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A Structural Basis
for
Electron Transfer in Bacterial Photosynthesis

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Abstract

Triplet data for the primary donor in single crystals of bacterial reaction centers of *Rhodobacter sphaeroides* and *Rhodopseudomonas viridis* are interpreted in terms of the corresponding x-ray structures. The analysis of electron paramagnetic resonance data from single crystals (triplet zero field splitting and cation and triplet linewidth of the primary special pair donor of bacterial reaction centers) is extended to systems of a non-crystalline nature. A unified interpretation based on frontier molecular orbitals concludes that the special pair behaves like a supermolecule in all wild-type bacteria investigated here. However, in heterodimers of *Rb. capsulatus* (His^{M200} changed to Leu or Phe with the result that the M-half of the special pair is converted to bacteriopheophytin) the special pair possesses the EPR properties more appropriately described in terms of a monomer. In all cases the triplet state and cation EPR properties appear to be dominated by the highest occupied molecular orbitals. These conclusions derived from EPR experiments are supplemented by data from Stark spectroscopy of reaction centers from *Rb. capsulatus*. The most red-shifted Stark band in the *Rb. capsulatus* heterodimer is relatively intense and is interpreted as a "pure" charge transfer band within the special pair donor. This explanation locates the energy of $|\mathrm{Bchl}^{-}{}_{M}>|\mathrm{Bchl}^{+}{}_{L}>$ or $|\mathrm{Bchl}^{+}{}_{M}>|\mathrm{Bchl}^{-}{}_{L}>$, the internal charge transfer state, anywhere from ~.1 ev to ~.3 ev above $^{1*}[|\mathrm{Bchl}_{M}>|\mathrm{Bchl}_{L}>]$, the first excited singlet state of the primary donor. This internal charge transfer state has been invoked previously in the initial mechanism of electron transfer in photosynthesis.

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Introduction[a]

The x-ray crystal structures of two photosynthetic bacterial reaction centers (RC's), *Rhodopseudomonas viridis* and *Rhodobacter sphaeroides*, are now known[1,2,3]. These structures have confirmed that the primary donor in these RCs consists of a dimeric bacteriochlorophyll special pair[4], $[|\mathrm{Bchl}_M>|\mathrm{Bchl}_L>]$, with approximate C2 symmetry. The subscripts M- and L- refer to the M-protein subunit and the L-protein subunit respectively. The charge separation process is initiated by the absorption of light by the special pair to form the excited singlet state of the special pair, designated $^{1*}[|\mathrm{Bchl}_M>|\mathrm{Bchl}_L>]$. The primary electron transfer occurs to form an initial radical pair species involving the special pair and a distant bacteriopheophytin in the L-protein subunit in less than 3.5 ps[5,6,7,8,9,10,11]. When the special pair was proposed to explain the magnetic resonance data over fifteen years ago[4], the initial charge separation state was invoked as $\mathrm{Bchl}^+\mathrm{Bchl}^-$ [12,13] where each Bchl is a member of the special pair. Similar CT states have again been invoked in some recent, more sophisticated models of the initial mechanism of electron transfer. Current detailed explanations of the initial electron transfer reaction rate of bacterial RCs are based on electron transfer theory[14,15]. Even though numerous experimental [5,6,7,16,17,18,19,20,21,22] and theoretical[23,24,25,26] studies have addressed the initial charge separation in RCs, the nature of the excited state of the primary donor still needs further illumination in order to obtain general agreement on the theoretical model for electron transfer.

CT states can be probed by applying a large, electric field external to the RCs and monitoring changes in spectroscopy and (or) the photosynthetic process. Kleuser and Bücher[27] studied electric field effects on the change in the optical absorption of chlorophyll a and chlorophyll b monolayers. Emrich *et al.*[28] used these results as well as their own electrochromic measurements of carotenoids to explain the light-induced absorption changes of spinach chloroplasts. Jackson and Crofts[29] studied the electrochromic effects of the carotenoid by generated external electric fields in the dark across membranes of *Rb. sphaeroides* chromatophores by ionic gradients operating through ionophorous antibiotics. More recently, electrochromism has been used to study the singlet excited state of the

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[a] Reaction center, (RC); bacteriochlorophyll, Bchl; bacteriopheophytin, Bphe, charge transfer, CT; electron paramagnetic resonance, (EPR); zero field splitting, (ZFS).

