \cos 144^\circ$ | $2 \cos 72^\circ$   | 0           |                                 | $(x^2 - y^2, xy)$ |
| $A_1''$  | 1 | 1                  | 1                  | 1      | -1         | -1                  | -1                  | -1          |                                 |                   |
| $A_2''$  | 1 | 1                  | 1                  | -1     | -1         | -1                  | -1                  | 1           | $z$                             |                   |
| $E_1''$  | 2 | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0      | -2         | $-2 \cos 72^\circ$  | $-2 \cos 144^\circ$ | 0           | ( $R_x, R_y$ )                  | $(xz, yz)$        |
| $E_2''$  | 2 | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0      | -2         | $-2 \cos 144^\circ$ | $-2 \cos 72^\circ$  | 0           |                                 |                   |

| $D_{6h}$ | $E$ | $2C_6$ | $2C_3$ | $C_2$ | $3C_2'$ | $3C_2''$ | $i$ | $2S_6$ | $2S_6$ | $\sigma_h$ | $3\sigma_d$ | $3\sigma_v$ | (x axis coincident with $C_2'$ ) |                               |
|----------|-----|--------|--------|-------|---------|----------|-----|--------|--------|------------|-------------|-------------|----------------------------------|-------------------------------|
| $A_{1g}$ | 1   | 1      | 1      | 1     | 1       | 1        | 1   | 1      | 1      | 1          | 1           | 1           | $R_z$                            | $x^2+y^2, z^2$                |
| $A_{2g}$ | 1   | 1      | 1      | 1     | -1      | -1       | 1   | 1      | 1      | 1          | -1          | -1          |                                  |                               |
| $B_{1g}$ | 1   | -1     | 1      | -1    | 1       | -1       | 1   | -1     | 1      | -1         | 1           | -1          |                                  |                               |
| $B_{2g}$ | 1   | -1     | 1      | -1    | -1      | 1        | 1   | -1     | 1      | -1         | -1          | 1           | $(R_x, R_y)$                     | $(xz, yz)$<br>$(x^2 - y, xy)$ |
| $E_{1g}$ | 2   | 1      | -1     | -2    | 0       | 0        | 2   | 1      | -1     | -2         | 0           | 0           |                                  |                               |
| $E_{2g}$ | 2   | -1     | -1     | 2     | 0       | 0        | 2   | -1     | -1     | 2          | 0           | 0           |                                  |                               |
| $A_{1u}$ | 1   | 1      | 1      | 1     | 1       | 1        | -1  | -1     | -1     | -1         | -1          | -1          | $z$                              |                               |
| $A_{2u}$ | 1   | 1      | 1      | 1     | -1      | -1       | -1  | -1     | -1     | -1         | 1           | 1           |                                  |                               |
| $B_{1u}$ | 1   | -1     | 1      | -1    | 1       | -1       | -1  | 1      | -1     | 1          | -1          | 1           |                                  |                               |
| $B_{2u}$ | 1   | -1     | 1      | -1    | -1      | 1        | -1  | 1      | -1     | 1          | 1           | -1          | $(x, y)$                         |                               |
| $E_{1u}$ | 2   | 1      | -1     | -2    | 0       | 0        | -2  | -1     | 1      | 2          | 0           | 0           |                                  |                               |
| $E_{2u}$ | 2   | -1     | -1     | 2     | 0       | 0        | -2  | 1      | 1      | -2         | 0           | 0           |                                  |                               |

