

Supplementary Information

Table 1: Assignment of IR modes in WL-PSI spectra of *Chroocidiopsis thermalis* PCC 7203

Mode Frequencies (cm ⁻¹)			Mode Assignments
Ground state (negative peaks)	Excited state (positive peaks)	Charge-separated state (positive peaks)	
1534 1609 and 1554	1512 and 1527 1594 and 1543		Chlorophyll macrocycle C=C stretching vibrations ^{1,2}
1672 and 1689	1637 and 1652		9-keto groups of chlorophylls ^{1,3}
1738	1728		10a-ester groups of chlorophylls ¹
		1710(+)	Upshifted keto carbonyl band of chlorophyll cation ¹
1700		1715	9-keto carbonyls of P _A and P _B chlorophylls of P700 ^{1,4}
1634		1648	
1745			10a-ester groups of P _A and P _B chlorophylls of P700 ^{1,4}
1731		1740	
1663, 1607, and 1590			C=O and C=C stretching modes of A ₁ ^{1,5}

The above assignments were based on the references listed below.

References

- 1 M. Di Donato, A. D. Stahl, I. H. M. Van Stokkum, R. Van Grondelle and M. L. Groot, *Biochemistry*, 2011, **50**, 480–490.
- 2 T. Noguchi, T. Tomo and Y. Inoue, *Biochemistry*, 1998, **37**, 13614–13625.
- 3 M. L. Groot, J. Breton, L. J. G. W. Van Wilderen, J. P. Dekker and R. Van Grondelle, *J. Phys. Chem. B*, 2004, **108**, 8001–8006.
- 4 J. Breton, *Biochim. Biophys. Acta*, 2001, **1507**, 180–193.
- 5 J. R. Burie, A. Boussac, C. Boullais, G. Berger, T. Mattioli, C. Mioskowski, E. Navedryk and J. Breton, *J. Phys. Chem.*, 1995, **99**, 4059–4070.