Bchl special pair. A large Stark effect was reported in the Q_y absorption of the photosynthetic bacteria *Rb. sphaeroides* by deLeeuv *et al.*[16] The value of the Stark effect in the special pair band was first quantitated by Lockhart *et al.*[17] and later confirmed by Lösche *et al.*[18] Both groups suggested that the large Stark effect may be due to a mixing of the charge-transfer state $|^{+}Bchl_M\rangle|^{-}Bchl_L\rangle$ and (or) $|^{-}Bchl_M\rangle|^{+}Bchl_L\rangle$ with the excited singlet state $^{1*}[|Bchl_M\rangle|Bchl_L\rangle]$ of the bacteriochlorophyll special pair.

Experimental Approach

In our opinion, the ultimate understanding of the initial steps in photosynthesis and electron transfer will require detailed knowledge of numerous molecular parameters. Of all such parameters the Hamiltonian matrix elements believed responsible for electron transfer are generally regarded as the most desirable. The standard experimental approach appropriate to the determination of the Hamiltonian matrix elements relevant to electron transfer is the direct measurement by spectroscopy of the kinetics of electron transfer. However, the direct and accurate connection between spectroscopic parameters and structure remains rather limited. This paucity reflects the fact that few detailed spectroscopic studies have been performed in single crystals of RCs. For that reason we have examined the triplet state in single crystals of reaction centers where a very accurate connection between structure and EPR spectroscopy is readily achieved. Extension of EPR to non-crystalline environments is based on rigorous and well established magnetic resonance spectroscopy in single crystals.

To examine our earlier hypothesis of a CT within the special pair we have investigated RCs in which the special pair of *Rb. capsulatus* has been genetically modified through site-directed mutagenesis[30]. We have probed two genetically modified RCs in which histidine M200, the axial ligand to the M-side Bchl of the special pair, was replaced with either leucine or phenylalanine. This "simple" amino acid substitution results in the replacement of the M-side Bchl with Bphe, forming a Bchl-Bphe heterodimer [8,30]. The heterodimer RCs also differ from wild-type in quantum yield and rate of electron transfer. The quantum yield of the electron transfer from $D \rightarrow D^{+}Bphe_L^{-}$ is ~50% in $His^{M200} \rightarrow$ Leu RCs, much lower than the ~100% yield for wild-type. The time constant for this electron transfer reaction is ~30 ps, about one order of magnitude slower than the 3.5 ps lifetime for wild-type [8]. These reasonably large differences in the electron transfer process make the heterodimer an excellent choice to test the credibility of various theoretical models of photosynthesis.

In particular, we have measured the Stark spectra and the triplet and cation EPR spectra of wild-type versus heterodimer containing RCs from *Rb. capsulatus.* The differences and similarities in the Stark spectrum, in the triplet EPR data and in the cation EPR linewidths of these three RCs of *Rb. capsulatus* as well as those of *Rp. viridis* and *Rb. sphaeroides* are discussed. Ultimately, these experimental results are intended to clarify the nature of the primary donor and its role in the initial act of photosynthesis. Thus the next step is the interpretation of the spectroscopic measurements in terms of structure and electron transfer. In this regard, Closs *et al.*[31] have shown a connection between the matrix elements of electron transfer and triplet energy transfer using a frontier molecular orbital approach. Consequently, another method of examining the matrix elements of electron transfer is by indirect inference from the rate constants for triplet energy transfer. Ultimately both approaches will require incorporation of the precise structural details of the molecular complex in which electron or triplet transfer occurs. In this paper no rate constants are measured; instead, the spectroscopic properties of excited singlet states, excited triplet states and cation states are described that can be interpreted in terms of frontier molecular orbitals using an approach similar to that of Closs et al.[31] for transfer rates.

The EPR experimental conditions are similar to those reported previously [4,12]. Wild-type, His^{M200} → Leu, and His^{M200} → Phe reaction centers of *Rb. capsulatus* were prepared by standard [32] procedures [8,30]. The Stark spectroscopy and normal spectroscopy were performed in liquid nitrogen by previously developed methods [17,18,33]. Our experimental system was verified with *Rb. sphaeroides* where we obtained results identical to previous work [17,18,19].

