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The heart of oxygenic photosynthesis illuminated

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Citation

Janssen, G. J. (2013, December 4). *The heart of oxygenic photosynthesis illuminated*. Retrieved from <https://hdl.handle.net/1887/22697>

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Author: Janssen, Geertje Jacoba

Title: The heart of oxygenic photosynthesis illuminated

Issue Date: 2013-12-04

THE HEART
OF
OXYGENIC
PHOTOSYNTHESIS
illuminated

Geertje Jacoba Janssen

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The Heart of Oxygenic Photosynthesis illuminated

Ph.D. Thesis, Leiden University, 4th December 2013

ISBN: 978909028000

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Cover design painting “Klaprozen” by Herman van der Wal

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THE HEART OF OXYGENIC PHOTOSYNTHESIS illuminated

PROEFSCHRIFT

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van de Rector Magnificus Prof. Mr. C.J.J.M. Stolker,
volgens besluit van het College voor Promoties
te verdedigen op Woensdag 4 December 2013
klokke 08:45

door

Geertje Jacoba Janssen

geboren te Londen, Verenigd Koninkrijk in 1984

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LIST OF ABBREVIATIONS

A	Electron acceptor
A ₀	Chl <i>a</i> primary electron acceptor in PSI
A ₁	Quinone secondary electron acceptor in PSI
ALA	δ-aminolevulinic acid
BBY	PSII enriched membrane
BChl	Bacteriochlorophyll
Chl <i>a</i>	Chlorophyll a
Car	Carotenoid
CS	Chemical shift
D	Electron donor
DD	Differential decay
DFT	Density functional theory
DNP	Dynamic nuclear polarization
DR	Differential relaxation
ENDOR	Electron nuclear double resonance
EPR	Electron paramagnetic resonance
ET	Electron transfer
<i>Hb.</i>	Heliobacter
ISC	Intersystem crossing
LCMS	Liquid Chromatography Mass Spectroscopy
MAS	Magic-angle spinning
n.a.	Natural abundance
ns	Nanosecond
NMR	Nuclear magnetic resonance

NPQ	non-photochemical quenching
OEC	Oxygen evolving complex
P _{D1}	Donor Chl <i>a</i> of PSII attached to the D1 branch of the RC
P _M	BChl <i>a</i> of P attached to the M branch of the RC
P _L	BChl <i>a</i> of P attached to the L branch of the RC
Phe <i>a</i>	Pheophytin <i>a</i>
Photo-CIDNP	Photochemically induced nuclear polarization
PSI	Photosystem I
PSII	Photosystem II
QM/MM	Quantum mechanics/molecular mechanics
<i>Rb.</i>	<i>Rhodobacter</i>
RC	Reaction center
rf	Radio-frequency
RPM	Radical pair mechanism
RT	Room temperature (293K)
TNP	Transient nuclear polarization
TOP	Transiently obscured polarization
TSM	Three-spin mixing
WT	Wild type
Φ	Bacteriopheophytin

LIST OF SYMBOLS

A_{zz}	(3,3) element of the hyperfine tensor
A_{zx}, A_{zy}	Pseudosecular elements of the hyperfine interaction
B	Absolute pseudosecular hf interaction

D	Magnitude of the electron-electron dipolar coupling
d	Electron-electron coupling
d_{vdW}	van der Waals distance
I	measured LCMS peak intensity
$I_{\%}$	relative LCMS peak intensity
I_t	calculated true LCMS peak intensity
J	Electron-electron exchange coupling
ρ_i	Electron spin density
S	Singlet radical state
T_0	Triplet state with magnetic quantum number 0
T_{ev}	Evolution time
T_S	Lifetime of the singlet radical state
T_T	Lifetime of the triplet radical state
τ_p	Laser pulse duration
ΔA	Hyperfine anisotropy
Δt	delay time between laser pulse and NMR detection
$\Delta\Omega$	Difference of the electron Zeeman interaction between the two radicals
ω_I	Nuclear Zeeman interaction