| $D_{3h}$ | $E$ | $2C_3$      | $2C_2$      | $C_2$ | $4C_2'$ | $4C_2''$ | $i$ | $2S_6$ | $2S_6$      | $2S_6$      | $\sigma_h$ | $4\sigma_v$ | $4\sigma_d$ | (x axis coincident with $C_2'$ ) |                                 |
|----------|-----|-------------|-------------|-------|---------|----------|-----|--------|-------------|-------------|------------|-------------|-------------|----------------------------------|---------------------------------|
| $A_{1g}$ | 1   | 1           | 1           | 1     | 1       | 1        | 1   | 1      | 1           | 1           | 1          | 1           | 1           | $R_z$                            | $x^2+y^2, z^2$                  |
| $A_{2g}$ | 1   | 1           | 1           | 1     | 1       | -1       | -1  | 1      | 1           | 1           | 1          | -1          | -1          |                                  |                                 |
| $B_{1g}$ | 1   | -1          | -1          | 1     | 1       | 1        | -1  | 1      | -1          | -1          | 1          | 1           | -1          |                                  |                                 |
| $B_{2g}$ | 1   | -1          | -1          | 1     | 1       | -1       | 1   | 1      | -1          | -1          | 1          | 1           | -1          | $(R_x, R_y)$                     | $(xz, yz)$<br>$(x^2 - y^2, xy)$ |
| $E_{1g}$ | 2   | $\sqrt{2}$  | $-\sqrt{2}$ | 0     | -2      | 0        | 0   | 2      | $\sqrt{2}$  | $-\sqrt{2}$ | 0          | -2          | 0           |                                  |                                 |
| $E_{2g}$ | 2   | 0           | 0           | -2    | 2       | 0        | 0   | 2      | 0           | 0           | -2         | 2           | 0           |                                  |                                 |
| $E_{1u}$ | 2   | $-\sqrt{2}$ | $\sqrt{2}$  | 0     | -2      | 0        | 0   | 2      | $-\sqrt{2}$ | $\sqrt{2}$  | 0          | -2          | 0           | $z$                              |                                 |
| $A_{1u}$ | 1   | 1           | 1           | 1     | 1       | 1        | -1  | -1     | -1          | -1          | -1         | -1          | -1          |                                  |                                 |
| $A_{2u}$ | 1   | 1           | 1           | 1     | 1       | -1       | -1  | -1     | -1          | -1          | -1         | 1           | 1           |                                  |                                 |
| $B_{1u}$ | 1   | -1          | -1          | 1     | 1       | 1        | -1  | -1     | 1           | 1           | -1         | -1          | -1          | $(x, y)$                         |                                 |
| $B_{2u}$ | 1   | -1          | -1          | 1     | 1       | -1       | 1   | -1     | 1           | -1          | -1         | 1           | -1          |                                  |                                 |
| $E_{1u}$ | 2   | $\sqrt{2}$  | $-\sqrt{2}$ | 0     | -2      | 0        | 0   | -2     | $-\sqrt{2}$ | $\sqrt{2}$  | 0          | 2           | 0           |                                  |                                 |
| $E_{2u}$ | 2   | 0           | 0           | -2    | 2       | 0        | 0   | -2     | 0           | 0           | 2          | -2          | 0           |                                  |                                 |
| $E_{1u}$ | 2   | $-\sqrt{2}$ | $\sqrt{2}$  | 0     | -2      | 0        | 0   | -2     | $\sqrt{2}$  | $-\sqrt{2}$ | 0          | 2           | 0           |                                  |                                 |

► The  $D_{nd}$  Groups

| $D_{2d}$ | $E$ | $2S_4$ | $C_2$ | $2C_2'$ | $2\sigma_d$ | (x axis coincident with $C_2'$ ) |                  |
|----------|-----|--------|-------|---------|-------------|----------------------------------|------------------|
| $A_1$    | 1   | 1      | 1     | 1       | 1           | $R_z$                            | $x^2 + y^2, z^2$ |
| $A_2$    | 1   | 1      | 1     | -1      | -1          |                                  |                  |
| $B_1$    | 1   | -1     | 1     | 1       | -1          |                                  |                  |
| $B_2$    | 1   | -1     | 1     | -1      | 1           | $z$                              | $xy$             |
| $E$      | 2   | 0      | -2    | 0       | 0           | $(x, y), (R_x, R_y)$             | $(xz, yz)$       |

| $D_{3d}$ | $E$ | $2C_3$ | $3C_2$ | $i$ | $2S_6$ | $3\sigma_d$ | (x axis coincident with $C_2$ ) |
|----------|-----|--------|--------|-----|--------|-------------|---------------------------------|
| $A_{1g}$ | 1   | 1      | 1      | 1   | 1      | $R_z$       | $x^2 + y^2, z^2$                |
| $A_{2g}$ | 1   | 1      | -1     | 1   | -1     |             |                                 |
| $E_g$    | 2   | -1     | 0      | 2   | -1     |             |                                 |
| $A_{1u}$ | 1   | 1      | 1      | -1  | -1     | $z$         |                                 |
| $A_{2u}$ | 1   | 1      | -1     | -1  | 1      |             |                                 |
| $E_u$    | 2   | -1     | 0      | -2  | 1      |             |                                 |