Results

In *Rb. sphaeroides* the triplet state of the special pair exhibits approximate C2 symmetry since the triplet state is located almost equally on both halves of the special pair[36]. In *Rp. viridis* the triplet state is located mainly on the L-side of the special pair[36], the flatter half of the special pair according to the x-ray structure [1]. Table I summarizes the EPR parameters used in this discussion [36].

The absorption, second derivative, and Stark spectra at 77 K for the Q_y absorption bands of wild-type, $\mathrm{His}^{M200} \rightarrow$ Leu, and $\mathrm{His}^{M200} \rightarrow$ Phe reaction centers from *Rb. capsulatus* have been determined by DiMagno *et al.*[34]. The Q_y Stark spectra for wild-type *Rb. capsulatus* exhibits similar features as *Rb. sphaeroides R-26*[17,18,19,20,35] and *Rp. viridis* [17,18,19]. The absorption, second derivative, and Stark spectra for $\mathrm{His}^{M200} \rightarrow$ Leu and $\mathrm{His}^{M200} \rightarrow$Phe RCs are nearly identical to each other. The Stark spectrum of the heterodimers are similar to the Stark spectrum of wild-type *Rb. capsulatus* in the accessary Bchl and the Bphe spectral regions, but differ dramatically in the special pair region for both the absorption and the Stark spectrum. These features suggest that the His^{M200} → Leu and $\mathrm{His}^{M200} \rightarrow$ Phe substitutions did not result in large structural changes.

Table II lists the angle, δ, between the transition moment vector, μ_{trans}, and the change in permanent dipole moment vector, $\Delta\mu_{app}$, as measured using the red most Stark band for the two *Rb. capsulatus* RCs where $\Delta\mu_{app}$ and the angle δ were determined as usual [17,18]. The results for wild-type *Rb. capsulatus* 11,530 cm^{-1} band at 77 K (δ=38.4°, $\Delta\mu_{app}$=6.7D) are the same as both *Rb. sphaeroides* and *Rp. viridis* [17,20] RCs within experimental error. Both $\mathrm{His}^{M200} \rightarrow$Leu and $\mathrm{His}^{M200} \rightarrow$ Phe RCs give the same value at ~11,000 cm^{-1} for δ and $\Delta\mu_{app}$ at 77 K (His200 → Leu: δ=20.3°, $\Delta\mu_{app} \geq 15.1$D; $\mathrm{His}^{M200} \rightarrow$ Phe: δ=22.6°, $\Delta\mu_{app} \geq 16.5$D), but the angle δ and the value $\Delta\mu_{app}$ differ substantially from wild-type *Rb. capsulatus* RCs. This 11,000 cm^{-1} band is an additional band not present in wild type and can be interpreted as a transition to a "pure" charge transfer state. We point out that no absorption peak appears in either heterodimer at 11,000 cm^{-1}. We also note that the Stark bands of the heterodimer in the spectral region (~11,000 to ~11,500 cm^{-1}) normally diagnostic of the special pair are strong, unlike the weak absorption tails in this same spectral region.

Discussion

To understand in elementary chemical terms what might be involved in describing the special pair and its role in electron transfer, a linear combination of simple molecular orbitals is usually employed. The excited states in the wild-type (subscript W) *Rp. viridis*, *Rb. sphaeroides* and *Rb. capsulatus* are expected to be linear combinations of the following frontier molecular orbitals;

$$|{}^*I>_W = |{}^*Bchl_M>|Bchl_L>,$$

$$|{}^*II>_W = |Bchl_M>|{}^*Bchl_L>,$$

$$|{}^*III>_W = |Bchl_M{}^+>|Bchl_L{}^->,$$

$$|{}^*IV>_W = |Bchl_M{}^->|Bchl_L{}^+>,$$

where * indicates either excited singlet or excited triplet. Possible excited state contributions to the heterodimer special pair mutant species of *Rb. capsulatus* (subscript H) are the following;

$$|{}^*I>_H = |{}^*Bphe_M>|Bchl_L> \qquad \text{(higher energy)},$$

$$|{}^*II>_H = |Bphe_M>|{}^*Bchl_L>,$$

$$|{}^*III>_H = |Bphe_M{}^+>|Bchl_L{}^-> \qquad \text{(higher energy)},$$

$$|{}^*IV>_H = |Bphe_M{}^->|Bchl_L{}^+>,$$

where * indicates either excited singlet or excited triplet. The heterodimer special pair states $|{}^*I>$ and $|{}^*III>$ are not considered likely participants in the eigenstates of the lowest first excited states because they are significantly higher energy due to the differences in redox potentials between bacteriopheophytin and bacteriochlorophyll[39]. Similarly, possible molecular orbitals that contribute to the wave function of the cation in wild type *Rp. viridis*, *Rb. sphaeroides*, and *Rb. capsulatus* are the following;

