

Biophysical Journal, Volume 97

Supporting Material

Single-molecule spectroscopy reveals that individual low-light LH2 complexes from *Rhodospseudomonas palustris* 2.1.6. have a heterogeneous polypeptide composition

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Supplementary Material

| | LH2* | LH3§ | Mixed LH2-LH3† |
|---|------------------------------------|------------------------------------|------------------------------------|
| R_α (Å) | 26.09 | 26.02 | 26.02 |
| R_β (Å) | 26.92 | 26.95 | 26.92 |
| A_α (rad) | -0.2043 | -0.2015 | -0.2015 |
| A_β (rad) | 0.1566 | 0.1592 | 0.1566 |
| Π_α (rad) | -3.4957 | -3.4598 | -3.4598 |
| Π_β (rad) | -0.5058 | -0.5620 | -0.5058 |
| Φ_α (rad) | -0.1361 | -0.0801 | -0.0801 |
| Φ_β (rad) | -0.1284 | -0.1288 | -0.1284 |
| dH (Å) | 0.00725 | -0.0785 | 0.00725 |
| $V_{n,i}; V_{n,e}$ (cm ⁻¹) | 254 ^a ;226 ^a | 256 ^b ;210 ^b | 270 ^c ;230 ^c |
| $W_\alpha; W_\beta$ (cm ⁻¹) | -35 ^a ;-26 ^a | -38 ^b ;22 ^b | -38 ^c ;-25 ^c |

Note: R_α and R_β , radius of α - and β -bound Bchl *a* circle in xy-plane; A_α and A_β , geometrical angle of the pigment of α - and β - bound Bchl *a* in xy-plane; Π_α and Π_β , in-plane dipole tilt from circular tangent of the α - and β - bound Bchl *a* in xy-plane; Φ_α and Φ_β , out-of-plane dipole tilt of the α - and β - bound Bchl *a* in z-plane; dH, height differences between centres α - and β - unit in z-plane. $V_{n,i}$ and $V_{n,e}$, the nearest-neighbour intra- and inter-dimer interaction; $W_\alpha; W_\beta$, the α -next-nearest-neighbour interaction and the β -next-nearest-neighbour interaction

* McDermott, S.M., et al., 1995, *Nature* 375, 517-521 and Papiz, M.Z., et al., 2003, *J Mol Biol* 326, 1523-1538. § McLuskey, K., et al., 2001, *Biochemistry* 40(30), 8783-8789.

^aHofmann, C., et al., 2004, *Chem Phys Lett* 395, 373-378. ^bde Ruijter, W.P.F., et al., 2007, *Chem Phys* 341, 320-325.

†^c This work

Table S1. The coordinate of the arrangement of Bchl *a* molecules in an LH2 complex according to the x-ray structural data.

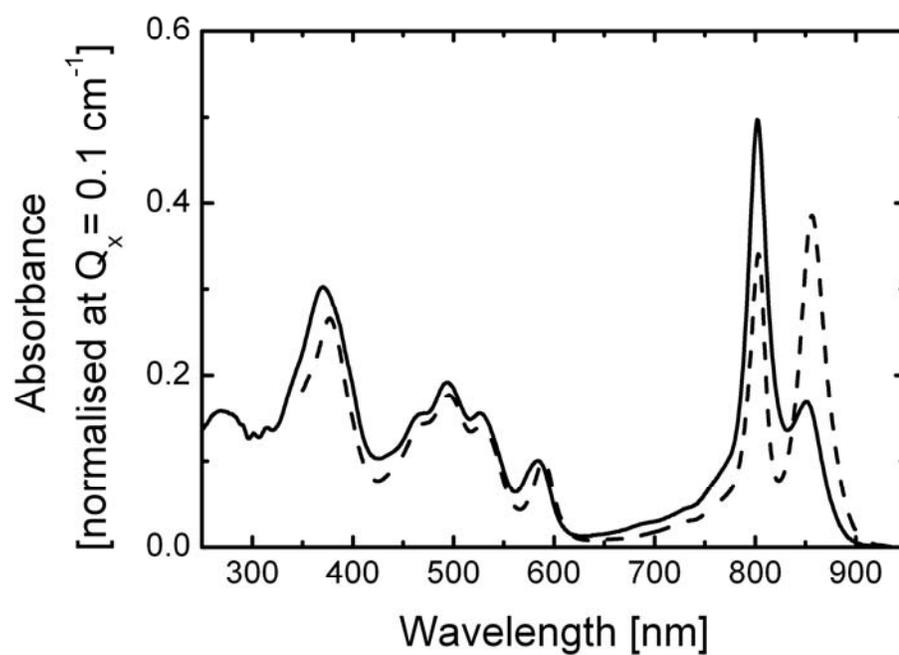


Figure S1. Room-temperature absorption spectra of *Rps. palustris* 2.1.6 grown at high-light (dashed line) and at low-light intensity (solid line). The absorption spectra are normalised at the Q_x-band around 590 nm.

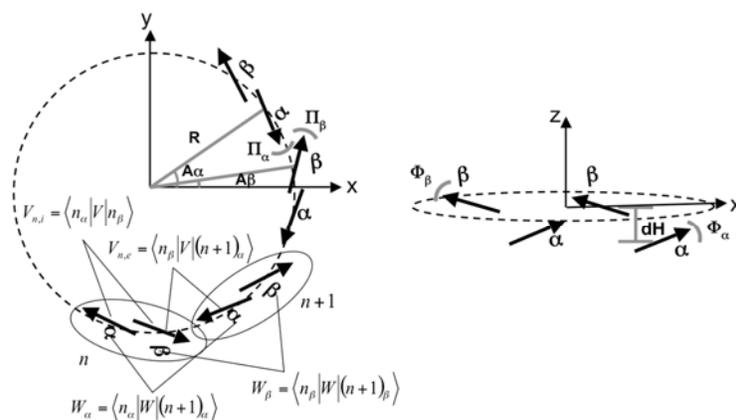


Figure S2. A schematic representation of the transition-dipole moments and the coordinate arrangement of the α - and β -bound Bchl *a* molecules in the xy -plane (left) and zy -plane (right). The $|n_\alpha\rangle$ etc. correspond to the wavefunctions of the electronically excited state localised on the α -bound Bchl *a* molecule in dimer n , respectively. The strongest contributions to the interaction result from the matrix elements for the intradimer nearest-neighbour interaction $V_{n,i}$, the interdimer nearest neighbour interaction $V_{n,e}$, the α -next-nearest-neighbour interaction W_α , and the β -next-nearest-neighbour interaction W_β , respectively. The geometrical arrangement of the α - and β -bound Bchl *a* molecules are defined by the radius of α - and β -unit circle in xy -plane R_u ($u = \alpha, \beta$), the geometrical angle of the pigment of α - and β -unit in xy -plane A_u , the in-plane tilt of the transition-dipole moment of the α - and β -Bchl *a* from the circular tangent in xy -plane Π_u , the height differences between the centres of the α - and β -Bchl *a* in the z -plane dH_u , and the out-of-plane tilt of the transition-dipole moment of the α - and β -Bchl *a* in the z -plane Φ . The actual values of these parameters are summarised in table 1 together with the respective data for LH2 and LH3 from *Rhodospseudomonas acidophila*. The circles with the dashed line help to orient our eyes.