
Oxygen-evolving Photosystem II core complexes: A new paradigm based on the spectral identification of the charge-separating state, the primary acceptor and assignment of low-temperature fluorescence.

Elmars Krausz,^{a,*} Joseph L. Hughes,^a Paul Smith,^b Ron Pace,^b and Sindra Peterson Årsköld^{a,c}

^a *Research School of Chemistry, Australian National University, Canberra, Australia.*

Fax: +61-26125-0750; Tel: +61-26125-3577; E-mail: krausz@rsc.anu.edu.au

^b *Faculties Chemistry, Australian National University, Canberra, Australia.*

^c *Department of Biochemistry, Center for Chemistry and Chemical Engineering, Lund University, Sweden*

Supplementary Information: Diagrams in Colour:

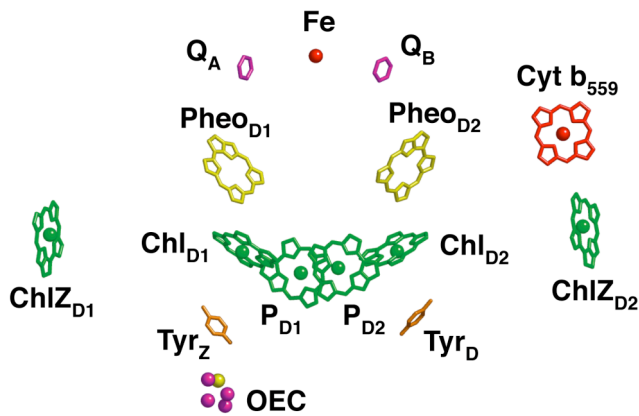


Fig. 1 Schematic (adapted from Ferreira et al.⁵) of chlorins and redox cofactors in the PSII reaction centre, viewed along the membrane plane and with the protein removed.

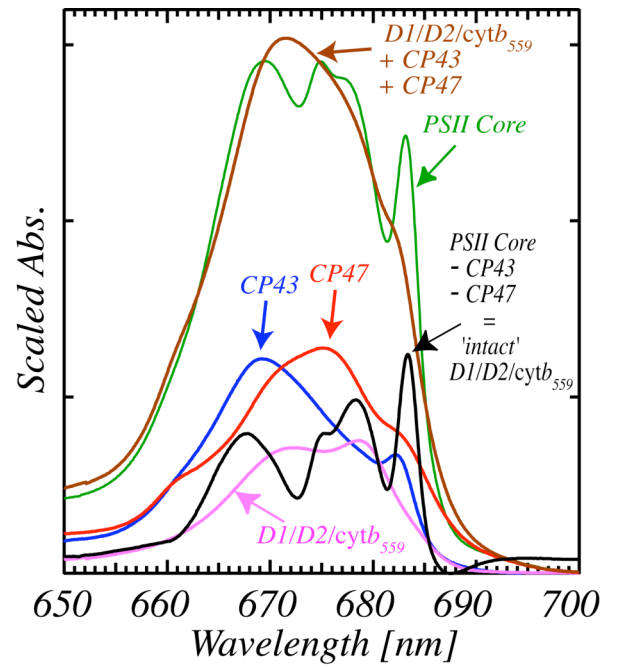


Fig. 3 Spectra of a spinach PSII core complex and its component sub-assemblies at 1.7 K, scaled to the correct chlorin content. Also shown are the sum of sub-assembly spectra (brown) and the modelled spectrum of the intact reaction centre (black). Adapted from Peterson Årsköld et al.³⁹

