



Coláiste na Tríonóide, Baile Átha Cliath  
Trinity College Dublin

Ollscoil Átha Cliath | The University of Dublin

Faculty of Engineering, Mathematics and Science

School of Physics

Nanoscience, Physics & Chemistry of Advanced Materials

Senior Sophister

Semester 1 2018

PYU44NP5

Comprehension and Problem Solving Paper

Paper Coordinator: Professor H. Zhang

10<sup>th</sup> December 2018

RDS Simmonscourt

9:30 – 12:30

**Instructions to Candidates:**

Complete the comprehension exercise in **Section A** and **answer 6** questions from **Section B** in 3 hours.

**Section A** accounts for 40% and **Section B** accounts for 60%.

*ANSWER EACH QUESTION IN A SEPARATE ANSWER BOOK*

Tables of physical constants and relative atomic masses and a periodic table are attached.

**Materials permitted for this examination:**

Spectroscopic tables, character tables, Booklets of Formulae and Tables are available from the invigilator for all students who require them. Graph paper is also available.

Non-programmable calculators are permitted for this examination – please indicate the make and model of your calculator on each answer book used.

## SECTION A

1. Read the short paper below from [Nature 553, 163 (2018)] and then answer the following questions/exercises (a)-(d);

(a) Write a brief summary of the article (approximately 1 page).

[10 marks]

(b) What are the advantages of lead halide perovskites as efficient light emitters?

[10 marks]

(c) What are the most suitable temperatures at which to explore the material's emission? Why? Explain your reasoning.

[10 marks]

(d) Photoexcitation promotes an electron into the conduction band, leaving a 'hole' in the valence band. If the interaction between the electron and the hole is assumed to be negligible—justified when each wavefunction is spread over an expanse of atoms—then the pair are free carriers. On the other hand, an attractive Coulombic interaction between the electron and hole 'quasi-particles' binds them into an exciton. The wavefunction of the bound state is hydrogenic, akin to that of a hydrogen atom.

(i) The binding energy is given as:

$$E_n = -\frac{\mu e^4}{32\pi\hbar^2\epsilon_0^2\epsilon_r^2n^2}$$

where  $n$  is the quantum number ( $n = 1$ , ground state) and  $\mu = \frac{m_e \cdot m_h}{m_e + m_h}$ .

Is the binding energy close to that of a hydrogen atom?

(where  $\mu = m_e, \epsilon_r = 1$  and  $E_1 = -13.6$  eV)? Why/Why not?

(ii) The Bohr radius (the most probable distance between the nucleus and the electron in a hydrogen atom in its ground state) is

$$a_1 = \frac{4\pi\epsilon_0\epsilon_r\hbar^2}{m_e e^2} \cong 0.53 \text{ \AA}$$

Estimate the size of an exciton.

[10 marks]

of RNA that binds to both the enzyme and the target DNA<sup>9</sup>. This approach is also known as CRISPR–Cas gene editing. The guide RNA matches the mutant but not the wild-type gene, enabling Gao and colleagues to solve the problem of ensuring that the mutant form of the gene is cut whereas the wild-type version is left untouched.

Another challenge was to get Cas9 into the inner ear. *In vivo* gene-editing approaches often rely on viruses to introduce nuclease-encoding sequences into the organism being edited<sup>10,11</sup>. However, Gao and colleagues reasoned that, when the nuclease has done its job in the cell, it will no longer be required, so introducing the protein itself should suffice. They turned to a technique they had used previously<sup>12</sup>, in which they packaged Cas9 protein bound to its guide RNA in a type of lipid droplet that can fuse with cells, enabling the editing machinery to enter. The authors injected these droplets into the inner ear of newborn Beethoven mice.

The inner ears of unedited adult Beethoven mice were barren of hair cells; however, their gene-edited adult siblings had inner-ear hair cells that were almost indistinguishable in shape and number from those in wild-type mice. The edited animals could be startled by a sudden loud noise, whereas their unedited siblings could not. More-sophisticated measurements also confirmed that hearing improved as a result of gene editing. Encouragingly, the engineered nuclease seems to have stayed true to its design and did not create undesired genetic changes of concern in the DNA of the hair cells.

A modest fraction of cells were edited. The authors propose that this low proportion of edited cells resulted in a beneficial ‘halo’-like effect on neighbouring unedited cells that still contained the mutant form of the gene, preventing the death and degeneration of these neighbouring cells. Although the mechanism underlying this proposed halo effect is unclear, the finding offers encouragement for the clinical adoption of this approach, because it suggests that the genetic repair of all hair cells is perhaps not needed to achieve a beneficial effect on hearing.

Gao and colleagues’ work provides an essential first step towards moving this type of approach nearer to the clinic by providing evidence that it is safe and effective in an animal that has a similar genetic mutation and comparable hearing loss to those in humans. How long could it be before individuals with this *TMC1* mutation might be treated using gene editing? One reason for optimism comes from the pace at which other gene-editing approaches have reached the clinic.

To give just a few examples from clinical trials, the gene *CCR5* has been inactivated in immune-system cells using a type of enzyme called a zinc-finger nuclease to try to reduce the viral load in people infected with

HIV<sup>13</sup>. Immune cells have also been edited to generate cancer-targeting cells<sup>14</sup>. However, these techniques required cells to be removed from the patient’s body for gene editing and then replaced. Ear cells cannot be removed, so a direct *in vivo* approach is needed, which is even more challenging to achieve than *ex vivo* gene editing.

Encouragingly, such *in vivo* gene editing (for a different condition) has been performed in a clinical trial using zinc-finger nucleases<sup>15</sup>, and the work leading up to that<sup>16</sup> makes clear the next steps for Gao and colleagues’ approach. A nuclease must be found that has clinical-grade potency and specificity in human cells. Lipids must be identified that can be safely injected along with the nuclease into the human inner ear. Next, this nuclease must be tested for safety in larger animals, such as primates. An *in vivo* virus-based gene therapy for direct injection into the eye<sup>17</sup> has been recommended for approval in the United States, and that work provides a road map for the scientific, medical and commercial considerations that need to be taken into account when moving to the clinic.

In 1902, the physician Archibald Garrod initiated the first study that demonstrated a link between a gene and a disease. Since then, more than 5,000 diseases have been linked to single-gene changes. However, without the tools to modify disease-causing forms of genes, geneticists have often been unable to see their knowledge put to use for clinical benefit. The

progress being made with genome editing is changing this. Although Beethoven never heard his famous *Ode to Joy*, it could be that — thanks in no small part to his murine namesake’s fateful encounter with Cas9 — we are getting closer to the day when individuals with deafness-causing mutations can be treated by gene editing to prevent hearing loss. ■

Fyodor Urnov is at the Altius Institute for Biomedical Sciences, Seattle, Washington 98121, USA.

e-mail: urnov@altius.org

1. Gao, X. *et al.* *Nature* **553**, 217–221 (2018).
2. Fettiplace, R. & Kim, K. X. *Physiol. Rev.* **94**, 951–986 (2014).
3. Kawashima, Y. *et al.* *J. Clin. Invest.* **121**, 4796–4809 (2011).
4. Kurima, K. *et al.* *Nature Genet.* **30**, 277–284 (2002).
5. Zhao, Y. *et al.* *PLoS ONE* **9**, e97064 (2014).
6. Vreugde, S. *et al.* *Nature Genet.* **30**, 257–258 (2002).
7. Pan, B. *et al.* *Neuron* **79**, 504–515 (2013).
8. Carroll, D. *Annu. Rev. Biochem.* **83**, 409–439 (2014).
9. Jiang, F. & Doudna, J. A. *Annu. Rev. Biophys.* **46**, 505–529 (2017).
10. Li, H. *et al.* *Nature* **475**, 217–221 (2011).
11. Ran, F. A. *et al.* *Nature* **520**, 186–191 (2015).
12. Zuris, J. A. *et al.* *Nature Biotechnol.* **33**, 73–80 (2014).
13. Tebas, P. *et al.* *N. Engl. J. Med.* **370**, 901–910 (2014).
14. Qasim, W. *et al.* *Sci. Transl. Med.* **9**, eaaj2013 (2017).
15. <https://clinicaltrials.gov/ct2/show/NCT03041324>
16. Sharma, R. *et al.* *Blood* **126**, 1777–1784 (2015).
17. Russell, S. *et al.* *Lancet* **390**, 849–860 (2017).

This article was published online on 20 December 2017.

