

Tutor Marked Assignment

Course and assignment no.

S205 TMA 05

Make sure you know how to complete and send in your TMA and PT3 form; detailed instructions are given in *Completing TMA and CMA forms* in your *Student Handbook*.

Covering: **Books 8 and 9**

Cut-off date:

Friday 18 July 2003

This assignment is made up of four questions. For each question, the following Table indicates:

- when you should attempt the question;
- the percentage of the total marks for this assignment allocated to the question; and
- the box number on the Assignment Form in which your tutor will indicate the marks that you obtain for the question.

Question number	When to attempt it	Percentage of total marks	Box No. on Assignment Form
1	after completing Book 8 Part 1 and the Spectroscopy CD-ROM	30	1
2	after completing the Spectroscopy CD-ROM	20	2
3	after completing the Spectroscopy CD-ROM	30	3
4	after completing Book 9 Sections 1-7	20	4

Question 1

This question carries 30 per cent of the marks for this assignment, and tests Learning Outcomes 2 and 3 of Book 8 Part 1, and Learning Outcomes 2 and 5 of Book 8 Part 2, the Spectroscopy CD-ROM.

Write up your results from the 'Spring stiffness experiment' in the *Harmonic oscillator model* program (Section 4 of Program 3 on CD-ROM0426). Be sure to use the computer-generated data in Section 4, rather than the physical experiment data in Section 6.

Use your plot to estimate the frequency of vibration when the force constant is 9.

Using the guidelines for writing up experiments in Book 8 Part 1, you should write up your results under the following headings:

- Title (1 mark)
- Aim(s) (1 mark)
- Method (7 marks)
- Results and discussion (19 marks)
- Conclusion (2 marks)

Note that 5 of these marks are allocated to the quality of your write up. Include a plot of your results with the write up: either a print-out from the computer, or a hand-drawn plot on graph paper is acceptable.

Question 2

This question carries 20 per cent of the marks for this assignment, and tests Learning Outcome 13 of Book 2, Learning Outcome 12 of Book 6, and Learning Outcomes 7-9 of Book 8 Part 2 (the Spectroscopy CD-ROM).

This question concerns the infrared and Raman spectra of the triatomic molecule $\text{F}-\text{Br}-\text{F}$. This representation does not necessarily show the correct bond order or the shape of the molecule. The bands in these spectra are as follows:

Infrared

596 cm^{-1}

198 cm^{-1}

Raman

442 cm^{-1}

Symmetric stretch

(a) (6 marks) Draw the Lewis structure of this molecule and use VSEPR theory to predict its shape. To which symmetry point group does it belong?

(b) (4 marks) Does the spectroscopic data confirm your prediction? Use the mutual exclusion rule to justify your answer.

(c) (10 marks) Assign the bands to antisymmetric stretch, symmetric stretch, and bending mode(s). Give your reasoning, and sketch all the modes.