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Spin-torch experiment on reaction centers of *Rhodobacter sphaeroides*

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References

- (1) Abragam, A. (1961) *Principles of Nuclear Magnetism*. Oxford: Oxford University Press.
- (2) ADF2009.01 (2009) SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>.
- (3) Alia, A., Matysik, J., Soede-Huijbregts, C., Baldus, M., Raap, J., Lugtenburg, J., Gast, P., van Gorkom, H. J., Hoff, A. J. and de Groot, H. J. M. (2001) Ultrahigh field MAS NMR dipolar correlation spectroscopy of the histidine residues in light-harvesting complex II from photosynthetic bacteria reveals partial internal charge transfer in the B850/His complex. *J. Am. Chem. Soc.*, 123, 4803-4809.
- (4) Alia, A., Roy, E., Gast, P., van Gorkom, H. J., de Groot, H. J. M., Jeschke, G. and Matysik, J. (2004) Photochemically induced dynamic nuclear polarization in photosystem I of plants observed by ^{13}C magic-angle spinning NMR. *J. Am. Chem. Soc.*, 126, 12819-12826.
- (5) Alia, A., Wawrzyniak, P. K., Janssen, G. J., Buda, F., Matysik, J. and de Groot, H. J. M. (2009) Differential charge polarization of axial histidines in bacterial reaction centers balances the asymmetry of the special pair. *J. Am. Chem. Soc.*, 131, 9626-9627.
- (6) Allen, J. P., Feher, G., Yeates, T. O., Komiya, H. and Rees, D. C. (1987) Structure of the reaction center from *Rhodobacter sphaeroides* R-26 the protein subunits. *Proc. Natl. Acad. Sci. U. S. A.*, 84, 6162-6166.
- (7) Andrew, E. R., Bradbury, A. and Eades, R. G. (1958) Nuclear magnetic resonance spectra from a crystal rotated at high speed. *Nature*, 182, 1659-1659.
- (8) Andrew, E. R., Bradbury, A. and Eades, R. G. (1959) *Nature*, 162, 1659.
- (9) Bahatyrova, S., Frese, R. N., Siebert, C. A., Olsen, J. D., van der Werf, K. O., van Grondelle, R., Niederman, R. A., Bullough, P. A., Otto, C. and Hunter, C. N. (2004) The native architecture of a photosynthetic membrane. *Nature*, 430, 1058-1062.
- (10) Baldus, M. and Meier, B. H. (1997) Broadband polarization transfer under magic-angle spinning: Application to total through-space-correlation NMR spectroscopy. *J. Magn. Reson.*, 128, 172-193.
- (11) Becke, A. D. (1988) Density-functional exchange-energy approximation with correct asymptotic-behavior. *Phys. Rev. A*, 38, 3098-3100.
- (12) Bennett, A. E., Griffin, R. G., Ok, J. H. and Vega, S. (1992) Chemical shift correlation spectroscopy in rotating solids: Radio frequency-driven dipolar recoupling and longitudinal exchange. *J. Chem. Phys.*, 96, 8624-8627.
- (13) Bennett, A. E., Rienstra, C. M., Auger, M., Lakshmi, K. V. and Griffin, R. G. (1995) Heteronuclear decoupling in rotating solids. *J. Chem. Phys.*, 103, 6951-6958.
- (14) Bennett, A. E., Rienstra, C. M., Griffiths, J. M., Zhen, W., Lansbury, J. P. T. and Griffin, R. G. (1998) Homonuclear radio frequency-driven recoupling in rotating solids. *J. Chem. Phys.*, 108, 9463-9479.