#### MATERIALS SCIENCE

## Rule-breaking perovskites

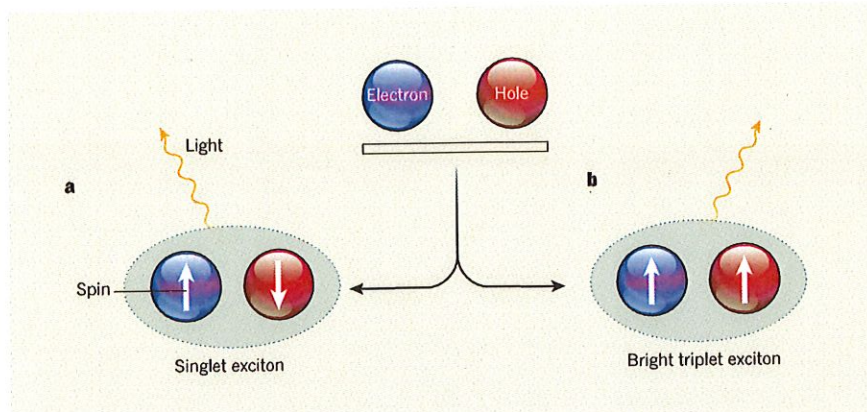
**A material from the perovskite family of semiconductors emits light much more efficiently than expected. The explanation for this anomalous behaviour could lead to improvements in light-emitting technology. SEE LETTER P.189**

MICHELE SABA

When a semiconductor absorbs light, a particle-like entity called an exciton can be produced. Excitons comprise an electron and a hole (the absence of an electron), and have two possible states: singlet and triplet. Triplet states were thought to be poor emitters of light, but, on page 189, Becker *et al.*<sup>1</sup> report that semiconductors known as lead halide perovskites have bright triplet excitons. The results could signify a breakthrough in optoelectronics because triplet states are three times more abundant than singlet states<sup>2</sup> and currently limit the efficiency of organic light-emitting diodes<sup>3</sup>.

Conventional wisdom holds that triplet states are dark because of the spin selection rule<sup>4</sup>, which forbids electrons from changing their intrinsic angular momentum (spin) during an optical transition — the process in which an atom or molecule switches from one energy state to another by emitting or absorbing light. The rule is taught in quantum-mechanics classes when atomic transitions are first introduced, and is so general that one might think that it is written in stone. Fortunately, there are loopholes that can be exploited.

The search for emissive triplet states has focused on a certain principle of quantum mechanics: if an electron’s spin is coupled



**Figure 1 | Exciton emission.** Semiconductors contain electrons and holes (absences of electrons) that can combine to form bound states called excitons. **a**, In singlet excitons, the intrinsic angular momenta (spins) of the electron and the hole point in opposite directions, which facilitates the emission of light. **b**, Conversely, in triplet excitons, the spins point in the same direction. Conventional wisdom holds that such states are dark, but Becker *et al.*<sup>1</sup> report that semiconductors known as lead halide perovskites emit light through bright triplet excitons.

to another form of angular momentum (namely, orbital momentum), the sum of the two momenta needs to be conserved, rather than the spin alone. The effect is known as spin-orbit coupling in atomic physics and as intersystem crossing in the study of organic semiconductors. It is responsible for weak emission from triplet states in atoms and organic molecules, especially when heavy elements are involved. However, until now, the strength of triplet emission was thought always to be inferior to that of singlet emission.

Lead halide perovskites seem to dispose of all conventional wisdom in materials science. Like organic semiconductors, they are relatively easy to fabricate, and their bandgap (a property that determines their conductivity and optical properties) can be tuned by varying their composition. Yet, like thin-layer (epitaxial) inorganic semiconductors, they are highly crystalline and exhibit efficient charge transport. It is as if their properties were selected from a materials scientist's wish list, combining the best aspects of organic molecules, nanocrystals and epitaxial inorganic semiconductors.

Becker and colleagues' study suggests that there is another feature of lead halide perovskites to be added to this list. The authors used a combination of theoretical and experimental work to show that nanocrystals of caesium lead halide perovskites ( $\text{CsPbX}_3$ , where X is chlorine, bromine or iodine) have bright triplet excitons (Fig. 1). This property results in an emission rate surpassing that of other known nanocrystals<sup>5</sup>.

The energy difference between the triplet and singlet states in  $\text{CsPbX}_3$  nanocrystals is relatively small (of the order of 1 millielectronvolt). Becker *et al.* therefore explored the material's emission at cryogenic temperatures (a few kelvin), to prevent

transitions between triplet and singlet states. It is unclear to what extent bright triplet states affect the material's emission efficiency at room temperature — when thermal energy greatly exceeds the singlet-triplet splitting energy and all states are equally populated. Nevertheless, the authors' findings are of fundamental relevance.

Future work will certainly investigate whether bright triplet states exist in other types of perovskite, such as hybrid perovskites that have organic, positively charged ions (cations). Such materials include the archetypal methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ), and are typically prepared not as nanocrystals, but as solid-state films<sup>6</sup>. Unlike  $\text{CsPbX}_3$  nanocrystals, these films comprise micrometre- or millimetre-sized crystalline domains, in which excitons dissociate into pairs of free electrons and holes at room temperature. More generally, Becker and colleagues' theoretical analysis might help scientists to identify other semiconducting materials (either organic or inorganic) that have bright triplet excitons.

Research into hybrid perovskites has been fuelled in the past few years by the successful incorporation of these materials into solar cells. Such devices can now convert more than 22% of the energy received from sunlight into electricity<sup>7</sup>, which is a record for perovskite solar cells. However, because of a concept known as quantum-mechanical reciprocity, there is an unavoidable energy loss in solar cells: that due to photoluminescence, which is the reverse of the absorption process<sup>8</sup>. As a consequence, the best solar cells are also the

best light emitters — an idea reinforced by Becker and colleagues' work.

Perovskite solar cells are now leaving academic labs and entering the market, thanks to substantial industrial efforts. The competition is mainly silicon solar cells, which have become so cheap that they negate some of the advantages of perovskite fabrication. For this reason, tandem solar cells (consisting of two sub-cells) and innovative architectures involving perovskites are being developed that can outperform commercial silicon devices in terms of efficiency, if not cost<sup>9</sup>.

Light emission is an application in which organic semiconductors and nanocrystals have already found commercial success, because of their ability to produce vivid colours and to be incorporated into thin panels. And yet the electric-current densities in organic light-emitting diodes are much lower than in their inorganic counterparts as a result of poor electrical conductivity. Perovskites could allow high current densities and efficiencies to be realized on large-area, thin panels<sup>10</sup>.

Becker and colleagues' study highlights the potential of perovskite materials as efficient light emitters. Although the findings might seem surprising at first sight, they should be seen as a natural consequence of quantum-mechanical reciprocity — that the class of material brought to the forefront by solar-cell technology could find applications in light emission. ■

Michele Saba is in the Department of Physics, University of Cagliari, I-09042 Monserrato, Italy.

e-mail: saba@unica.it

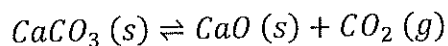
1. Becker, M. A. *et al.* *Nature* **553**, 189–193 (2018).
2. Pope, M. & Swenberg, C. E. *Electronic Processes in Organic Crystals* (Oxford Univ. Press, 1999).
3. Reineke, S., Thomschke, M., Lüssem, B. & Leo, K. *Rev. Mod. Phys.* **85**, 1245–1293 (2013).
4. Demtröder, W. *Atoms, Molecules and Photons* (Springer, 2010).
5. Rainò, G. *et al.* *ACS Nano* **10**, 2485–2490 (2016).
6. Stoumpos, C. C. & Kanatzidis, M. G. *Acc. Chem. Res.* **48**, 2791–2802 (2015).
7. Correa-Baena, J.-P. *et al.* *Science* **358**, 739–744 (2017).
8. Rau, U. *Phys. Rev. B* **76**, 085303 (2007).
9. Eperon, G. E., Hörantner, M. T. & Snaith, H. J. *Nature Rev. Chem.* **1**, 0095 (2017).
10. Colella, S., Mazzeo, M., Rizzo, A., Gigli, G. & Listorti, A. *J. Phys. Chem. Lett.* **7**, 4322–4334 (2016).

#### CORRECTION

The News & Views article 'Cancer: Tumour lymph vessels boost immunotherapy' by Christine Mousson and Shannon J. Turley (*Nature* **552**, 340–342; 2017) cited reference 2 incorrectly. The correct reference is: S. L. Topalian, C. G. Drake & D. M. Pardoll *Cancer Cell* **27**, 450–461 (2015).

## SECTION B

1. Calcium carbonate decomposes according to the reaction below.

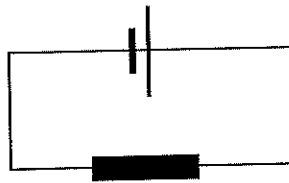


	$\Delta_f G^\circ$ (kJ mol <sup>-1</sup> ) @298 K	$\Delta_f G^\circ$ (kJ mol <sup>-1</sup> ) @1000 K
CaCO <sub>3</sub> (s)	-1129	-951.2
CaO (s)	-604	-531.1
CO <sub>2</sub> (g)	-394.5	-395.8

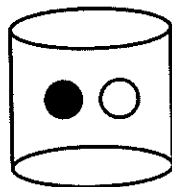
- (a) Use the thermodynamic data in the table to calculate the equilibrium constant  $K$  for this reaction at  $T = 298$  K.  
[2 marks]
- (b) Calculate  $\Delta H^\circ$  and  $\Delta S^\circ$  for the decomposition reaction; assume that their values remain constant over the interval 298-1000 K.  
[2 marks]
- (c) 0.010 mol of CaCO<sub>3</sub> and 0.020 mol of CaO are placed in an empty 10.0 L sealed container and heated to 1000 K. Calculate the pressure in the container and the mass of CaCO<sub>3</sub> and CaO obtained at equilibrium.  
[4 marks]
- (d) If an additional 0.1 bar of CO<sub>2</sub> are pumped into the container, what is the final mass of CaCO<sub>3</sub> and CaO after equilibrium is re-established?  
[2 marks]

2. For each of the following situations, state whether the given integrals over electric and/or magnetic fields ( $\vec{E}$  and  $\vec{B}$ ) are zero or non-zero and explain your reasoning. Some of the situations require a careful answer.