| $D_{3d}$ | $E$ | $2S_6$      | $2C_4$ | $2S_8^3$    | $C_2$ | $4C_2'$ | $4\sigma_d$ | (x axis coincident with $C_2'$ ) |                   |
|----------|-----|-------------|--------|-------------|-------|---------|-------------|----------------------------------|-------------------|
| $A_1$    | 1   | 1           | 1      | 1           | 1     | 1       | 1           |                                  | $x^2 + y^2, z^2$  |
| $A_2$    | 1   | 1           | 1      | 1           | 1     | -1      | -1          | $R_z$                            |                   |
| $B_1$    | 1   | -1          | 1      | -1          | 1     | 1       | -1          |                                  |                   |
| $B_2$    | 1   | -1          | 1      | -1          | 1     | -1      | 1           | $z$                              |                   |
| $E_1$    | 2   | $\sqrt{2}$  | 0      | $-\sqrt{2}$ | -2    | 0       | 0           | $(x, y)$                         |                   |
| $E_2$    | 2   | 0           | -2     | 0           | 2     | 0       | 0           |                                  | $(x^2 - y^2, xy)$ |
| $E_3$    | 2   | $-\sqrt{2}$ | 0      | $\sqrt{2}$  | -2    | 0       | 0           | $(R_x, R_y)$                     | $(xz, yz)$        |

| $D_{3d}$ | 1 | $2C_3$             | $2C_2'$            | $5C_2$ | $i$ | $2S_6^5$            | $2S_6$              | $5\sigma_d$ | (x axis coincident with $C_2$ ) |                   |
|----------|---|--------------------|--------------------|--------|-----|---------------------|---------------------|-------------|---------------------------------|-------------------|
| $A_{1g}$ | 1 | 1                  | 1                  | 1      | 1   | 1                   | 1                   | 1           |                                 | $x^2 + y^2, z^2$  |
| $A_{2g}$ | 1 | 1                  | 1                  | -1     | 1   | 1                   | 1                   | -1          | $R_z$                           |                   |
| $E_{1g}$ | 2 | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0      | 2   | $2 \cos 72^\circ$   | $2 \cos 144^\circ$  | 0           | $(R_x, R_y)$                    | $(xz, yz)$        |
| $E_{2g}$ | 2 | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0      | 2   | $2 \cos 144^\circ$  | $2 \cos 72^\circ$   | 0           |                                 | $(x^2 - y^2, xy)$ |
| $A_{1u}$ | 1 | 1                  | 1                  | 1      | -1  | -1                  | -1                  | -1          |                                 |                   |
| $A_{2u}$ | 1 | 1                  | 1                  | -1     | -1  | -1                  | -1                  | 1           | $z$                             |                   |
| $E_{1u}$ | 2 | $2 \cos 72^\circ$  | $2 \cos 144^\circ$ | 0      | -2  | $-2 \cos 72^\circ$  | $-2 \cos 144^\circ$ | 0           | $(x, y)$                        |                   |
| $E_{2u}$ | 2 | $2 \cos 144^\circ$ | $2 \cos 72^\circ$  | 0      | -2  | $-2 \cos 144^\circ$ | $-2 \cos 72^\circ$  | 0           |                                 |                   |

| $D_{3d}$ | $E$ | $2S_{12}$   | $2C_6$ | $2S_8$ | $2C_3$ | $2S_6^5$    | $C_2$ | $6C_2'$ | $6\sigma_d$ | (x axis coincident with $C_2$ ) |                   |
|----------|-----|-------------|--------|--------|--------|-------------|-------|---------|-------------|---------------------------------|-------------------|
| $A_1$    | 1   | 1           | 1      | 1      | 1      | 1           | 1     | 1       | 1           |                                 | $x^2 + z^2, z^2$  |
| $A_2$    | 1   | 1           | 1      | 1      | 1      | 1           | 1     | -1      | -1          | $R_z$                           |                   |
| $B_1$    | 1   | -1          | 1      | -1     | 1      | -1          | 1     | 1       | -1          |                                 |                   |
| $B_2$    | 1   | -1          | 1      | -1     | 1      | -1          | 1     | -1      | 1           | $z$                             |                   |
| $E_1$    | 2   | $\sqrt{3}$  | 1      | 0      | -1     | $-\sqrt{3}$ | -2    | 0       | 0           | $(x, y)$                        |                   |
| $E_2$    | 2   | 1           | -1     | -2     | -1     | 1           | 2     | 0       | 0           |                                 | $(x^2 - y^2, xy)$ |
| $E_3$    | 2   | 0           | -2     | 0      | 2      | 0           | -2    | 0       | 0           |                                 |                   |
| $E_4$    | 2   | -1          | -1     | 2      | -1     | -1          | 2     | 0       | 0           |                                 |                   |
| $E_5$    | 2   | $-\sqrt{3}$ | 1      | 0      | -1     | $\sqrt{3}$  | -2    | 0       | 0           | $(R_x, R_y)$                    | $(xz, yz)$        |