- (15) Bielecki, A., Kolbert, A. C. and Levitt, M. H. (1989) Frequency-switched pulse sequences: Homonuclear decoupling and dilute spin NMR in solids. *Chem. Phys. Lett.*, 155, 341-346.
- (16) Blankenship, R. E., Babcock, G. T., Warden, J. T. and Sauer, K. (1975) Observation of a new EPR transient in chloroplasts that may reflect electron-donor to photosystem II at room-temperature. *FEBS Lett.*, 51, 287-293.
- (17) Blankenship, R. E., Madigan, M. T. and Bauer, C. E., eds. (1995) *Anoxygenic Photosynthetic Bacteria*. Dordrecht: Kluwer Academic Publishers.
- (18) Blankenship, R. E. (2002) *Molecular Mechanisms of Photosynthesis*. Oxford, London: Blackwell Science Ltd.
- (19) Bloembergen, N. (1949) The interaction of nuclear spins in a crystalline lattice. *Physica*, 15, 386-426.
- (20) Brinkmann, A. and Levitt, M. H. (2001) Symmetry principles in the nuclear magnetic resonance of spinning solids: Heteronuclear recoupling by generalized Hartmann-Hahn sequences. *J. Chem. Phys.*, 115, 357-384.
- (21) Camara-Artigas, A., Magee, C., Goetsch, A. and Allen, J. P. (2002a) The structure of the heterodimer reaction center from *Rhodobacter sphaeroides* at 2.55 angstrom resolution. *Photosynth. Res.*, 74, 87-93.
- (22) Camara-Artigas, A., Brune, D. and Allen, J. P. (2002b) Interactions between lipids and bacterial reaction centers determined by protein crystallography. *Proc. Natl. Acad. Sci. U. S. A.*, 99, 11055-11060.
- (23) Caravatti, P., Deli, J., Bodenhausen, G. and Ernst, R. R. (1982) Direct evidence of microscopic homogeneity in disordered solids. *J. Am. Chem. Soc.*, 104, 5506-5507.
- (24) Caravatti, P., Neuenschwander, P. and Ernst, R. R. (1985) Characterization of heterogeneous polymer blends by two-dimensional proton spin diffusion spectroscopy. *Macromolecules*, 18, 119-122.
- (25) Carravetta, M., Edén, M., Zhao, X., Brinkmann, A. and Levitt, M. H. (2000) Symmetry principles for the design of radiofrequency pulse sequences in the nuclear magnetic resonance of rotating solids. *Chem. Phys. Lett.*, 321, 205-215.
- (26) Castellani, F., van Rossum, B., Diehl, A., Schubert, M., Rehbein, K. and Oschkinat, H. (2002) Structure of a protein determined by solid-state magic-angle-spinning NMR spectroscopy. *Nature*, 420, 98-102.
- (27) Chapter.2 This thesis.
- (28) Chapter.3 This thesis.
- (29) Cheung, T. T. P. (1981) Spin diffusion in NMR in solids. *Phys. Rev. B*, 23, 1404.
- (30) Closs, G. L. and Closs, L. E. (1969) Induced dynamic nuclear spin polarization in reactions of photochemically and thermally generated triplet diphenylmethylenes. *J. Am. Chem. Soc.*, 91, 4549.
- (31) Cooper, D. E., Rands, M. B. and Woo, C. P. (1975) Sulfide reduction in *ferromongery* effluent by red sulfur bacteria. *J. Water Pollut. Con. F.*, 47, 2088-2100.

- (32) Cotton, T. M. and Van Duyne, R. P. (1979) An electrochemical investigation of the redox properties of bacteriochlorophyll and bacteriopheophytin in aprotic solvents. *J. Am. Chem. Soc.*, 101, 7605-7612.
- (33) Crocker, E., Patel, A. B., Eilers, M., Jayaraman, S., Getmanova, E., Reeves, P. J., Ziliox, M., Khorana, H. G., Sheves, M. and Smith, S. O. (2004) Dipolar assisted rotational resonance NMR of tryptophan and tyrosine in Rhodopsin. *J. Biomol. NMR*, 29, 11-20.
- (34) Crofts, A. R., Meinhardt, S. W., Jones, K. R. and Snozzi, M. (1983) The role of the Quinone pool in the cyclic electron-transfer chain on *Rhodospseudomonas sphaeroides* a modified q-cycle mechanism. *Biochim. Biophys. ACTA*, 723, 202-218.
- (35) Crosby, R. C., Reese, R. L. and Haw, J. F. (1988) Cross polarization magic angle spinning proton NMR-spectroscopy of solids. *J. Am. Chem. Soc.*, 110, 8550-8551.
- (36) Daviso, E., Diller, A., Alia, A., Matysik, J. and Jeschke, G. (2008a) Photo-CIDNP MAS NMR beyond the T_1 limit by fast cycles of polarization extinction and polarization generation. *J. Magn. Reson.*, 190, 43-51.
- (37) Daviso, E., Jeschke, G. and Matysik, J. (2008b) Photochemically induced dynamic nuclear polarization (Photo-CIDNP) magic-angle spinning NMR. In: T. Aartsma and J. Matysik, eds. *Biophysical techniques in photosynthesis II*. Dordrecht: Springer, 385-399.
- (38) Daviso, E., Alia, A., Prakash, S., Diller, A., Gast, P., Lugtenburg, J., Matysik, J. and Jeschke, G. (2009a) Electron-nuclear spin dynamics in a bacterial photosynthetic reaction center. *J. Phys. Chem. C*, 113, 10269-10278.
- (39) Daviso, E., Prakash, S., Alia, A., Gast, P., Jeschke, G. and Matysik, J. (2009b) Nanosecond-Flash ^{15}N Photo-CIDNP MAS NMR on Reaction Centers of *Rhodobacter sphaeroides* R-26. *Appl. Magn. Reson.*, 37, 49-63.
- (40) Daviso, E., Prakash, S., Alia, A., Gast, P., Neugebauer, J., Jeschke, G. and Matysik, J. (2009c) The electronic structure of the primary electron donor of reaction centers of purple bacteria at atomic resolution as observed by photo-CIDNP ^{13}C NMR. *Proc. Natl. Acad. Sci. U. S. A.*, 106, 22281-22286.
- (41) Daviso, E., Diller, A., Gast, P., Alia, A., Lugtenburg, J., Muller, M. G. and Matysik, J. (2010) Action Spectroscopy on Dense Samples of Photosynthetic Reaction Centers of *Rhodobacter sphaeroides* WT Based on Nanosecond Laser-Flash ^{13}C Photo-CIDNP MAS NMR. *Appl. Magn. Reson.*, 38, 105-116.
- (42) de Boer, I., Bosman, L., Raap, J., Oschkinat, H. and de Groot, H. J. M. (2002) 2D ^{13}C - ^{13}C MAS NMR correlation spectroscopy with mixing by true ^1H spin diffusion reveals long-range intermolecular distance restraints in ultra high magnetic field. *J. Magn. Reson.*, 157, 286-291.
- (43) De Paepe, G., Lewandowski, J. R., Loquet, A., Bockmann, A. and Griffin, R. G. (2008) Proton assisted recoupling and protein structure determination. *J. Chem. Phys.*, 129, 245101-245121.
- (44) Deisenhofer, J., Epp, O., Miki, K., Huber, R. and Michel, H. (1985) Structure of the protein subunits in the photosynthetic reaction center of *Rhodospseudomonas viridis* at 3 Å resolution. *Nature*, 318, 618-624.