(a) An electric circuit containing a battery and a resistor, as shown below, has a steady current flowing. Consider  $\oint \vec{E} \cdot d\vec{\ell}$  for an integration loop which passes through the centre of the wire, the resistor and the battery i.e. along the centre of the circuit.

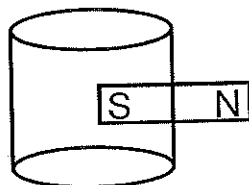


(b) Two charges (one positive, one negative and of equal magnitude) are placed a small distance apart inside a cylindrical closed surface ('pill box'). Evaluate  $\int \vec{E} \cdot d\vec{S}$  integrated over the entire surface of the pill box. The charges are stationary.



(c) Now one of the charges in part (b) rotates at constant velocity about a vertical axis so that it executes horizontal circles inside the closed surface. State whether  $\int \vec{B} \cdot d\vec{S}$  over the top (circular) surface of the pill box and  $\oint \vec{E} \cdot d\vec{\ell}$  along the edge of the top surface are zero or not.

(d) A bar magnet is arranged so that its south pole is inside a cylindrical closed surface and its north pole is outside. Evaluate  $\int \vec{B} \cdot d\vec{S}$  integrated over the entire surface.



[10 marks]

3. (a) A solution of spherical 25 nm radius polystyrene nanoparticles is given as 10 % nanoparticles by volume. Calculate the number of nanoparticles in 1 mL of solution.

[5 marks]

- (b) The 25 nm radius polystyrene nanoparticles are diluted in a solution containing 100 mM NaCl. This colloidal suspension is observed to be unstable, with the nanoparticles quickly coagulating. Discuss strategies for stabilizing this colloidal suspension.

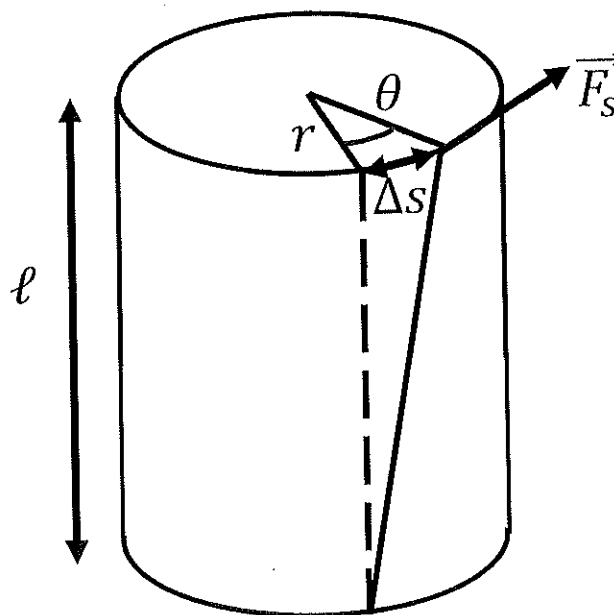
[5 marks]

4. (a) A force, shown as  $F_s$  here, produces a torsional deformation of a solid cylinder. Show that the torque about the top surface of the cylinder is given by:

$$\tau = \frac{\pi r^4 G \theta}{2 \ell}$$

where  $G$  is the shear modulus of the cylinder.

- (b) In a skiing accident, a shear force of  $10^4$  N is applied to a femoral bone. The radius of the bone is 1 cm, the shear modulus of bone is  $1 \times 10^9$  N m<sup>-2</sup> and the largest strain that the bone can withstand before fracture is 0.01. Show whether or not the bone will fracture.



**Hint:** Remember that an elastic modulus is stress divided by strain.

[10 marks]

5. Consider a molecular solid with a simple six-coordinate cubic lattice ( $a = b = c$ ) described by the pair interaction potential  $w(r)$ :

$$w(r) = -A/r^6 + B/r^{12}, \quad \text{where } A = 1 \times 10^{-78} \text{ J m}^6 \text{ and } B = 2 \times 10^{-136} \text{ J m}^{12}$$

Assuming only nearest neighbor interactions, calculate the following:

- (a) The molar cohesive energy of this molecular solid
- (b) The surface energy of the (110) facet of this molecular solid

[10 marks]

6. After diffusing impurities into a particular semiconductor, the density of a given impurity  $p(x)$  at a distance  $x$  below the surface varies according to

$$p(x) = \left(\frac{0.8}{l}\right) \exp\left[-\frac{x}{l}\right] + 0.2\delta(x - d) \quad x \geq 0$$

$$p(x) = 0 \quad x < 0$$

where  $d$  and  $l$  are two distances. The delta function arises because a fraction of the impurities have, during the diffusion process, become trapped on an accidental grain boundary at a distance  $d$  below the surface.

- (a) Make a carefully labelled sketch of the fraction of *cumulative total impurities* to be found at a distance  $x$  from the surface which displays all of its important features. [You do not need to give an analytic expression for this functional]
- (b) Find the mean depth of an impurity i.e. the mean value of  $x$ .
- (c) Characterise the spread in impurities by finding the variance of  $x$ .

[10 marks]



7. CO adsorbs with different characteristics on the {100} surface of two different fcc metals as detailed in the table below. Sketch a possible surface structure for each of the surfaces and explain the data.

Surface	Surface coverage $\theta$	Vibrational frequency	Work function change relative to clean surface
A	0.25	1846 $\text{cm}^{-1}$	0.5 eV
B	0.50	2088 $\text{cm}^{-1}$	-0.5 eV

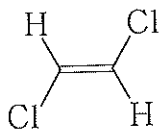
[10 marks]

8. A particle has only two possible quantum states, one of energy  $0$  and one of energy  $\epsilon$ . The particle is in thermal contact with a reservoir at temperature  $T$ .

- Write down the partition function of the two states of this particle
- Evaluate the mean (internal) energy  $U$  as a function of  $T$
- Compute the heat capacity at constant volume,  $C_V$ .
- When a plot of  $C_V$  vs. temperature is made, a single peak is observed to occur. Can you explain *physically* why such a peak should occur?

[10 marks]

9. Trans 1,2-dichloroethene belongs to the  $C_{2h}$  point group



- (a) Use group theory to determine the representations capturing all modes of motion.

- (b) Identify the modes of motions corresponding to vibrations and in each case state whether the vibration is (i) IR active and (ii) Raman active.

[10 marks]

10. A 50 mm diameter, 200 mm long solenoid is made by closely winding 1 mm diameter copper wire. The magnetic field at the centre of a solenoid is given by  $B = \mu_0 n I$ , where  $n$  is the number of turns per unit length and  $I$  is the current.

- (a) Calculate the magnetic field at the centre of the solenoid when the current is 1000 A.

- (b) Calculate the tension in the coil for 1000 A. Hint: it may be useful to consider the forces acting on a short section of wire.

- (c) Given that the tensile strength of copper is  $2 \times 10^8 \text{ N m}^{-2}$ , at what value of current will the coil break?

[10 marks]

11. How would you prepare silicon rubber starting from dichloromethylvinylsilane and dichloromethylsilane? Draw schemes of the relevant chemical processes.

[10 marks]

12. The total wavefunction of the 1s electron in a hydrogen atom has the spherically symmetric form

$$\Psi_{1s} = 2 \left( \frac{1}{a_0} \right)^{\frac{3}{2}} e^{-r/a_0}$$

where  $a_0$  is the Bohr radius and is given by  $a_0 = 0.0529 \text{ nm}$

Calculate the *most probable radial distance* of the electron from the hydrogen nucleus (proton) and the *mean radial distance* of the electron from the nucleus. Explain any difference in these values by a sketch or otherwise.

Hint: (a) Define  $P(r)$  as the probability of finding the electron at a radius  $r$  from the nucleus. (b) The expectation value may be given by:  $\langle r \rangle = \int_0^\infty r \frac{dP(r)}{dr} dr$   
(c) Integration by parts is given by  $\int u dv = uv - \int v du$  with appropriate choice of  $u$  and  $v$ .