$$|{}^+I>_W = |{}^+Bchl_M>|Bchl_L>,$$

$$|{}^+II>_W = |Bchl_M>|{}^+Bchl_L>.$$

Finally, the possible MOs for the cation of heterodimer are the following:

$$|{}^+I>_H = |{}^+Bphe_M>|Bchl_L> \qquad \text{(higher energy)}$$

$$|{}^+II>_H = |Bphe_M>|{}^+Bchl_L>$$

Here state $|{}^+I>$ is again not considered a likely participant in the working description of the heterodimer and thus we expect the system to behave like a monomeric Bchl species. Table III lists the **approximate** percentages of each wavefunction consistent with the magnetic resonance observations. Values in Table III for the triplet state are based on experiments in single crystals[36].

The unusually small ZFS for the triplet state in *Rp. viridis* can be explained by ~77% of $|Bchl_M>|{}^{3*}Bchl_L>$ mixed with ~23% of $|Bchl_M{}^+>|Bchl_L{}^->$, i.e., a special pair mechanism[36]. Such a supermolecule mechanism is confirmed by phosphorescence measurements of Takiff and Boxer [37].

Consequently, alternative monomer (i.e., non-supermolecule) explanations involving different molecular orbitals induced by a special protein environment are ruled out. Because of the vector nature of the ZFS tensor, the 23% charge transfer state reduces the ZFS in magnitude but does not alter its direction significantly away from the L-side macrocycle. On the other hand the heterodimer special pair has ZFS completely characteristic of a monomer of Bchl. This indicates 100% $|\mathrm{Bphe}_M\rangle|^{3*}\mathrm{Bchl}_L\rangle$ and no participation of charge transfer. In both cases the C2 symmetry appears to be completely broken in the triplet state; however, from the point of view of the ZFS the special pair in *Rp. viridis* behaves like a supermolecule dimer whereas the heterodimer special pair behaves like a simple monomer. In both cases a generalized special pair model can explain the triplet (single crystals only) and cation (general) EPR linewidth equally well. The second moment of the EPR lineshape is given by

$$M_{sp} = f^2 M_m + (1-f)^2 M_m ,$$

where M_{sp} and M_m are the second moments of the special pair and the monomer respectively. In these systems the observed linewidth is proportional to the square root of the second moment. In such a general model the fraction of occupancy of any one type of state (charge transfer, cation, triplet, or singlet) on the L-side is f and on the M-side is 1-f. The f can range from 0 to 1 where f = 0.5 describes the special pair with C2 symmetry. Thus, the triplet or cation delocalization can range from approximate C2 special pair as in *Rb. sphaeroides* to complete localization on the L-side of the special pair as in the heterodimer mutants of *Rp. capsulatus.* Using values of f determined from Table III the above equation offers a reasonable explanation of the experimental linewidths of Table I. In other words, the observed range of delocalization can be rationalized in terms of a simple frontier molecular orbital description.

The nature of the first excited singlet excited state can be examined by Stark spectroscopy. Based on such Stark spectroscopy here we present recent results for RCs of *Rb. capsulatus.* The magnitude of $\Delta\mu_{app}$ for RCs of *Rb. capsulatus* ($\mathrm{His}^{M200} \rightarrow$ Leu) and *Rb. capsulatus* ($\mathrm{His}^{M200} \rightarrow$ Phe) is larger than wild-type RCs for the red most band. For the Leu heterodimer this red most Stark band centered at ~11,020 cm^{-1} strongly suggests the formation of a charge-transfer state within the heterodimer that evolves within several hundred femtoseconds after the excitation flash [8]. The other Stark band at ~12,110 cm^{-1} is interpreted as the "normal" exciton band characteristic of the special pair. Previous calculations indicate that the relative energy of the charge-transfer state might be above the lowest excited singlet state of the special pair in wild-type RCs[38]. When the constituents of the charge-transfer state change from $Bchl_L^+Bchl_M^- \rightarrow Bchl_L^+Bphe_M^-$ in the heterodimer, the energy of the charge-transfer state will decrease by ~.1 *to* ~ .3 eV[39] and this should *narrow* the energy gap between the "normal" exciton and "pure" CT states. This decrease in energy of the charge-transfer state is expected to mix the corresponding oscillators in the heterodimer relative to wild-type RCs, thus giving some oscillator strength to the normally invisible charge transfer band. Such a picture is compatible with the extensive red tail in the normal optical spectrum in the heterodimer mutant. This conclusion is also consistent with the investigation by Kirmaier *et al.*[8], who suggested the pure charge-transfer state ($^+Bchl_L^-Bphe_M$) in the heterodimer to explain the time resolved transient absorption difference spectra and the decreased rate of electron transfer (~30 ps) to the initial radical pair state.