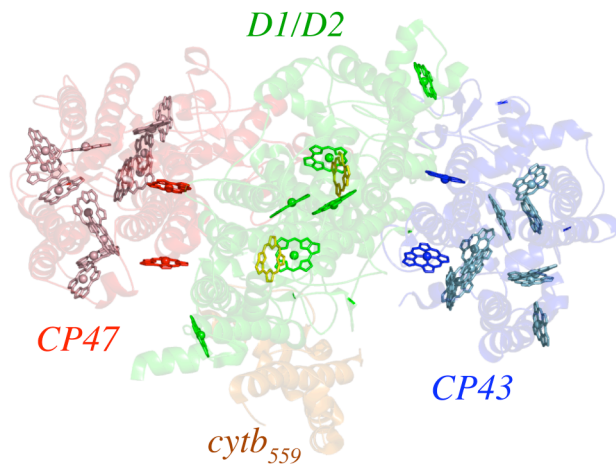


Fig. 2 Top view of the PSII core complex chlorins, with proteins in the background. Darker red and blue pigments in CP47 and CP43 are 'linker' pigments to the reaction centre. Structure adapted from Ferreira et al.⁵

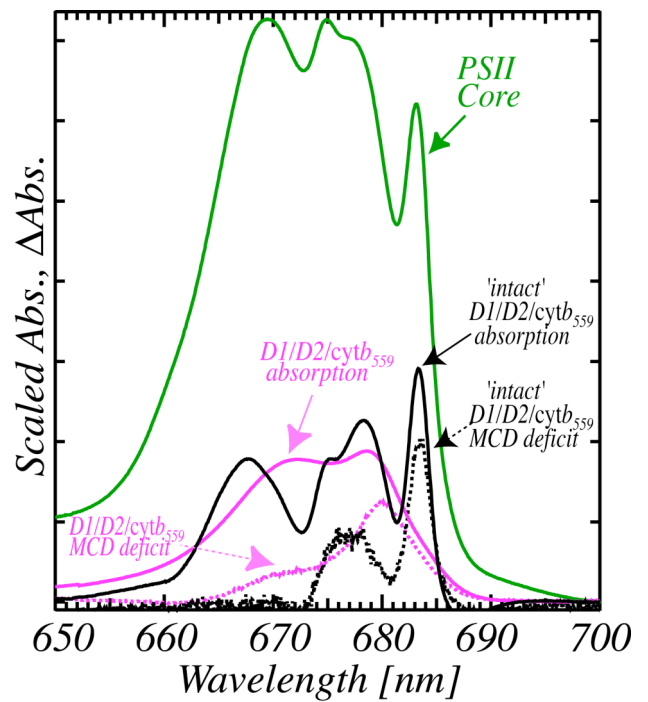


Fig. 4 Absorption (solid lines) and MCD deficit spectra (dashed lines) as indicated (see text). Adapted from Peterson Årsköld et al.³⁹

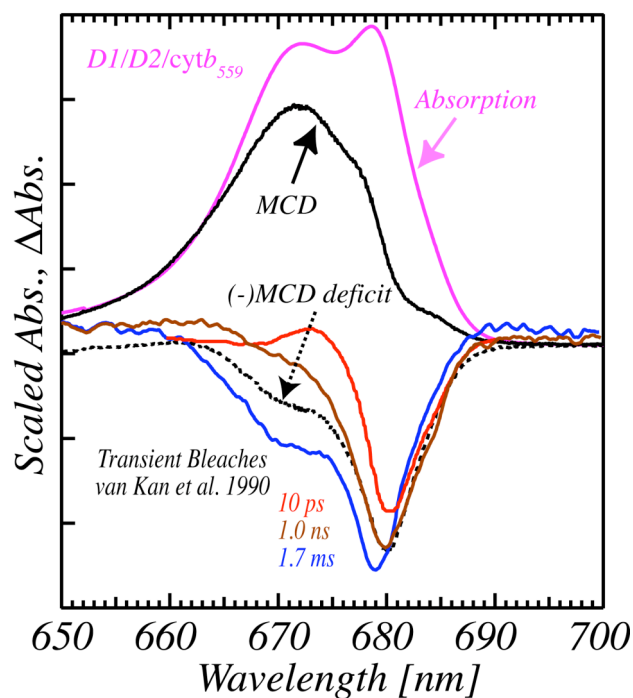


Fig. 5 Top: Absorption and scaled MCD spectra at 1.7 K of a 6-chl *a* D1/D2/cytb₅₅₉ sub-assembly. Bottom: The (inverted) MCD deficit spectrum (dashed) is compared to pulse laser-induced transient bleaches, recorded by van Kan et al.,³¹ at times after excitation as indicated.

