SECTION C

Long-answer questions

Attempt **ONE** *of the following three questions, and* **ONE** *other question from this Section* **or** *from Sections B and D. All questions carry 15 per cent of the total marks for the examinable component. Section C tests the material in Book 5 (Part 1), Book 6 and Book 8. You are advised to spend no more than* **30 minutes** *on each question. Write your answer(s) in a separate answer book from those used for Sections A, B and D.*

Question 16

The decomposition of hydrogen peroxide (H_2O_2) under certain conditions in aqueous solution at 300 K has the following time-independent stoichiometry:

$$2H_2O_2(aq) = 2H_2O(l) + O_2(g) \qquad (11)$$

(*a*) (*2 marks*) Express the rate of reaction, *J*, in terms of the rate of change of concentration of both H_2O_2 and O_2.

(*b*) (*8 marks*) It is found that the partial order with respect to H_2O_2 is 1, and that, overall, the reaction is first order. Given this information, write down the form of the experimental rate equation, and then outline the steps that would be required to determine a value for the experimental rate constant for the decomposition reaction at 300 K.

(*c*) (*5 marks*) If the reaction conditions are kept the same, but the decomposition is carried out at 310 K, how would you expect the rate of reaction to change? Give the reasons for your answer, and clearly identify the factor that will be most influential in causing the change.

Question 17

(*a*) (*2 marks*) Which bond and angle terms would you need in order to describe methanal, $H_2C{=}O$, in molecular mechanics?

(*b*) (*3 marks*) Describe the bonding at the carbon atom in methanal in terms of hybrid orbitals.

(*c*) (*4 marks*) Use the flow chart given in the S205 *Data Book* (p. 37) to establish the symmetry point group of methanal.

(*d*) (*3 marks*) Sketch a π bonding orbital for CO.

(*e*) (*3 marks*) An *ab initio* Hartree–Fock calculation using a small basis set on CO, gives a partial charge of +0.05 on carbon. Use the formula given on the *Data Sheet* that accompanies this examination paper to calculate the dipole moment of CO. How might you improve this calculation to obtain an answer closer to experiment? (The bond distance in CO is 1.14 Ångstrom.)