[10 marks]

Use the following values for fundamental constants, conversion factors, relative atomic masses and other data for examination purposes:

### Constants

Gas Constant	$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$
Boltzmann's Constant	$k_B = 1.381 \times 10^{-23} \text{ J K}^{-1}$
Planck's Constant	$h = 6.626 \times 10^{-34} \text{ J s}$
	$\hbar = h/2\pi = 1.055 \times 10^{-34} \text{ J s}$
Velocity of light	$c = 2.998 \times 10^8 \text{ m s}^{-1}$
Charge of electron	$e = -1.602 \times 10^{-19} \text{ C}$
Rest mass of electron	$m_e = 9.109 \times 10^{-31} \text{ kg}$
Rest mass of proton	$m_p = 1.673 \times 10^{-27} \text{ kg}$
Atomic Mass Unit	$1 \text{ u} = 1.66054 \times 10^{-27} \text{ kg}$
Vacuum permittivity	$\epsilon_0 = 8.854 \times 10^{-12} \text{ J}^{-1} \text{ C}^2 \text{ m}^{-1}$
Vacuum permeability	$\mu_0 = 4\pi \times 10^{-7} \text{ J s}^2 \text{ C}^{-2} \text{ m}^{-1}$
Bohr magneton	$\beta = 9.274 \times 10^{-24} \text{ J T}^{-1}$
Nuclear magneton	$\beta_n = 5.051 \times 10^{-27} \text{ J T}^{-1}$
Rydberg constant	$R_\infty = 2.178 \times 10^{-18} \text{ J} = 1.097 \times 10^5 \text{ cm}^{-1}$
Avogadro's constant	$N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$
Faraday constant	$F = N_A e = 9.648 \times 10^4 \text{ C mol}^{-1}$
Bohr radius	$a_0 = 5.292 \times 10^{-11} \text{ m}$
Molar volume at S.T.P.	$M_v = 22.414 \text{ dm}^3 \text{ mol}^{-1}$

### Conversion factors etc.

$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J} = 9.648 \times 10^4 \text{ J mol}^{-1}$
$1 \text{ cm}^{-1} = 1.986 \times 10^{-23} \text{ J} = 11.96 \text{ J mol}^{-1} = 1.240 \times 10^{-4} \text{ eV}$
$1 \text{ \AA} = 0.1 \text{ nm} = 10^{-10} \text{ m}$
$1 \text{ standard atmosphere} = 1.013 \times 10^5 \text{ N m}^{-2} \text{ (Pa)} = 760 \text{ torr} = 1013 \text{ mbar}$
$1 \text{ L} = 1 \text{ dm}^3 = 10^{-3} \text{ m}^3$
$1 \text{ Debye (D)} = 3.336 \times 10^{-30} \text{ C m}$
$1 \text{ calorie} = 4.184 \text{ J}$
$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 8.206 \times 10^{-2} \text{ L atm K}^{-1} \text{ mol}^{-1}$

### Approximate values of relative atomic masses

(Values in brackets are mass numbers of longest lived isotopes).

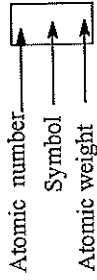
Ac (227)	Ge 72.6	Po (209)
Ag 107.9	H 1.0	Pr 140.9
Al 27.0	He 4.0	Pt 195.1
Am (243)	Hf 178.5	Pu (244)
Ar 40.0	Hg 200.6	Ra (226)
As 74.9	Ho 164.9	Rb 85.5
At (210)	I 126.9	Re 186.2
Au 197.0	In 114.8	Rh 102.9
B 10.8	Ir 192.2	Rn (222)
Ba 137.3	K 39.1	Ru 101.1
Be 9.0	Kr 83.8	S 32.0
Bi 209.0	La 138.9	Sb 121.8
Bk (247)	Li 6.9	Sc 45.0
Br 79.9	Lu 175.0	Se 79.0
C 12.0	Lw (257)	Si 28.1
Ca 40.1	Md (258.1)	Sm 150.4
Cd 112.4	Mg 24.3	Sn 118.7
Ce 140.1	Mn 54.9	Sr 87.6
Cf (242.1)	Mo 95.9	Ta 180.9
Cl 35.5	N 14.0	Tb 158.9
Cm (247)	Na 23.0	Tc (97.9)
Co 58.9	Nb 92.9	Te 127.6
Cr 52.0	Nd 144.2	Tl 204.4
Cs 132.9	Ne 20.2	Th 232.0
Cu 63.5	Ni 58.7	Ti 47.9
Dy 162.5	No (259.1)	Tm 168.9
Er 167.3	Np (237)	U 238.0
Es (252.1)	O 16.0	V 50.9
Eu 152.0	Os 190.2	W 183.9
F 19.0	P 31.0	Xe 131.3
Fe 55.9	Pa (231)	Y 88.9
Fm (257)	Pb 207.2	Yb 173.0
Fr (223)	Pd 106.4	Zn 65.4
Ga 69.7	Pm (145)	Zr 91.2
Gd 157.3		

# The Periodic Table of the Elements

18

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																																																
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																																																
H 1.0079	He 4.0026	Li 6.941	Be 9.01218	Na 22.98977	Mg 24.305	Al 26.9815	Si 28.0855	P 30.9738	S 32.06	Cl 35.453	Ar 39.948	K 39.0983	Ca 40.08	Sc 44.9559	Ti 47.88	V 50.9415	Cr 51.996	Mn 54.938	Fe 55.847	Co 58.9332	Ni 58.69	Cu 63.546	Zn 65.38	Ga 69.72	Ge 72.59	As 74.9216	Se 78.96	Br 79.904	Kr 83.80	Rb 85.4678	Sr 87.62	Y 88.9059	Zr 91.22	Nb 92.9064	Mo 95.94	Tc (97.9)	Ru 101.07	Rh 102.9055	Pd 106.42	Ag 107.868	Cd 112.41	In 114.82	Sn 118.69	Sb 121.75	Te 127.60	I 126.9045	Xe 131.29	Cs 132.9054	Ba 137.33	#La 138.9055	Hf 178.49	Ta 180.9479	W 183.85	Re 186.207	Os 190.2	Ir 192.22	Pt 195.08	Au 196.9665	Hg 200.59	Tl 204.383	Pb 207.2	Bi 208.9804	Po (209)	At (210)	Rn (222)
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																																																
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54																																																
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86																																																
87	88	89	89	*Ac 227.0278	Fr (223)	Ra 226.025	Ba 137.33	#La 138.9055	Hf 178.49	Ta 180.9479	W 183.85	Re 186.207	Os 190.2	Ir 192.22	Pt 195.08	Au 196.9665	Hg 200.59	Tl 204.383	Pb 207.2	Bi 208.9804	Po (209)	At (210)	Rn (222)																																										

Key



( ) mass numbers of most stable isotope

## # LANTHANUM SERIES

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce 140.12	Pr 140.9077	Nd 144.24	Pm (145)	Sm 150.36	Eu 151.96	Gd 157.25	Tb 158.9254	Dy 162.50	Ho 164.9304	Er 167.26	Tm 168.9342	Yb 173.04	Lu 174.967

## \* ACTINIUM SERIES

90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th 232.0381	Pa 231.0359	U 238.0389	Np 237.0482	Pu (244)	Am (243)	Cm (247)	Bk (247)	Cf (242.1)	Es (254)	Fm (257)	Md (258.1)	No (259.1)	Lr (260)

# APPENDIX A

## Point Group Character Tables

### 1. The Nonaxial Groups

$C_1$	$E$
$A$	1

$C_s$	$E$	$\sigma_h$	
$A'$	1	1	$x, y, R_z$ $x^2, y^2, z^2, xy$
$A''$	1	-1	$z, R_x, R_y$ $yz, xz$

$C_i$	$E$	$i$	
$A_g$	1	1	$R_x, R_y, R_z$ $x^2, y^2, z^2, xy, xz, yz$
$A_u$	1	-1	$x, y, z$

### 2. 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	$x, y, R_x, R_y$ $yz, xz$

$C_3$	$E$	$C_3$	$C_3^2$	
$A$	1	1	1	$z, R_z$ $x^2 + y^2, z^2$
$E$	$\begin{bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{bmatrix}$	$\epsilon$	$\epsilon^*$	$(x, y), (R_x, R_y)$ $(x^2 - y^2, xy), (yz, xz)$

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

$D_3$	$E$	$2C_3$	$3C_2$	$x^2 + y^2, z^2$
$A_1$	1	1	1	$x^2 + y^2, z^2$
$A_2$	1	1	-1	$z, R_z$
$E$	2	-1	0	$(x^2 - y^2, xy), (xz, yz)$

$D_4$	$E$	$2C_4$	$C_2 (= C_4^2)$	$2C_2'$	$2C_2''$	$x^2 + y^2, z^2$
$A_1$	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	$(xz, yz)$

$D_5$	$E$	$2C_5$	$2C_3$	$2C_2$	$5C_2$	$x^2 + y^2, z^2$
$A_1$	1	1	1	1	1	$x^2 + y^2, z^2$
$A_2$	1	1	1	1	-1	$z, R_z$
$E_1$	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	$2 \cos 144^\circ$	0	$(xz, yz)$
$E_2$	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	$2 \cos 72^\circ$	0	$(x^2 - y^2, xy)$

$D_6$	$E$	$2C_6$	$2C_3$	$C_2$	$3C_2'$	$3C_2''$	$x^2 + y^2, z^2$
$A_1$	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	$(xz, yz)$
$E_2$	2	-1	-1	2	0	0	$(x^2 - y^2, xy)$