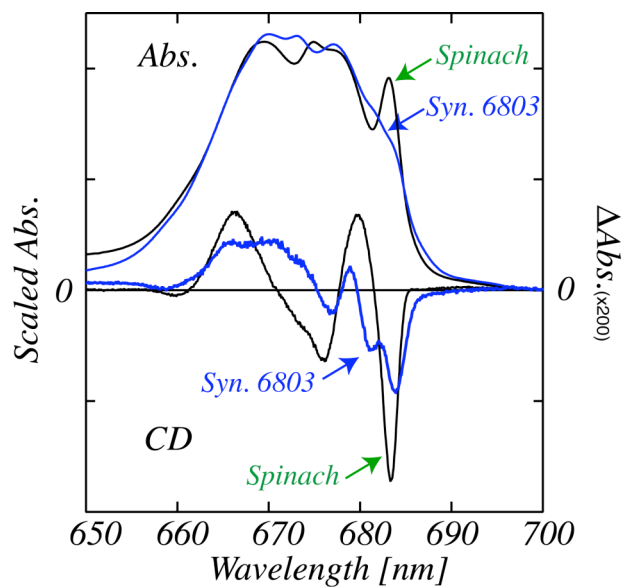


Fig. 6 Absorption and CD spectra of spinach and Syn. 6803 core complexes at 1.7 K. Adapted from Peterson Årsköld et al.³⁹

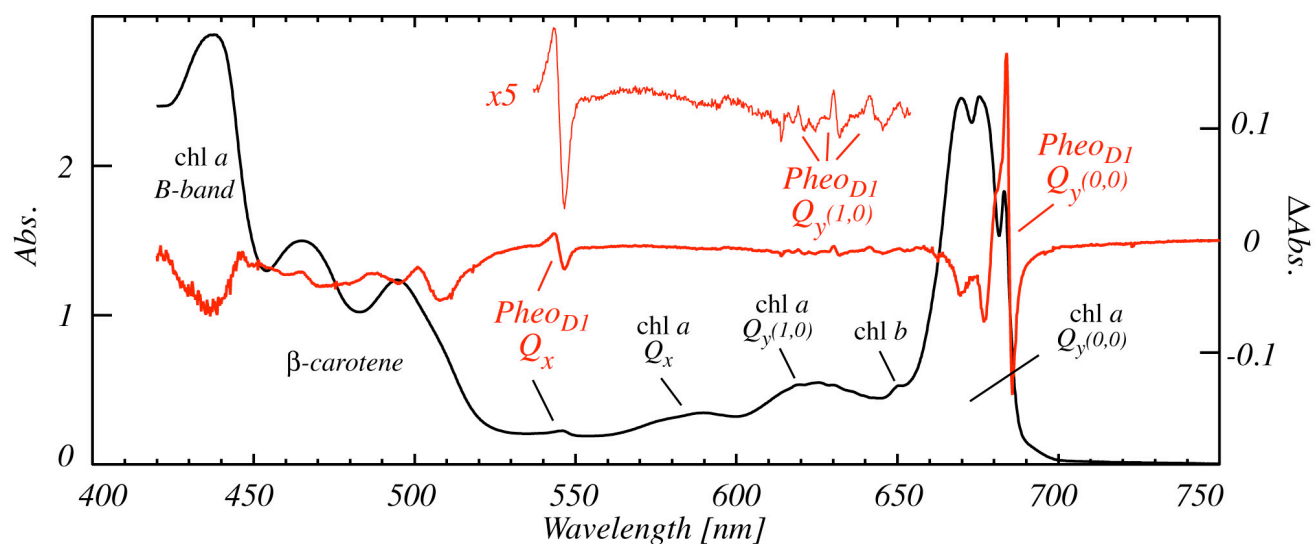


Fig. 7 Absorption (black, left-hand scale) and changes in absorption (red, right-hand scale) after illumination of a spinach core complex at 1.7 K with 15 mJ/cm² at 660 nm. Changes between 530 and 650 nm are also shown multiplied by 5.

