

A1

This question was answered poorly on the whole, with many candidates obviously leaving this question till they were nearly out of time. Part (a) was answered surprisingly badly, with many candidates not remembering the form of the eigenvalues of the angular momentum operators, nor the limits on the angular momentum quantum numbers. Despite this, reasonable numbers of candidates were OK with (b) and (c), although marks were lost for not being able to remember basic properties of the spherical harmonics. Only a few candidates gave good answers to (d), by demonstrating that the p_x and p_y orbitals are eigenfunctions of L^2 but not of L_z .

A2

The question was well answered on the whole. Most candidates were OK with (a) and (b) (i), although marks were lost for algebraic errors in b(i). There were a wide variety of answers to b(ii) (demonstrating that some candidates understood the variation principle much better than others). Candidates found part (b)(iii) challenging, although there were a few good answers.

A3

The A3 paper 1B questions were overall well answered by the students. The mean and median of the scores for Q A3 were 14 and 15 respectively. There are few extreme scores, with ~20 candidates scored ≤ 10 and and 18 scoring ≥ 18 .

Some found question A3b (ii) and A3c(i & ii) tricky to answer.

A4

Almost all candidates were able to identify the correct point groups and determining the IRs of the d orbitals and ligands was straightforward for most too. The MO diagram was done well, although the instruction to only show the orbitals deriving principally from the metal d orbitals was almost universally ignored. Calculating the effective magnetic moment proved tricky, as few students had the correct electron count. It was also common to ignore the possibility of a high spin state for the square planar complex, despite that being explored in a supervision question. Still, most candidates correctly asserted that the complex is square planar even if some of the reasoning was a little spurious.

The normal modes part was generally answered poorly. Although this was a major topic in the lectures and the subject of many supervision questions, quite a number of students appeared to have no idea how to approach it. There was reasonable knowledge of the rule of mutual exclusion, although some candidates asserted that both geometries possess a centre of inversion. The better students were able to recognise that very little work was required for the second part as the relevant representation matches the ligand orbitals from part (a). It was rare for candidates to get anywhere with the final part, and among those that did, it was a select group indeed who realised that a CN ligand consists of two atoms.

A5

On average this question was not answered well, with a noticeable number of candidates submitting barely anything. There is some evidence to suggest such candidates had not allocated enough time to give the question a proper attempt. Future candidates are reminded that there is no particular reason to attempt the paper in question order, and that starting with what may be the easier questions is probably a good idea.

The benzene part was a mixed bag, with some candidates having no idea how to begin and others clearly finding it straightforward. Several candidates wasted

time by determining the IRs of the orbitals, which was not required. The commonest mistake was to not show that some of the contributions for the degenerate orbitals are twice the size, despite this point being stressed in the lectures. In calculating the delocalisation energy, a large number of candidates compared with a system of six isolated carbons rather than a system with three localised bonds. Mentions of an empirical guideline for aromaticity were not relevant and were ignored.

The majority of candidates could identify the point group of pyrazine and provide appropriate symmetry orbitals. There were a small number of interesting suggestions including 3 and 5 fold rotation axes and even tetrahedral symmetry. It was pleasing to see only a very small number of candidates committing the cardinal sin of not separating the C and N basis sets. In contrast, finding the MO energies proved impossible for most, particularly calculating the Hamiltonian matrix elements in the SO basis set. Confusion about the localised system to compare pyrazine to was high, with a minority recognising that considering localised C-N bonds was necessary. There were then interesting and varied suggestions about the appropriate energy for a localised C-N bonding orbital, with only a tiny number solving the appropriate secular determinant.

A6-A8

No reports received.

A9

This question was about the geometry of a two dimensional Bravais lattice, the corresponding unit cell in real and reciprocal space and the construction of Brillouin zones. The 2D reciprocal space exercise was preceded by a one-dimensional example, by way of introduction. The question was answered rather well. Almost every student understood the basic concepts. In fact, there was large number of scripts receiving full marks (15 out of 123). However, a substantial fraction of the students, while getting the correct orientation of the lattice vectors made a mistake with the determination of the length. This was by far the most common error, which is perhaps an indication that translational symmetry remains a somewhat unfamiliar operation.

A10

The key issue probed in this question is the crucial distinction between the thermal occupation of an extended state as given by the Fermi-Dirac distribution and the density of states. The generalization to fractional occupation was evidently not difficult to make, but most students struggled with the concept of a density of states. This was clear from the rather poor answers to questions ai, aii and bii. Similarly, a number of answers to question aiv left out the integral over states, although this mistake was relatively rare. The question about the switch over from extrinsic to intrinsic behaviour of a doped semiconductor with increasing temperature (question bi) was done well, except that a number of answers seem to imply that all donor electrons end up in the conduction band at high temperature, indicating that the idea of a thermal distribution was perhaps not as clear as it should be. Question 10, more than question 9, addressed the fundamental difference between the electronic states of molecule and a solid. It is evidently a bit of a challenge for chemistry students, and contrary to question 9, there was only a single script with full marks.