4. The  $C_{nv}$  Groups

$C_{2v}$	$E$	$C_2$	$\sigma_v(xz)$	$\sigma_v(yz)$	$x^2, y^2, z^2$
$A_1$	1	1	1	1	$x^2, y^2, z^2$
$A_2$	1	1	-1	-1	$xy$
$B_1$	1	-1	1	-1	$xz$
$B_2$	1	-1	-1	1	$yz$

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

3. The  $D_n$  Groups

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

$C_5$	$E$	$C_5$	$C_5^2$	$C_5^3$	$C_5^4$	$\epsilon = \exp(2\pi i/5)$
$A$	1	1	1	1	1	$x^2 + y^2, z^2$
$E_1$	1	$\epsilon$	$\epsilon^2$	$\epsilon^4$	$\epsilon^3$	$(yz, xz)$
$E_2$	1	$\epsilon^2$	$\epsilon^4$	$\epsilon$	$\epsilon^3$	$(x^2 - y^2, xy)$

$C_6$	$E$	$C_6$	$C_3$	$C_2$	$C_3^2$	$C_6^5$	$\epsilon = \exp(2\pi i/6)$
$A$	1	1	1	1	1	1	$x^2 + y^2, z^2$
$B$	1	-1	1	-1	1	-1	$z, R_z$
$E_1$	1	$\epsilon$	$\epsilon^2$	$\epsilon^4$	$\epsilon^5$	$\epsilon^3$	$(xz, yz)$
$E_2$	1	$\epsilon^2$	$\epsilon^4$	$\epsilon$	$\epsilon^5$	$\epsilon^3$	$(x^2 - y^2, xy)$

$C_7$	$E$	$C_7$	$C_7^2$	$C_7^3$	$C_7^4$	$C_7^5$	$C_7^6$	$\epsilon = \exp(2\pi i/7)$
$A$	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$E_1$	1	$\epsilon$	$\epsilon^2$	$\epsilon^4$	$\epsilon^6$	$\epsilon^5$	$\epsilon^3$	$z, R_z$
$E_2$	1	$\epsilon^2$	$\epsilon^4$	$\epsilon^6$	$\epsilon^5$	$\epsilon^3$	$\epsilon$	$(xz, yz)$
$E_3$	1	$\epsilon^3$	$\epsilon^6$	$\epsilon$	$\epsilon^5$	$\epsilon^2$	$\epsilon^4$	$(x^2 - y^2, xy)$

$C_8$	$E$	$C_8$	$C_4$	$C_8^3$	$C_2$	$C_8^5$	$C_4^3$	$C_8^7$	$\epsilon = \exp(2\pi i/8)$
$A$	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$B$	1	-1	1	-1	1	-1	1	-1	$z, R_z$
$E_1$	1	$\epsilon$	$\epsilon^2$	$\epsilon^4$	$\epsilon^6$	$\epsilon^5$	$\epsilon^3$	$\epsilon$	$(xz, yz)$
$E_2$	1	$\epsilon^2$	$\epsilon^4$	$\epsilon^6$	$\epsilon^5$	$\epsilon^3$	$\epsilon$	$\epsilon^2$	$(x^2 - y^2, xy)$
$E_3$	1	$\epsilon^3$	$\epsilon^6$	$\epsilon$	$\epsilon^5$	$\epsilon^2$	$\epsilon^4$	$\epsilon^3$	



$C_{4v}$	E	$2C_4$	$C_2$	$2\sigma_v$	$2\sigma_d$	
$A_1$	1	1	1	1	1	$z$
$A_2$	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	$(xz, yz)$

$C_{3v}$	E	$2C_3$	$3\sigma_v$	$5\sigma_v$	
$A_1$	1	1	1	1	$z$
$A_2$	1	1	-1	-1	$R_z$
$E_1$	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x, y), (R_x, R_y)$
$E_2$	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	$(x^2 + y^2, z^2)$ $(xz, yz)$ $(x^2 - y^2, xy)$

$C_{6v}$	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	$x^2 + y^2, z^2$
$B_2$	1	-1	1	-1	1	1	$(xz, yz)$
$E_1$	2	1	-1	-2	0	0	$(x, y), (R_x, R_y)$
$E_2$	2	-1	-1	2	0	0	$(x^2 - y^2, xy)$

5. The  $C_{nh}$  Groups

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

$C_{3h}$	E	$C_3$	$C_2$	$\sigma_h$	$S_6^5$	$S_3$	
$A'$	1	1	1	1	1	1	$R_z$
$E'$	2	$\epsilon$	$\epsilon^*$	1	$\epsilon$	$\epsilon^*$	$(x, y)$
$A''$	1	1	1	-1	-1	-1	$z$
$E''$	2	$\epsilon$	$\epsilon^*$	-1	$\epsilon$	$\epsilon^*$	$(R_x, R_y)$

$C_{4h}$	E	$C_4$	$C_2$	$C_4^3$	$i$	$S_4^3$	$\sigma_h$	$S_4$	$S_2$	
$A_g$	1	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$B_g$	1	-1	1	-1	1	-1	1	-1	-1	$x^2 - y^2, xy$
$E_g$	2	$i$	-1	$-i$	1	$i$	-1	$-i$	$i$	$(xz, yz)$
$A_u$	1	1	1	1	-1	-1	-1	-1	-1	$z$
$B_u$	1	-1	1	-1	-1	1	1	1	1	$(x, y)$
$E_u$	2	$i$	-1	$-i$	-1	$-i$	1	$i$	$-i$	

$C_{5h}$	E	$C_5$	$C_2$	$C_5^3$	$C_4$	$\sigma_h$	$S_5^4$	$S_5^3$	$S_2$	$S_5^2$	
$A'$	1	1	1	1	1	1	1	1	1	1	$R_z$
$E_1'$	4	$\epsilon$	$\epsilon^*$	$\epsilon^2$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon^2$	$\epsilon$	$\epsilon^*$	$(x, y)$
$E_2'$	4	$\epsilon^2$	$\epsilon$	$\epsilon^*$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon$	$z$
$A''$	1	1	1	1	-1	-1	-1	-1	-1	-1	$(R_x, R_y)$
$E_1''$	4	$\epsilon$	$\epsilon^*$	$\epsilon^2$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon^2$	$\epsilon$	$\epsilon^*$	$(xz, yz)$
$E_2''$	4	$\epsilon^2$	$\epsilon$	$\epsilon^*$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon$	$\epsilon^*$	$\epsilon$	$(x^2 - y^2, xy)$

$C_{6h}$	E	$C_6$	$C_3$	$C_2$	$C_3^2$	$C_6^5$	$i$	$S_6^5$	$\sigma_h$	$S_6^4$	$S_6^3$	$S_2$	
$A_g$	1	1	1	1	1	1	1	1	1	1	1	1	$R_z$
$B_g$	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	$(R_x, R_y)$
$E_{1g}$	2	$\epsilon$	$\epsilon^*$	-1	$\epsilon^*$	$\epsilon$	1	$\epsilon^*$	-1	$\epsilon$	$\epsilon^*$	$\epsilon$	$z$
$E_{2g}$	2	$\epsilon^2$	$\epsilon$	-1	$\epsilon^*$	$\epsilon$	1	$\epsilon^*$	-1	$\epsilon$	$\epsilon^*$	$\epsilon$	$(x^2 - y^2, xy)$
$A_u$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	$z$
$B_u$	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	$(x, y)$
$E_{1u}$	2	$\epsilon$	$\epsilon^*$	-1	$\epsilon^*$	$\epsilon$	-1	$\epsilon^*$	1	$\epsilon$	$\epsilon^*$	$\epsilon$	$(R_x, R_y)$
$E_{2u}$	2	$\epsilon^2$	$\epsilon$	-1	$\epsilon^*$	$\epsilon$	-1	$\epsilon^*$	1	$\epsilon$	$\epsilon^*$	$\epsilon$	$(x^2 - y^2, xy)$

6. 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	$R_z$
$B_{2g}$	1	-1	1	-1	1	-1	1	-1	$R_y$
$B_{3g}$	1	-1	-1	1	1	-1	-1	1	$R_x$
$A_u$	1	1	1	1	-1	-1	-1	-1	z
$B_{1u}$	1	1	-1	-1	-1	-1	1	1	y
$B_{2u}$	1	-1	1	-1	-1	1	-1	-1	x
$B_{3u}$	1	-1	-1	1	-1	1	1	-1	

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

$D_{4h}$	E	$2C_4$	$C_2$	$2C_2'$	$2C_2''$	i	$2S_4$	$\sigma_h$	$2\sigma_v$	$2\sigma_d$	
$A_{1g}$	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	$R_z$
$B_{1g}$	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	$(R_x, R_y)$
$A_{1u}$	1	1	1	1	-1	-1	-1	-1	-1	-1	z
$A_{2u}$	1	1	-1	-1	-1	-1	-1	1	1	-1	
$B_{1u}$	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	$2C_5$	$2C_3'$	$5C_2$	$\sigma_h$	$2S_5$	$2S_5'$	$5\sigma_v$	
$A_1'$	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°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	$(x, y)$
$E_2'$	2	2 cos 144°	2 cos 72°	0	2	2 cos 144°	2 cos 72°	0	
$A_1''$	1	1	1	1	-1	-1	-1	-1	z
$A_2''$	1	1	-1	-1	-1	-1	-1	1	
$E_1''$	2	2 cos 72°	2 cos 144°	0	-2	-2 cos 72°	-2 cos 144°	0	$(R_x, R_y)$
$E_2''$	2	2 cos 144°	2 cos 72°	0	-2	-2 cos 144°	-2 cos 72°	0	

