A1 Ave mark 9.1/20. Candidates struggled with this question, with many using it as the 'question of last resort'. Nevertheless, there were some good first class answers, including one scoring full marks. Most candidates were OK with (a), (b) (i) and (ii), but only a minority worked out how to use the Hermiticity of H to derive the result of b(iii). Many candidates made a reasonable attempt at b(iv), with some losing marks for not identifying H(1). Only a few candidates successfully completed part (c).

A2 Ave mark 11.4/20. This question was well answered on the whole, except for c(i), in which many candidates demonstrated a poor understanding of the Born-Oppenheimer approximation. Many answers to (a) demonstrated confusion between the Pauli Principle and the Pauli exchange principle. Part b(i) and (ii) received a variety of responses, with many candidates being unsure of the definition of L, S, J etc. Most candidates scored full marks for (b)(iii).

A3 The mode of the mark distribution is around 10-12 (based on bin size of 2 marks). There were few extreme scores, with ~10 candidates scoring <= 6 and >= 18. Some candidates found question A3a (ii &iii) and A3b(ii) tricky to answer.

A4 Ave mark 11.9/20. On the whole candidates answered this question well. A common mistake was to forget that there are four degenerate MOs; many candidates seemed reluctant to exploit the block diagonal form of the secular determinant. Unfortunately, there were a number of candidates who performed very badly, which is reflected in the noticeable difference between the mean and the median. There were some hints that should have helped candidates get out of the blocks (e.g., the A1u symmetry orbital was given in the question, as were the degenerate SOs). Even in cases where candidates failed to reduce the representation correctly, follow on marks were awarded, allowing reasonable progress in the question to be made.

A5 Ave mark 10.9/20. The highest mark was 20 (obtained by 2 students) and the lowest was 0.5. 33%, 14%, 14%, 15% of students obtained a 1st, 2.1, 2.2 and 3rd respectively. [a (i)] was in general well answered. Few students obtained full marks for [a (ii)] – most failed to account for the H atoms. Several students did not understand what was required in [b (i)] and failed to identify the IR active modes of Benzene (many simply chose E_{1U} and discounted A_{2U}).

A6 This was a question which probed understanding of surface adsorption. Most students answered well the first part concerning the partition function. The second part concerned with surface coverage was found to be more challenging by many students but was still in many cases well answered.

A7 This question focused on chemical equilibrium and was generally well answered. Most students were able to derive the required expression for the equilibrium constant. The derivation of the degree of ionisation was more challenging, and difficulties were encountered in some cases in obtaining the numerical values.

A8 (no report received)

A9 The question was well done with many candidates showing good command of the material.

(a)

i. Some easy marks, but rather too many people described β in such a way as to confuse it with the overlap integral S. Most people understood that for the p band you needed an change of sign, but some people over did it by changing the sign of β and the sign in the expression for E_k.

ii. Again some easy marks, but some lost marks as a result of careless and inconsistent labelling.

iii. Easy marks.

(b)

i. Common errors here were not to remember that the mixing varies with k, and that in particular it is zero at k = 0 and k = π/a.

ii. Generally well done, but some people got muddled over how curves would look as a result of the avoided crossing.

iii. This is essentially a repeat of ii, but with some specific values to be added to the graph. Oddly, some people who got the plot incorrect in ii in fact did iii correctly, and did not go back to correct what must have by then been obviously wrong. The part which people often failed to comment on at all was how the mixing changes as a function of k, and how the s or p character of the bands therefore changes significantly in the range $k = 0$ to $k = \pi/a$.

iv. If iii was done correctly, then this part followed easily.

A10 The question was well done with many candidates showing good command of the material.

(a)

i. Easy marks for everyone

ii. This is straight from the notes and an integration is required to get the activation energy as $E_g/2$. There were a variety of dubious/inventive ways of getting this result which were not accepted. Many people forgot to answer the part about how the band gap could be estimated using the temperature dependence of the conductivity.

(b)

i. Easy marks

ii. More easy marks, but to get them all it was necessary to be clear that the spacing between the donor levels and the bottom of the conduction band is much less than the band gap.

iii. These are transitions between the donor levels, with the limit being the electron moving into the conduction band; rather too many people decided that these were transitions due to excitons (for which partial credit was given). Many people correctly determined the assignment, the values of the effective Rydberg constant, and the dielectric constant.

iv. Generally done well.

(c) Many people had sensible things to say here, but rather too many had the acceptor energy levels running the wrong way.