### THE CUBIC GROUPS

#### ► Tetrahedral Groups

| T | $E$  | $4C_3$ | $4C_3^2$ | $3C_2$ | $\varepsilon = \exp(2\pi i/3)$ |                                 |
|---|--|--------|----------|--------|--------------------------------|---------------------------------|
| A | 1  | 1      | 1        | 1      |                                | $x^2 + y^2 + z^2$               |
| E | $\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & 1 \\ 1 & \varepsilon^* & \varepsilon & 1 \end{Bmatrix}$ |        |          |        |                                | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| T | 3  | 0      | 0        | -1     | $(R, R_y, R_z), (x, y, z)$     | $(xy, xz, yz)$                  |

| $T_h$ | $E$  | $4C_3$ | $4C_3^2$ | $3C_2$ | $i$ | $4S_6$ | $4S_6^5$ | $3\sigma_h$ | $(\epsilon = \exp(2\pi i/3))$ |                                 |
|-------|--|--------|----------|--------|-----|--------|----------|-------------|-------------------------------|---------------------------------|
| $A_g$ | 1  | 1      | 1        | 1      | 1   | 1      | 1        | 1           |                               | $x^2 + y^2 + z^2$               |
| $A_u$ | 1  | 1      | 1        | 1      | -1  | -1     | -1       | -1          |                               |                                 |
| $E_g$ | $\begin{Bmatrix} 1 & \epsilon & \epsilon^* & 1 & 1 & \epsilon & \epsilon^* & 1 \\ 1 & \epsilon^* & \epsilon & 1 & 1 & \epsilon^* & \epsilon & 1 \end{Bmatrix}$         |        |          |        |     |        |          |             |                               | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $E_u$ | $\begin{Bmatrix} 1 & \epsilon & \epsilon^* & 1 & -1 & -\epsilon & -\epsilon^* & -1 \\ 1 & \epsilon^* & \epsilon & 1 & -1 & -\epsilon^* & -\epsilon & -1 \end{Bmatrix}$ |        |          |        |     |        |          |             |                               |                                 |
| $T_g$ | 3  | 0      | 0        | -1     | 3   | 0      | 0        | -1          | $(R_x, R_y, R_z)$             | $(xz, yz, xy)$                  |
| $T_u$ | 3  | 0      | 0        | -1     | -3  | 0      | 0        | 1           | $(x, y, z)$                   |                                 |

| $T_d$ | $E$ | $8C_3$ | $3C_2$ | $6S_4$ | $6\sigma_d$ |                   |                                 |
|-------|-----|--------|--------|--------|-------------|-------------------|---------------------------------|
| $A_1$ | 1   | 1      | 1      | 1      | 1           |                   | $x^2 + y^2 + z^2$               |
| $A_2$ | 1   | 1      | 1      | -1     | -1          |                   |                                 |
| $E$   | 2   | -1     | 2      | 0      | 0           | $(R_x, R_y, R_z)$ | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $T_1$ | 3   | 0      | -1     | 1      | -1          | $(x, y, z)$       |                                 |
| $T_2$ | 3   | 0      | -1     | -1     | 1           |                   | $(xy, xz, yz)$                  |

► Octahedral Groups

| $O$   | $E$ | $6C_4$ | $3C_2(=C_4^2)$ | $8C_3$ | $6C_2$ |                              |                                 |
|-------|-----|--------|----------------|--------|--------|------------------------------|---------------------------------|
| $A_1$ | 1   | 1      | 1              | 1      | 1      |                              | $x^2 + y^2 + z^2$               |
| $A_2$ | 1   | -1     | 1              | 1      | -1     |                              |                                 |
| $E$   | 2   | 0      | 2              | -1     | 0      | $(R_x, R_y, R_z), (x, y, z)$ | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $T_1$ | 3   | 1      | -1             | 0      | -1     |                              |                                 |
| $T_2$ | 3   | -1     | -1             | 0      | 1      |                              | $(xy, xz, yz)$                  |