$D_{6h}$	E	$2C_6$	$2C_3$	$C_2$	$3C_2'$	$3C_2''$	i	$2S_6$	$2S_6'$	$\sigma_h$	$3\sigma_v$	$3\sigma_d$	
$A_{1g}$	1	1	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	-1	-1	$R_z$
$B_{1g}$	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	
$E_{1g}$	2	1	-1	-2	0	0	2	1	-1	-2	0	0	$(R_x, R_y)$
$E_{2g}$	2	-1	1	2	0	0	-2	-1	1	2	0	0	$(x^2 - y^2, xy)$
$A_{1u}$	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	
$E_{1u}$	2	1	-1	-2	0	0	-2	-1	1	-2	0	0	$(x, y)$
$E_{2u}$	2	-1	1	2	0	0	2	1	-1	2	0	0	

$D_{8h}$	E	$2C_8$	$2C_4$	$2C_2$	$4C_2'$	$4C_2''$	i	$2S_8$	$2S_8'$	$2S_8''$	$2S_8'''$	$\sigma_h$	$4\sigma_d$	$4\sigma_v$	
$A_{1g}$	1	1	1	1	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	1	1	-1	-1	$R_z$
$B_{1g}$	1	-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	-1	
$E_{1g}$	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	$(R_x, R_y)$
$E_{2g}$	2	0	0	-2	2	0	0	2	0	0	-2	2	0	0	$(xz, yz)$
$E_{3g}$	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	-2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	$(x^2 - y^2, xy)$
$A_{1u}$	1	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	1	
$B_{1u}$	1	-1	-1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	z
$B_{2u}$	1	-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	0	$(x, y)$
$E_{2u}$	2	0	0	-2	2	0	0	2	0	0	-2	2	0	0	
$E_{3u}$	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	-2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	

7. The  $D_{nd}$  Groups

$D_{2d}$	E	$2S_4$	$C_2$	$2C_2'$	$2\sigma_d$	
$A_1$	1	1	1	1	1	$x^2 + y^2, z^2$
$A_2$	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	$(xz, yz)$

$D_{3d}$	$E$	$2C_3$	$3C_2$	$i$	$2S_6$	$3\sigma_d$	
$A_{1g}$	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A_{2g}$	1	1	-1	1	1	-1	$R_z$ ( $R_x, R_y$ )
$E_g$	2	-1	0	2	-1	0	$(x^2 - y^2, xy)$ , ( $xz, yz$ )
$A_{1u}$	1	1	1	-1	-1	-1	$z$
$A_{2u}$	1	1	-1	-1	-1	1	$(x, y)$
$E_u$	2	-1	0	-2	1	0	

$D_{4d}$	$E$	$2S_8$	$2C_4$	$2S_8^3$	$C_2$	$4C_2$	$4\sigma_d$	
$A_1$	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	$z$
$B_2$	1	-1	1	-1	1	-1	1	$(x, y)$
$E_1$	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	$(x^2 - y^2, xy)$
$E_2$	2	0	-2	0	2	0	0	$(xz, yz)$
$E_3$	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0	

$D_{5d}$	$E$	$2C_5$	$2C_2^2$	$5C_2$	$i$	$2S_{10}$	$2S_{10}^3$	$5\sigma_d$	
$A_{1g}$	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A_{2g}$	1	1	1	-1	1	1	1	-1	$R_z$ ( $R_x, R_y$ )
$E_{1g}$	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x^2 - y^2, xy)$
$E_{2g}$	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	$(xz, yz)$
$A_{1u}$	1	1	1	1	-1	-1	-1	-1	$z$
$A_{2u}$	1	1	1	-1	-1	-1	-1	1	$(x, y)$
$E_{1u}$	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	-2	$-2 \cos 72^\circ$	$-2 \cos 144^\circ$	0	
$E_{2u}$	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	-2	$-2 \cos 144^\circ$	$-2 \cos 72^\circ$	0	

$D_{6d}$	$E$	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2C_2$	$6C_2$	$6\sigma_d$	
$A_1$	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A_2$	1	1	1	1	1	1	-1	-1	$R_z$
$B_1$	1	-1	1	-1	1	1	1	-1	$z$
$B_2$	1	-1	1	-1	1	-1	-1	1	$(x, y)$
$E_1$	2	$\sqrt{3}$	1	0	-1	-2	0	0	
$E_2$	2	1	-1	-2	-1	1	2	0	$(x^2 - y^2, xy)$
$E_3$	2	0	-2	0	2	-2	0	0	
$E_4$	2	$-\sqrt{3}$	-1	0	-1	2	0	0	$(xz, yz)$
$E_5$	2	$-\sqrt{3}$	1	0	-1	-2	0	0	

8. The  $S_n$  Groups

$S_4$	$E$	$S_4$	$C_2$	$S_4^3$	
$A$	1	1	1	1	$x^2 + y^2, z^2$
$B$	1	-1	1	-1	$x^2 - y^2, xy$
$E$	$\begin{Bmatrix} 1 & i \\ 1 & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -1 \\ -1 & -i \end{Bmatrix}$	$\begin{Bmatrix} -1 & -1 \\ -1 & -1 \end{Bmatrix}$	$\begin{Bmatrix} -i & 1 \\ 1 & -i \end{Bmatrix}$	$(xz, yz)$

$S_6$	$E$	$C_3$	$C_3^2$	$i$	$S_6^5$	$S_6^4$	$S_6^3$	$S_6^2$	$\epsilon = \exp(2\pi i/3)$
$A_g$	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$E_g$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & 1 \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & 1 \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$(x^2 - y^2, xy)$ , ( $xz, yz$ )
$A_u$	1	1	1	-1	-1	-1	-1	-1	$z$
$E_u$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & 1 \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & 1 \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$(x^2 - y^2, xy)$ ( $xz, yz$ )

$S_8$	$E$	$S_8$	$C_4$	$S_8^3$	$C_2$	$S_8^5$	$C_2^3$	$S_8^7$	$S_8^6$	$\epsilon = \exp(2\pi i/8)$
$A$	1	1	1	1	1	1	1	1	1	$x^2 + y^2, z^2$
$B$	1	-1	1	-1	1	-1	1	-1	-1	$R_z$ $z$
$E_1$	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} i & -\epsilon^* \\ -i & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon^* & -i \\ -\epsilon & -i \end{Bmatrix}$	$\begin{Bmatrix} -1 & -\epsilon^* \\ -1 & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon^* & -i \\ -\epsilon & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -\epsilon^* \\ -i & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & 1 \\ \epsilon & 1 \end{Bmatrix}$	$(x, y)$ , ( $R_x, R_y$ )
$E_2$	$\begin{Bmatrix} 1 & i \\ 1 & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -1 \\ -i & -1 \end{Bmatrix}$	$\begin{Bmatrix} -1 & -i \\ -1 & -i \end{Bmatrix}$	$\begin{Bmatrix} -i & -1 \\ -i & -1 \end{Bmatrix}$	$\begin{Bmatrix} -1 & -i \\ -1 & -i \end{Bmatrix}$	$\begin{Bmatrix} -i & -1 \\ -i & -1 \end{Bmatrix}$	$\begin{Bmatrix} 1 & -i \\ 1 & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -1 \\ i & -1 \end{Bmatrix}$	$\begin{Bmatrix} -i & -1 \\ -i & -1 \end{Bmatrix}$	$(x^2 - y^2, xy)$
$E_3$	$\begin{Bmatrix} 1 & -\epsilon \\ 1 & -\epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon & 1 \\ -\epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} i & -\epsilon^* \\ -i & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon^* & -i \\ -\epsilon & -i \end{Bmatrix}$	$\begin{Bmatrix} -1 & -\epsilon^* \\ -1 & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon^* & -i \\ -\epsilon & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -\epsilon^* \\ -i & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & 1 \\ \epsilon & 1 \end{Bmatrix}$	$(xz, yz)$

9. The Cubic Groups

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

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

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

O	E	8C <sub>3</sub>	3C <sub>2</sub> (=C <sub>2</sub> <sup>2</sup> )	6C <sub>4</sub>	6C <sub>2</sub>	$x^2 + y^2 + z^2$
A <sub>1</sub>	1	1	1	1	1	$x^2 + y^2 + z^2$
A <sub>2</sub>	1	1	1	-1	-1	$(2z^2 - x^2 - y^2, x^2 - y^2)$
E	2	-1	2	0	0	$(xz, yz)$
T <sub>1</sub>	3	0	-1	1	-1	$(R_x, R_y, R_z), (x, y, z)$
T <sub>2</sub>	3	0	-1	-1	1	$(xy, xz, yz)$

