General discussion summary

The general discussion was led by J. Barber (*Department of Biological Sciences, Imperial College of Science, Technology and Medicine, London, UK*) and focused on two main points arising from the structural studies on photosystem II.

- (i) The location of Ca^{2+} relative to the Mn cluster
- (ii) Which chlorins within the core of the PSII reaction centre can be attributed to P_{680} ?

Regarding the first issue, P. Fromme (*Max-Volmer Laboratorium für Chemie und Biochemie, Technische Universität Berlin, Berlin, Germany and Department of Chemistry and Biochemistry, Arizona State University, Tempe, USA*) explained that with the present X-ray map it is not possible to distinguish an electron-density for Ca^{2+} within the background high density generated by the Mn-cluster. C. Dismukes (*Department of Chemistry, Princeton University, Princeton, NJ, USA*) pointed out that Ca^{2+} is required for the photoinduced assembly of the Mn-cluster and that EPR studies have shown that magnetic and ligand field changes occur on Ca^{2+} -binding which suggests that Ca^{2+} and Mn are physically very close to each other and may share the same ligands, possibly water.

The question of what is, and where is, P_{680} , generated considerable discussion. W. Junge (*Abteilung Biophysik, Universität Osnabrück, Osnabrück, Germany*) made the point that all four chlorophylls within the reaction centre core must have high redox potentials, differing by only *ca.* 40–60 mV. To address the question, therefore, of where P_{680}^+ is located would require a titration against temperature. At high temperature, the radical cation could be delocalized, while at low temperature it may localize at the lowest potential chlorophyll. He also suggested that the high potential of the four chlorophylls is likely to be due to H-bonding and that the lack of a special pair was not a key issue for generating the high potentials.

R. van Grondelle (*Department of Biophysics, Free University, Amsterdam, The Netherlands*) made the point, based on analogies with experiments performed on mutated reaction centres of *Rhodobacter sphaeroides*, that the initial donor to pheophytin could be the accessory chlorophyll. Indeed, he and his colleagues have conducted a careful analysis of the Stark spectrum measured with the isolated D1/D2 complex and concluded that the primary charge transfer is between the 'accessory' chlorophyll and pheophytin on the active branch. This concept was reinforced by D. Klug (*Department of Chemistry, Imperial College of Science, Technology and Medicine, London*), who has come to the same conclusion based on time-resolved optical spectroscopy. Further confirmation of the general idea that the excited accessory chlorophyll acts as the primary donor comes from recent work of B. Diner and co-workers (*Central Research and Development Department, E. I. du Pont de Nemours and Company, Wilmington, Delaware, USA*). B. Diner explained that His198 on the D1 protein and His197 on the D2 protein are the likely ligands for the 'special pair equivalent' chlorophylls P_A and P_B , respectively. By mutating these histidine residues, he has concluded that after the primary charge separation involving the accessory chlorophylls, the radical cation migrates to the P_A chlorophyll, where it is localized. His work indicates that this localization of the P_{680}^+ on P_A chlorophyll occurs at low and at room temperatures.