The values for $\Delta\mu_{app}$ listed in Table II assume that all of the red most Stark lineshapes are pure second derivatives. The largest error in determining $\Delta\mu_{app}$ was in obtaining the weighted second derivative of the absorption spectrum, especially in the case of the broad featureless absorption spectra of the mutants. In the case of the two heterodimer RCs, no second derivative signal could be measured without significant noise. Thus, limits were established for the size of the second derivative as -2.4×10^{-7} for $His^{M200} \rightarrow$ Phe RC and -1.7×10^{-7} for $His^{M200} \rightarrow$ Leu RCs. These values correspond to minima for $\Delta\mu_{app}$ of 16.5 for $His^{M200} \rightarrow$ Phe and 15.1 for $His^{M200} \rightarrow$ Leu RCs. Approximately 40 Debye is an estimate of the value of $\Delta\mu_{app}$ for a pure charge separation within the special pair. Based on the estimated error in experimental and simulated data, we are only able to bracket the value for $\Delta\mu_{app}$ for the heterodimers between ~15 and ~40 Debye. We note that the value for $\Delta\mu_{app}$ is larger in the heterodimer than in wild-type, again consistent with an increase in the amount of charge-transfer character in the excited singlet of RCs of the heterodimers.

Although no crystal structure exists for *Rb. capsulatus*, linear dichroism shows that the orientation of pigments with respect to the membrane direction in wild-type, His^{M200} → Leu, and His^{M200} → Phe RCs are similar to each other and to RCs in *Rb. sphaeroides* R26 [40]. Thus, the Stark data will be described using the crystal structure of *Rb. sphaeroides* RCs, which should act as a good model for *Rb. capsulatus* because *Rb. sphaeroides* contains the same type of bacteriochlorophyll and bacteriopheophytin and a similar protein sequence in the vicinity of the special pair. From the crystal structure of *Rb. sphaeroides* R26 RCs, the angle between Q_Y transition moments of the members of the special pair is ~38°. The observed change in the angle δ between wild-type *Rb. capsulatus* and the *Rb. capsulatus* His^{M200} → Phe, $\delta_{wild\text{-}type} - \delta_{Phe}$, is 15.8°; and the change in the angle δ between wild-type *Rb. capsulatus* and the *Rb. capsulatus* His_{M200} → Leu, $\delta_{wild\text{-}type} - \delta_{Leu}$, is 18.1° in reasonable agreement with one half of 38° observed in the x-ray structure of *R26* RCs. The change of δ between the wild-type and heterodimer RCs can be attributed to the breaking of the apparent C_2 symmetry due to either the change in the Q_Y transition moment or the change in the direction of $\Delta\mu_{app}$ from a dimer to monomer-like special pair. Since a larger value for $\Delta\mu_{app}$ in heterodimer RCs, is observed, the change in δ most likely is due to the different direction of $\Delta\mu_{app}$ in dimeric-like versus monomeric-like donor. This observation supports the claim of charge-transfer n the initially excited singlet state in wild type bacterial reaction centers[12,13,36] and that this charge transfer state is above the first excited singlet as predicted by Parson and Warshel [38].