O <sub>h</sub>	E	8C <sub>3</sub>	6C <sub>2</sub>	6C <sub>4</sub>	3C <sub>2</sub> (=C <sub>2</sub> <sup>2</sup> )	i	6S <sub>4</sub>	8S <sub>6</sub>	3σ <sub>h</sub>	6σ <sub>d</sub>	$x^2 + y^2 + z^2$
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
A <sub>2g</sub>	1	-1	-1	1	1	1	-1	1	-1	-1	$(2z^2 - x^2 - y^2, x^2 - y^2)$
E <sub>g</sub>	2	-1	0	2	2	0	-1	2	0	0	$(xz, yz, xy)$
T <sub>1g</sub>	3	0	-1	-1	3	1	0	-1	-1	-1	$(R_x, R_y, R_z)$
T <sub>2g</sub>	3	0	-1	-1	3	-1	0	-1	1	1	$(x, y, z)$
A <sub>1u</sub>	1	1	1	1	1	-1	-1	-1	-1	-1	
A <sub>2u</sub>	1	-1	-1	1	1	-1	-1	-1	1	1	
E <sub>u</sub>	2	-1	0	2	-2	0	1	-2	0	0	
T <sub>1u</sub>	3	0	-1	-1	-3	-1	0	1	1	1	
T <sub>2u</sub>	3	0	-1	-1	-3	1	0	1	-1	-1	

10. The Groups C<sub>∞v</sub> and D<sub>∞h</sub> for Linear Molecules

C <sub>∞v</sub>	E	2C <sub>∞</sub> <sup>φ</sup>	∞σ <sub>v</sub>	∞σ <sub>v</sub>	z	$x^2 + y^2, z^2$
A <sub>1</sub> ≡Σ <sup>+</sup>	1	1	∞	1	z	$(xz, yz)$
A <sub>2</sub> ≡Σ <sup>-</sup>	1	1	∞	-1	R <sub>z</sub>	$(x^2 - y^2, xy)$
E <sub>1</sub> ≡Π	2	2 cos φ	∞	0	(x, y), (R <sub>x</sub> , R <sub>y</sub> )	
E <sub>2</sub> ≡Δ	2	2 cos 2φ	∞	0		
E <sub>3</sub> ≡Φ	2	2 cos 3φ	∞	0		
...	...	...	∞	...		

D <sub>∞h</sub>	E	2C <sub>∞</sub> <sup>φ</sup>	∞σ <sub>v</sub>	i	2S <sub>∞</sub> <sup>φ</sup>	∞C <sub>2</sub>	$x^2 + y^2, z^2$
Σ <sub>g</sub> <sup>+</sup>	1	1	∞	1	1	1	$x^2 + y^2, z^2$
Σ <sub>g</sub> <sup>-</sup>	1	1	∞	-1	1	-1	$(xz, yz)$
Π <sub>g</sub>	2	2 cos φ	∞	2	-2 cos φ	0	$(x^2 - y^2, xy)$
Δ <sub>g</sub>	2	2 cos 2φ	∞	2	2 cos 2φ	0	
...	...	...	∞	...	...	...	
Σ <sub>u</sub> <sup>+</sup>	1	1	∞	1	-1	-1	z
Σ <sub>u</sub> <sup>-</sup>	1	1	∞	-1	-1	1	(x, y)
Π <sub>u</sub>	2	2 cos φ	∞	0	2 cos φ	0	
Δ <sub>u</sub>	2	2 cos 2φ	∞	0	-2 cos 2φ	0	
...	...	...	∞	...	...	...	

11. The Icosahedral Groups

I	E	12C <sub>5</sub>	12C <sub>2</sub> <sup>2</sup>	20C <sub>3</sub>	15C <sub>2</sub>	$\eta^{\pm} = \frac{1}{2}(1 \pm 5^{1/2})$
A	1	1	1	1	1	$x^2 + y^2 + z^2$
T <sub>1</sub>	3	η <sup>+</sup>	η <sup>-</sup>	0	-1	$(x, y, z), (R_x, R_y, R_z)$
T <sub>2</sub>	3	η <sup>-</sup>	η <sup>+</sup>	0	-1	$(2z^2 - x^2 - y^2, x^2 - y^2, xy, yz, zx)$
G	4	-1	-1	1	0	
H	5	0	0	-1	1	

I <sub>h</sub>	E	12C <sub>5</sub>	12C <sub>2</sub> <sup>2</sup>	20C <sub>3</sub>	15C <sub>2</sub>	i	12S <sub>10</sub>	12S <sub>6</sub> <sup>5</sup>	20S <sub>6</sub>	15σ	$\eta^{\pm} = \frac{1}{2}(1 \pm 5^{1/2})$
A <sub>g</sub>	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
T <sub>1g</sub>	3	η <sup>+</sup>	η <sup>-</sup>	0	-1	3	η <sup>-</sup>	η <sup>+</sup>	0	-1	$(R_x, R_y, R_z)$
T <sub>2g</sub>	3	η <sup>-</sup>	η <sup>+</sup>	0	-1	3	η <sup>+</sup>	η <sup>-</sup>	0	-1	$(2z^2 - x^2 - y^2, x^2 - y^2, xy, yz, zx)$
G <sub>g</sub>	4	-1	-1	1	0	4	-1	-1	1	0	
H <sub>g</sub>	5	0	0	-1	1	5	0	0	-1	1	

A <sub>u</sub>	1	1	1	1	1	1	1	1	1	1	
T <sub>1u</sub>	3	η <sup>+</sup>	η <sup>-</sup>	0	-1	-1	-1	-1	-1	-1	
T <sub>2u</sub>	3	η <sup>-</sup>	η <sup>+</sup>	0	-1	-1	-1	-1	-1	-1	
G <sub>u</sub>	4	-1	-1	1	0	-4	1	1	-1	0	
H <sub>u</sub>	5	0	0	-1	1	-5	0	0	1	-1	

Note: In these groups and others containing C<sub>s</sub>, the following relationships may be useful:

$$\eta^+ = 1/2(1 + 5^{1/2}) = 1.61803 \dots = -2 \cos 144^\circ$$

$$\eta^- = 1/2(1 - 5^{1/2}) = -0.61803 \dots = -2 \cos 72^\circ$$

$$\eta^+ \eta^- = 1 + \eta^+, \quad \eta^- \eta^- = 1 + \eta^-, \quad \eta^+ \eta^- = -1$$

Chemical Shifts of Methyl, Methylene and Methine Protons

Methyl Protons	$\delta$	Methylene Protons	$\delta$	Methine Protons	$\delta$
Proton		Proton		Proton	
$\text{CH}_3 - \text{C}$	0.9	$-\text{C} - \text{CH}_2 - \text{C}$	1.4	$\text{C} - \text{CH} - \text{C}$	1.5
$\text{CH}_3 - \text{C} - \text{C} = \text{C}$	1.1	$-\text{C} - \text{CH}_2 - \text{C} - \text{C} = \text{C}$	1.7		
$\text{CH}_3 - \text{C} - \text{O}$	1.3	$-\text{C} - \text{CH}_2 - \text{C} - \text{O}$	1.9	$-\text{C} - \text{CH} - \text{C} - \text{O}$	2.0
$\text{CH}_3 - \text{C} = \text{C}$	1.6	$-\text{C} - \text{CH}_2 - \text{C} = \text{C}$	2.3		
$\text{CH}_3 - \text{Ar}$	2.3	$-\text{C} - \text{CH}_2 - \text{Ar}$	2.7	$-\text{CH} - \text{Ar}$	3.0
$\text{CH}_3 - \text{CO} - \text{R}$	2.2	$-\text{C} - \text{CH}_2 - \text{CO} - \text{R}$	2.4	$-\text{C} - \text{CH} - \text{CO} - \text{R}$	2.7
$\text{CH}_3 - \text{CO} - \text{Ar}$	2.6	$-\text{C} - \text{CH}_2 - \text{CO} - \text{Ar}$	2.2	$-\text{C} - \text{CH} - \text{CO} - \text{Ar}$	3.3
$\text{CH}_3 - \text{CO} - \text{O} - \text{R}$	2.0	$-\text{C} - \text{CH}_2 - \text{CO} - \text{O} - \text{R}$	2.2		
$\text{CH}_3 - \text{CO} - \text{O} - \text{Ar}$	2.4				
$\text{CH}_3 - \text{CO} - \text{N} - \text{R}$	2.0	$-\text{C} - \text{CH}_2 - \text{CO} - \text{N} - \text{R}$	2.2		
$\text{CH}_3 - \text{O} - \text{R}$	3.3	$-\text{C} - \text{CH}_2 - \text{O} - \text{R}$	3.4	$-\text{C} - \text{CH} - \text{O} - \text{R}$	3.7
		$-\text{C} - \text{CH}_2 - \text{O} - \text{H}$	3.6	$-\text{C} - \text{CH} - \text{O} - \text{H}$	3.9
$\text{CH}_3 - \text{O} - \text{C} = \text{C}$	3.8				
$\text{CH}_3 - \text{O} - \text{Ar}$	3.8	$-\text{C} - \text{CH}_2 - \text{O} - \text{Ar}$	4.3		
$\text{CH}_3 - \text{O} - \text{CO} - \text{R}$	3.7	$-\text{C} - \text{CH}_2 - \text{O} - \text{CO} - \text{R}$	4.1	$-\text{C} - \text{CH} - \text{O} - \text{CO} - \text{R}$	4.8
$\text{CH}_3 - \text{N}$	2.3	$-\text{C} - \text{CH}_2 - \text{N}$	2.5	$-\text{C} - \text{CH} - \text{N}$	2.7
$\text{CH}_3 - \text{N}^+$	3.3				
$\text{CH}_3 - \text{N} - \text{Ar}$	3.0				
$\text{CH}_3 - \text{S}$	2.1	$-\text{C} - \text{CH}_2 - \text{S}$	2.4	$-\text{C} - \text{CH} - \text{S}$	3.2
		$-\text{C} - \text{CH}_2 - \text{NO}_2$	4.4	$-\text{C} - \text{CH} - \text{NO}_2$	4.7
$\text{CH}_3 - \text{C} - \text{NO}_2$	1.6	$-\text{C} - \text{CH}_2 - \text{C} - \text{NO}_2$	2.1		
$\text{CH}_3 - \text{C} = \text{C} - \text{CO}$	2.0	$-\text{C} - \text{CH}_2 - \text{C} = \text{C} - \text{CO}$	2.4		
$\text{C} = \text{C}(\text{CH}_3) - \text{CO}$	1.8	$\text{C} = \text{C}(\text{CH}_3) - \text{CO}$	2.4		
		$\text{C} - \text{CH}_2 - \text{Cl}$	3.6		
		$\text{C} - \text{CH}_2 - \text{Br}$	3.5	$\text{C} - \text{CH} - \text{Br}$	4.3
		$\text{C} - \text{CH}_2 - \text{I}$	3.2	$\text{C} - \text{CH} - \text{I}$	4.3
$\text{CH}_3 - \text{N} - \text{CO} - \text{R}$	2.9	$\text{C} - \text{CH}_2 - \text{C} \equiv \text{N}$	2.3	$\text{C} - \text{CH} - \text{C} \equiv \text{N}$	2.7
				$\text{C} - \text{CH} - \text{N} - \text{CO} - \text{R}$	4.1