| $O_h$    | $E$ | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2(=C_4^2)$ | $i$ | $6S_4$ | $8S_6$ | $3\sigma_h$ | $6\sigma_d$ |                                 |
|----------|-----|--------|--------|--------|----------------|-----|--------|--------|-------------|-------------|---------------------------------|
| $A_{1g}$ | 1   | 1      | 1      | 1      | 1              | 1   | 1      | 1      | 1           | 1           | $x^2 + y^2 + z^2$               |
| $A_{2g}$ | 1   | 1      | -1     | -1     | 1              | 1   | -1     | 1      | 1           | -1          |                                 |
| $E_g$    | 2   | -1     | 0      | 0      | 2              | 2   | 0      | -1     | 2           | 0           | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $T_{1g}$ | 3   | 0      | -1     | 1      | -1             | 3   | 1      | 0      | -1          | -1          | $(R_x, R_y, R_z)$               |
| $T_{2g}$ | 3   | 0      | 1      | -1     | -1             | 3   | -1     | 0      | -1          | 1           | $(xz, yz, xy)$                  |
| $A_{1u}$ | 1   | 1      | 1      | 1      | 1              | -1  | -1     | -1     | -1          | -1          |                                 |
| $A_{2u}$ | 1   | 1      | -1     | -1     | 1              | -1  | 1      | -1     | -1          | 1           |                                 |
| $E_u$    | 2   | -1     | 0      | 0      | 2              | -2  | 0      | 1      | -2          | 0           |                                 |
| $T_{1u}$ | 3   | 0      | -1     | 1      | -1             | -3  | -1     | 0      | 1           | 1           | $(x, y, z)$                     |
| $T_{2u}$ | 3   | 0      | 1      | -1     | -1             | -3  | 1      | 0      | 1           | -1          |                                 |



**Pemalar Asas dalam Kimia Fizik**

| Simbol               | Keterangan        | Nilai  |
|----------------------|-------------------|--|
| $N_A$                | Nombor Avogadro   | $6.022 \times 10^{23} \text{ mol}^{-1}$  |
| F                    | Pemalar Faraday   | 96,500 C mol <sup>-1</sup> , atau<br>coulomb per mol, elektron   |
| e                    | Cas elektron      | $4.80 \times 10^{-10}$ esu<br>$1.60 \times 10^{-19}$ C atau coulomb  |
| $m_e$                | Jisim elektron    | $9.11 \times 10^{-28}$ g<br>$9.11 \times 10^{-31}$ kg  |
| $m_p$                | Jisim proton      | $1.67 \times 10^{-24}$ g<br>$1.67 \times 10^{-27}$ kg  |
| h                    | Pemalar Planck    | $6.626 \times 10^{-27}$ erg s<br>$6.626 \times 10^{-34}$ J s   |
| c                    | Halaju cahaya     | $3.0 \times 10^{10}$ cm s <sup>-1</sup><br>$3.0 \times 10^8$ m s <sup>-1</sup>   |
| R                    | Pemalar gas       | $8.314 \times 10^7$ erg K <sup>-1</sup> mol <sup>-1</sup><br>$8.314$ J K <sup>-1</sup> mol <sup>-1</sup><br>$0.082$ l atm K <sup>-1</sup> mol <sup>-1</sup><br>$1.987$ cal K <sup>-1</sup> mol <sup>-1</sup> |
| k                    | Pemalar Boltzmann | $1.380 \times 10^{-16}$ erg K <sup>-1</sup> molekul <sup>-1</sup><br>$1.380 \times 10^{-23}$ J K <sup>-1</sup> molekul <sup>-1</sup>   |
| g                    |                   | 981 cm s <sup>-2</sup><br>9.81 m s <sup>-2</sup>   |
| 1 atm                |                   | 76 cmHg<br>$1.013 \times 10^6$ dyne cm <sup>-2</sup><br>101,325 N m <sup>-2</sup>  |
| $2.303 \frac{RT}{F}$ |                   | 0.0591 V, atau volt, pada 25 °C  |

**Berat Atom yang Berguna**

|            |            |            |            |            |
|------------|------------|------------|------------|------------|
| H = 1.0    | C = 12.0   | I = 126.9  | Fe = 55.8  | As = 74.9  |
| Br = 79.9  | Cl = 35.5  | Ag = 107.9 | Pb = 207.0 | Xe = 131.1 |
| Na = 23.0  | K = 39.1   | N = 14.0   | Cu = 63.5  | F = 19.0   |
| O = 16.0   | S = 32.0   | P = 31.0   | Ca = 40.1  | Mg = 24.0  |
| Sn = 118.7 | Cs = 132.9 | Te = 128.0 |            |            |