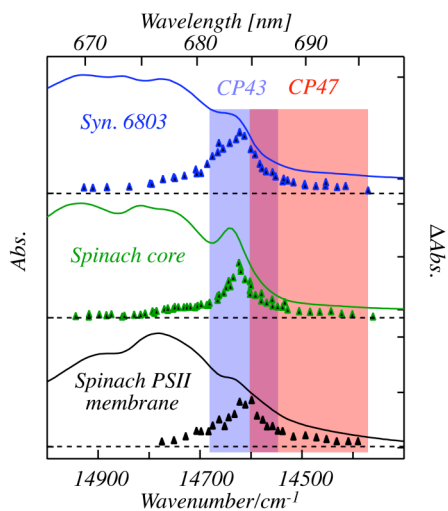


Fig. 8 Panels show absorption (solid lines) and corresponding hole-burning action spectra (triangles) for core complexes of *Syn. 6803*, spinach and PSII-enriched membrane preparations. Hole-burning in shaded areas is attributed to CP43 and CP47 'slow-transfer' pigments. Adapted from Hughes et al.¹²

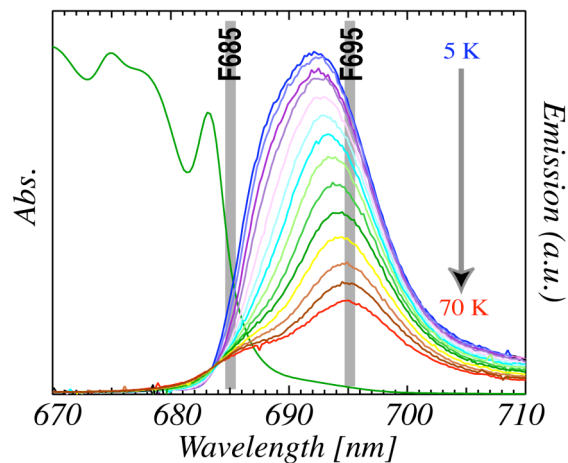


Fig. 10 Absorption at 1.7 K (left) and temperature dependent emission spectra (right) taken of a spinach PSII core complex preparation in 5 K increments from 5 K to 70 K. Excitation was with an unfocused 1mW laser at 633nm. Adapted from Krausz et al.⁶³

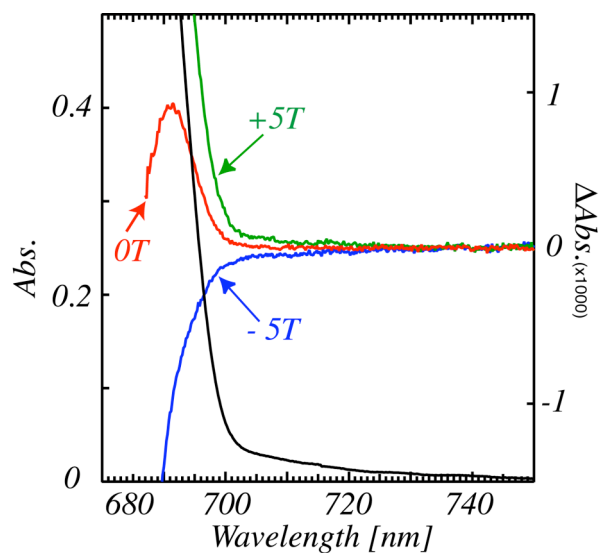


Fig. 9 Long-wavelength absorption (black, left-hand scale) and CD (red, right-hand scale) spectra of the PSII core-complex preparation used in Fig. 7 with a peak OD near 680 nm of ~15. Green and blue traces are CD spectra recorded with applied magnetic fields of +5T and -5T (see text).