Infrared Carbonyl Frequencies

Group	Frequency	Group	Frequency	Group	Frequency	Group	Frequency	Group	Frequency		
Aldehyde $\text{X} = \text{H}$	1740 - 1720	Ketone $\text{X} = \text{Alk}$	1725 - 1705	Acid $\text{X} = \text{OH}$	1725 - 1700 (monomer 1760)	Ester $\text{X} = \text{OR}$	1750 - 1735	Amide $\text{X} = \text{N} <$	Prim. 1690 Sec. 1700 - 1670 Tert. 1670 - 1630	Acid chloride $\text{X} = \text{Cl}$	1815 - 1790
	1745 - 1695		1700 - 1680 ( $\text{X} = \text{Ar}$ 1760 - 1600)		1700 - 1680		1730 - 1715				1790 - 1750
	1705 - 1680		1685 - 1665		1715 - 1690		1715 - 1715		+ 15 $\text{cm}^{-1}$ over saturated system		
							1800 - 1750				
			$\text{X} = \text{CH}_2$ n=4 1780 n=5 1750 - 1740 n=6 1725 - 1705								
			n=5 1710 - 1690 n=6 1695 - 1680								

Infrared Spectroscopy (all figures in  $\text{cm}^{-1}$ )

Group	Frequency	Group	Frequency	Group	Frequency
OH	2500 - 3700	$\text{C} = \text{C}$ alkenyl	1590 - 1690	$\text{CH}_3$	1360 - 1490
$\text{NH}, \text{NH}_2$	3200 - 3500	$\text{C} = \text{C}$ aromatic	1440 - 1625	OH	1000 - 1450
$\equiv \text{CH}$	3300	$\text{N} = \text{N}$	1570 - 1640	$\text{COO}^-$	1300 - 1420
CH aromatic	3030 - 3080	$\text{C} = \text{N}$	1470 - 1690	$\text{C} - \text{N}$	1020 - 1420
CH alkenyl	3010 - 3100	NH	1510 - 1640	$\text{C} - \text{O}$	1050 - 1430
CH aliphatic	2840 - 2975	$\text{COO}^-$	1540 - 1620	$\text{NO}_2$	1250 - 1385
$\text{C} \equiv \text{N}$	2040 - 2270	$\text{NO}_2$	1500 - 1650	CH aromatic	660 - 900
$\text{C} \equiv \text{C}$	2100 - 2270	CH	1340 - 1490	CH alkenyl	665 - 1000
$\text{C} \equiv \text{O}$	1540 - 1870	CH oil	1280 - 1430	$\text{C} - \text{Cl}$	600 - 800

Proton - Proton Coupling Constants

Group	J (Hz)
	10 - 18
	2 - 9 (6 - 7 if free rotation)
	0 - 3.5
	11 - 18
	6 - 14
	0.5 - 2
	2 - 3
	1 - 3
	4 - 8 typically (1 - 11 range) Hz (depends on dihedral angle)
	o- 7 - 10 m- 2 - 3 p- 0 - 1

Estimation of Chemical Shift ( $\delta$ ) for Protons of  $-\text{CH}_2-$  and  $-\text{CH}-$  Groups  
 $\delta_{\text{CH}_2} = 0.23 + C_1 + C_2$        $\delta_{\text{CH}} = 0.23 + C_1 + C_2 + C_3$

X	C	X	C	X	C
$-\text{CH}_3$	0.5	$-\text{SR}$	1.6	$-\text{OR}$	2.4
$-\text{CF}_3$	1.1	$-\text{C} \equiv \text{C}-\text{Ar}$	1.7	$-\text{Cl}$	2.5
$> \text{C} = \text{C} <$	1.3	$-\text{CN}$	1.7	$-\text{OH}$	2.6
$-\text{C} \equiv \text{C}-\text{R}$	1.4	$-\text{CO}-\text{R}$	1.7	$-\text{N} = \text{C} = \text{S}$	2.9
$-\text{COOR}$	1.5	$-\text{I}$	1.8	$-\text{OCOR}$	3.1
$-\text{NR}_2$	1.6	$-\text{Ph}$	1.8	$-\text{OPh}$	3.2
$-\text{CONR}_2$	1.6	$-\text{Br}$	2.3		

Approximate Chemical Shifts of Protons Attached to Unsaturated Linkages

Proton	$\delta$	Proton	$\delta$
R - CHO	9.4 - 10.0	-C = CH -	4.5 - 6.0
Ar - CHO	9.7 - 10.5	-C = CH - CO	5.8 - 6.7
H - CO - O	8.0 - 8.2	-CH = C - CO	6.5 - 8.0
H - CO - N	8.0 - 8.2	-CH = C - O	4.0 - 5.0
-C $\equiv$ C - H	1.8 - 3.1	-C = CH - O	6.0 - 8.1
Aromatic protons	6.0 - 9.0	-CH = C - N	3.7 - 5.0
		-C = CH - N	5.7 - 8.0

Chemical Shifts of *Ortho*, *Meta* and *Para* Protons in Mono-substituted Benzenes (in p.p.m. from Benzene,  $\delta = 7.27$  p.p.m.)<sup>†</sup>

Substituent	$\Delta_{ortho}$	$\Delta_{meta}$	$\Delta_{para}$
$\text{NO}_2$	0.94	0.18	0.39
CHO	0.58	0.20	0.26
COOH	0.80	0.16	0.25
$\text{COOCH}_3$	0.71	0.08	0.20
COCl	0.82	0.21	0.35
$\text{CCl}_3$	0.80	0.20	0.20
$\text{COCH}_3$	0.62	0.10	0.25
CN	0.26	0.18	0.30
$\text{CONH}_2$	0.65	0.20	0.22
$\text{NH}_2^+$	0.40	0.20	0.20
$\text{CH}_2\text{X}^*$	0.0 - 0.1	0.0 - 0.1	0.0 - 0.1
$\text{CH}_3$	-0.16	-0.09	-0.17
$\text{CH}_2\text{CH}_3$	-0.15	-0.06	-0.18
$\text{CH}(\text{CH}_3)_2$	-0.14	-0.09	-0.18
$\text{C}(\text{CH}_3)_3$	-0.09	0.05	-0.23
F	-0.30	-0.02	-0.23
Cl	0.01	-0.06	-0.08
Br	0.19	-0.12	-0.05
I	0.39	-0.25	-0.02
$\text{NH}_2$	-0.76	-0.25	-0.63
$\text{OCH}_3$	-0.46	-0.10	-0.41
OH	-0.49	-0.13	-0.20
OCOR	-0.20	0.10	-0.20
$\text{NHCH}_3$	-0.80	-0.30	-0.60
$\text{N}(\text{CH}_3)_3$	-0.60	-0.10	-0.62