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Proposal for verifying dipole properties of light-harvesting antennas

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ABSTRACT

For light harvesters with a reaction center complex (LH1-RC complex) of three types, we propose an experiment to verify our analysis based upon antenna theories that automatically include the required structural information. Our analysis conforms to the current understanding of light-harvesting antennas in that we can explain known properties of these complexes. We provide an explanation for the functional roles of the notch at the light harvester, a functional role of the polypeptide called PufX or W at the opening, a functional role of the special pair, a reason that the cross section of the light harvester must not be circular, a reason that the light harvester must not be spherical, reasons for the use of dielectric bacteriochlorophylls instead of conductors to make the light harvester, a mechanism to prevent damage from excess sunlight, an advantage of the dimeric form, and reasons for the modular design of nature. Based upon our analysis we provide a mechanism for dimerization. We predict that the dimeric form of light-harvesting complexes is favored under intense sunlight. We further comment upon the classification of the dimeric or S-shape complexes. The S-shape complexes should not be considered as the third type of light harvester but simply as a composite form.

1. Introduction

Photosynthesis is divided into light-dependent reactions and the Calvin cycle (carbon fixation reactions) [1,2]. The primary step of the light-dependent reaction includes energy transfer and electron transfer. The Calvin cycle is a sequence of chemical processes, whereas the energy transfer step might be analyzed physically.

To consider the interaction of light and a single atom we can approximate the system as a two-level system. However, if the number of atoms grows and the system becomes extended in space, the interference from individual effects will include time-lag. Biological systems often fall into this later case. A theory to sum-up individual effects of light-matter interaction is called antennas theory. In an antenna theory the most important information is the geometry of the antenna which will produce the time-lag. A proposal has appeared in which DNA is considered as a fractal antenna when placed in electromagnetic fields [3].

Beginning about 1995, a reasonably complete picture of the bacterial light-harvesting (LH) systems has been acquired [4–6]. Many such structures have been subsequently analyzed [7]. The light harvesters with a reaction center complex (LH1-RC) is particularly interesting as it is a fully fledged antenna, even without LH2. Therefore, the LH1-RC complex serves as a minimum model we should consider.

Such antenna of three basic types have been discovered:

- The most common form of LH1-RC complex exists as monomeric form with RC surrounded by a closed elliptical ring such as for *Blastochloris viridis* [8], *Phaeospirillum (Phs.) molischianum*; previous name *Rhodospirillum (Rsp.)* [9,10], *R. rubrum* [11], *Rhodobacter (Rba.) veldkampii* [12,13], *R. capsulatus* [14], *R. vinaykumarii* [14], and *Thermochromatium (Tch.) tepidum* [15].
- In *Rhodopseudomonas (Rps.) palustris*, the complex is found in a monometric form that contains an opening [16]. The cross section of this LH1-RC complex is elliptical; the RC is surrounded with an incomplete double ring of helices. Some species, such as *R. sphaeroides*, have a polypeptide component termed “W” is found at the opening, similar to the PufX polypeptide in several *Rba.* species for which a precise function has long been debated [14,17-20]. The elliptical LH1 complex has an outer long axis of length 110 Å and a short axis of length 95 Å; the greatest dimension of the inside of this LH1 is 78 Å. A gap of 4 Å is found between the RC and the ring, as the RC has a long dimension of 70 Å and the orientation of the long axis of the LH1 ellipse coincides with the long axis of the RC. The height of the cylindrical (more precisely toroidal) shape of the molecule can be obtained with software such as Jmol or PyMOL, using the data from PDB, to be about half the width of the molecule.
- A dimeric form exists in *R. sphaeroides* [14,21-24], *R. blasticus* [25], *Rhodobacter changlensis* and *Rhodobacter azotoformans* [14].

We show the structures of a number of these complexes in Fig. 1. In

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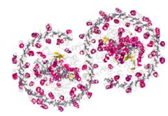
protein	PDB ID	symmetry	cartoon
Tch. tepidum [15]	4V8K	C16	
Rps. palustris [16]	1PYH		
Rba. sphaeroides [19]	4V9G		

Fig. 1. Three types of LH1-RC complex. The molecules are identified by the PDB ID assigned by Protein Data Bank http://www.rcsb.org/pdb/.

some species, such as *Rhodobaca bogoriensis*, monomeric and dimeric forms have been shown to coexist [18].

The standard model to consider energy transfer within light-harvesting complexes in the photosynthesis community is the exciton theory. For instance, Komatsu et al. used exciton theory to calculate the absorption spectra and energy transfer rates of an array of LH2 [26]. They approximated the ring as an array of dipoles. The problem of this model is it involves a calibration procedure, which is *ad hoc*, even though the authors claim their calculation is *ab initio*.

