Paper 2A

Q17

Most people knew about the r^{-6} terms begin due to the dispersion interaction, and that the r^{-12} term was empirical; people were less confident about the origin of the exponential term in the Buckingham potential. Unfortunately, the question was widely misunderstood in two ways: "Explain the origins of the terms" was taken to be asking for a definition of the parameters; "… comment on their suitability for modelling gaseous hydrogen" was taken to be asking about the dissociation of H_2, rather than modelling the interactions between H_2 molecules.

Q18

Generally well done. People quickly identified that it was the non-bonding MO that was relevant and had a strategy for finding the coefficients. Most people interpreted "Determine which site is the most reactive" as being applied to each individual molecule, whereas the intention was to identify the sit out of both **A** and **B** which was most reactive.

Q21

(a) This was familiar ground which most people had little trouble with. There were a few very odd MO diagrams for NH invoking hydrogen 2s and 2p orbitals.
(b) This is based on the familiar idea of PQR branches, but with the twist that the expression for the rotational energies was modified by the presence of orbital angular momentum. Most people managed to derive the required expressions and sketch the spectrum, but far too few acted on the clear statement in the question about the range of J and as a result were not able to sketch the spectrum properly.
(c) Most people spotted that there was a band head in the R branch and managed to get out a reasonable value of the rotational constant. Assigning the Q branch lines fell foul of not understanding the range of J values.

Overall the question was a good discriminator, yielding a wide range of marks.

Q22

(a) The key point that this requires a time resolved experiment in the absence of quenching was missed by almost everybody.
(b) This is based on familiar ground and most people identified a suitable straight-line plot. The thing that tripped 90% of candidates was converting torr to mol dm^{-3}: it is very surprising that, at this stage, a trivial manipulation of this kind represents such a challenge.
(c) This is less familiar territory but most people knew more or less what to do.

The question was not such a good discriminator with few people achieving really good marks.

Paper 2B

Q25

Straightforward and generally well done.

Q26

Some people got into a muddle working out the term symbols (e.g. by not applying the Clebsch–Gordon series correctly). Otherwise well answered.

Q27

Generally well answered.

Q33

There was an error in the expression in (b)(i) – the first term should have been q^4, not q^2. This was identified quickly during the exam, but a few candidates noted on their scripts that they had already completed this part of the question. The appropriate compensation was made.

(a) This produced some rather incoherent responses.
(b) Generally well done.
(c) Likewise

Q34

(a) Produced rather a muddle of results, with few people pointing out that *J* was a quantum number and giving its range.
(b) Likewise surprisingly incoherent – several candidates talked about normal modes.
(c) Fine
(d) Generally well done apart from a few numerical slips.
(e) People know that *B* decreased with increasing *v* but most attributed this to centrifugal distortion. Very few identified the asymmetry of the potential energy function as the origin.
(f) Fine

Q35

(a) Straightforward and well done
(b) Straightforward and well done
(c) The algebra in (ii) defeated a significant number of candidates
(d) Most people knew what to do – i.e. combining the results of (b) and (c), but there were a lot of slips in doing this. Candidates needed to recall the relationship between *k* and *ω* to complete the proof.
(e) Those who made it here without previous errors could complete this easily.