Conclusions

Because of the difference in redox potentials between the bacteriochlorophyll and bacteriopheophytin, the sharing of spin density should be unequal in the oxidized heterodimer. This result is confirmed[41] in EPR experiments on the two heterodimers for both the triplet and the cation. The EPR linewidth from wild-type RC suggested a special pair dimer $^+[Bchl_L Bchl_M]^4$, while the EPR linewidth from the heterodimer containing RCs indicated monomeric $Bchl^+{}_L$ electron donor.[41] The asymmetric charge distribution of the oxidized heterodimer confirm the notion that an internal CT state within the heterodimer special pair would be more favored due to the difference in redox potentials of the different heterodimer constituents. Both the Stark data and the transient absorption data suggest a rather asymmetric heterodimer special pair. In our measurements, δ appears to be more like monomeric pigments rather than the special pair of *Rb. sphaeroides*. *Rp. viridis*, and wild type *Rb. capsulatus* [17,18,34].

The simple MO description that explains the size and directions of the ZFS also offers a simple explanation of both the triplet and cation epr linewidth. This frontier orbital approach suggests that triplet state is dominated by HOMO orbitals since certainly the cation is. The symmetry can be broken in two distinct ways: by small changes in the environment whereby the energies of the orbitals to be mixed between the two halves of the special pair are very similar, or by much larger changes where the two molecular orbitals are significantly different as in the heterodimer special pair where one half is bacteriopheophytin and one half is bacteriochlorophyll. In the former case the triplet behaves like a supermolecule, and in the latter case the triplet behaves as a simple monomer as clearly evidenced by the triplet zero field parameter. This also suggests that the triplet is dominated by the HOMO since the charge transfer in the supermolecule is less likely to involve the much higher triplet charge transfer state. The energy of the state $|\mathrm{Bchl}^{+}{}_{M}\rangle|\mathrm{Bchl}^{-}{}_{L}\rangle$ should be ~.1 to ~.3 ev above the lowest excited singlet state, $^{1*}[|\mathrm{Bchl}_{M}\rangle|\mathrm{Bchl}_{L}\rangle]$, in wild-type reaction centers if the red-most Stark band arises from a "pure" CT state, $|\mathrm{Bphe}^{-}{}_{M}\rangle|\mathrm{Bchl}^{+}{}_{L}\rangle$, in the heterodimer containing reaction centers as we have suggested here.

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Table I
EPR Properties of Bacteriochlorophylls a and b and the Primary Donors in *Rp. viridis*, *Rb. sphaeroides* and *Rb. capsulatus* Reaction Centers

	TRIPLET			CATION
	D	E (gauss)	ΔH_{pp}	ΔH_{pp}
Bchl b in vitro	227	59	--	13.9
Bphe b in vitro	226	53	--	--
$Bchl_M Bchl_L$ (*viridis* - ^1H)	165	40	11.3	11.5^*
$Bchl_M Bchl_L$ (*viridis* - ^2H)	165	40	6.8^*	4.6^*
Bchl a in vitro	240	57	--	13.0
Bphe a in vitro	274	48	--	13.5
$Bchl_M Bchl_L$ (*sphaeroides* - ^1H)	199	33	10.3^*	9.6^*
$Bchl_M Bchl_L$ (*capsulatus* - ^1H)	210	37	--	10.6
$Bphe_M Bchl_L$ (*capsulatus* - ^1H) (His → Phe)	225	64	--	12.0
$Bphe_M Bchl_L$ (*capsulatus* - ^1H) (His →Leu)	225	64	--	12.2

*, single crystal data.

Table II
A comparison of the direction and magnitude of the apparent dipole moments, $\Delta\mu_{app}$, in photosynthetic bacteria.[a]

Photosynthetic Bacteria	δ,°	$\Delta\mu_{app}$, D	ν, cm^{-1}
Rb. capsulatus wild-type	38.4 ± 2.3	6.7 ± 1.0	11,530
Rb. capsulatus His^{M200} → Leu	20.3 ± 3.3	$\geq$ 15.1	11,020
Rb. capsulatus His^{M200} → Phe	22.6 ± 2.4	$\geq$ 16.5	11,147

Table III
Approximate Wavefunctions of the Triplet and Cation of the Primary Donor

	TRIPLET				CATION	
	I	II	III[a,b]	IV[a,b]	I[a,b]	II[a,b]
Rb. sphaeroides	32	55	13	0	38.5	61.5
Rp. viridis	0	77	23	0	11.5	88.5
Rb. capsulatus (wild-type)	c	c	c	c	c	c
Rb. capsulatus (heterodimer)	0	100	0	0	0	100

a, charge asymmetry is assumed and is not determined by EPR.
b, asymmetry can be reversed from that given here.