We address the three forms mentioned, in particular the dimer form from a classical electrodynamic point following the analysis of non-reciprocal properties in a previous paper [27], in the following. Our analysis takes the structural information into consideration and requires no *ad hoc* parameter. We hence propose an experiment to verify our theory.

2. Loop Antennas

Two simplified shapes shown in the figure resemble the *R. palustris* (1PYH) LH1-RC complex shown in Fig. 1. Fig. 2 (a) is simple and can be solved with algebraic methods, whereas Fig. 2 (b), although resembling the LH1-RC complex more closely, has a resonant frequency only

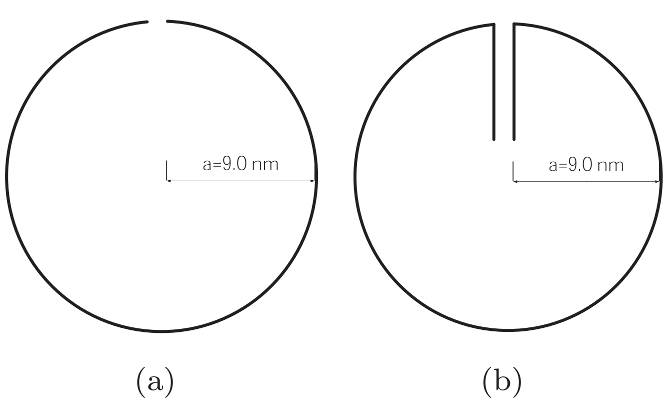


Fig. 2. Antennas of two idealized shapes. According to experimental data, the exterior length of the long axis of the *R. palustris* LH1-RC complex is 110 Å, while the short axis is 95 Å; the longest dimension of the inner LH1 is 78 Å. We choose 90 Å as the average value in our figures. (a) Is a simple loop antenna, while (b) is called a loop antenna with line feed. The opening can be filled with other material to adjust the resonance frequency, whereas the LH1 has a PufX/W over there. The feed line, though resembling the special pair in the RC, modifies only slightly the resonant frequency, but the notch is essential.

slightly modified from that of Fig. 2 (a). We hence consider only Fig. 2 (a). The notch is essential not only for concentrating but also to take out the energy received by the $LH1-RC$ complex [28]. The molecule of 1PYH shown in Fig. 1 also has a notch. Chemists describe the function of the opening as enabling the passage of quinones (charge carriers) to the RC [21]. Without this opening, such as the molecule 4V8K, other mechanisms have to be employed to retrieve the energy received. In engineering the opening can be filled with a spacer material to adjust the resonance frequency, which is interpreted as impedance matching in antenna theory [29], while in biology a polypeptide called PufX or W is often found over there. Our analysis here show that PufX/W and the notch arise from distinct physics; one does not imply the other.

In engineering, antennas of such shapes are well studied: they are called loop antennas and loop antennas with line feed, respectively [30]. The line feed resembles the special pair from the light harvester to the reaction center.

Loop antennas can be further divided into two categories depending upon their size relative to the wavelength of operation. If an antenna has a radius smaller than the wavelength of operation, it is called a small-loop antenna; otherwise, a resonant-loop antenna. As the wavelength, λ, of operation of LH1 or LH2, $800-900$ *nm*, is much larger than the radius of the antenna, 9.0 *nm*, the light-harvesting antenna is a small-loop antenna, more precisely deep sub-wavelength antenna, which has a small radiation resistance and a large reactance; its impedance is hence difficult to match with that of the transmitter. As a result such antennas serve mainly as a receiving antenna for which an impedance mismatch loss can be tolerated. A small-loop antenna is equivalent to a short-dipole antenna of which the receiving (radiation) pattern has a toroidal shape, with electric and magnetic fields interchanged, and thus serves as a magnetic dipole with the direction of dipole orthogonal to the loop plane.

There are a complete way and a simple way for arriving at the electromagnetic properties of such an antenna. We begin with the complete way.

Let the radius of the loop located at the origin be a, the plane of the loop be $x-y$, and the angle from the x $-$axis be ϕ. If the current I around the loop is uniform and in phase, the only component of the vector potential is A_ϕ, as shown in Fig. 3 (a). The infinitesimal value of A_ϕ at a point away from the loop by distance r caused by two diametrically opposed infinitesimal dipoles is

$$\mathrm{d}A_\phi = \frac{\mu \mathrm{d}M}{4\pi r}, \tag{1}$$

in which $\mathrm{d}M = 2j[I]a\cos\phi[\sin(2\pi a\cos\phi\sin\theta/\lambda)]\mathrm{d}\phi$, θ is the angle