- (45) Deisenhofer, J. and Norris, J. R. (1993) *The Photosynthetic Reaction Center*. San Diego: Academic.
- (46) Deleeuw, D., Malley, M., Buttermann, G., Okamura, M. Y. and Feher, G. (1982) The stark-effect in reaction centers from *R. spheroides*. *Biophys. J.*, 37, A111.
- (47) Diller, A., Alia, A., Roy, E., Gast, P., de Groot, H., van Gorkom, H., Jeschke, G. and Matysik, J. (2007a) The origin of the high redox force of photosystem II: A photo-CIDNP MAS NMR analysis. 91, PS246.
- (48) Diller, A., Roy, E., Gast, P., van Gorkom, H. J., de Groot, H. J. M., Glaubitz, C., Jeschke, G., Matysik, J. and Alia, A. (2007b) ¹⁵N photochemically induced dynamic nuclear polarization magic-angle spinning NMR analysis of the electron donor of photosystem II. *Proc. Natl. Acad. Sci. U. S. A.*, 104, 12767-12771.
- (49) Diller, A., Alia, A., Gast, P., Jeschke, G. and Matysik, J. (2008) ¹³C Photo-CIDNP MAS NMR on the LH1-RC Complex of *Rhodopseudomonas acidophila*. *Photosynthesis. Energy from the Sun*, 55-58.
- (50) Douglass, D. C. and McBrierty, V. J. (1978) Cross Relaxation in Poly(vinylidene fluoride) from Transient Overhauser Measurements. *Macromolecules*, 11, 766.
- (51) Duer, M. J. (2004) *Introduction to solid state NMR spectroscopy*. Oxford: Blackwell Publishing Ltd.
- (52) Eden, M. and Levitt, M. H. (1999) Pulse sequence symmetries in the nuclear magnetic resonance of spinning solids: Application to heteronuclear decoupling. *J. Chem. Phys.*, 111, 1511-1519.
- (53) Egorova-Zachernyuk, T., Rossum, B. v., Erkelens, C. and Groot, H. d. (2008) Characterisation of uniformly ¹³C, ¹⁵N labelled bacteriochlorophyll *a* and bacteriopheophytin *a* in solution and in solid state: complete assignment of the ¹³C, ¹H and ¹⁵N chemical shifts. *Magn. Reson. Chem.*, 46, 1074-1083.
- (54) Egorova-Zachernyuk, T. A., van Rossum, B., Boender, G.-J., Franken, E., Ashurst, J., Raap, J., Gast, P., Hoff, A. J., Oschkinat, H. and de Groot, H. J. M. (1997) Characterization of pheophytin ground states in *Rhodobacter sphaeroides* R26 photosynthetic reaction centers from multispin pheophytin enrichment and 2-D ¹³C MAS NMR dipolar correlation spectroscopy. *Biochemistry*, 36, 7513-7519.
- (55) Ermler, U., Fritzsche, G., Buchanan, S. K. and Michel, H. (1994) Structure of the photosynthetic reaction-center from *Rhodobacter sphaeroides* at 2.65-Angstrom resolution cofactors and protein-cofactor interactions. *Structure*, 2, 925-936.
- (56) Ernst, M. and Meier, B. H. (1998) Spin diffusion in solids. In: I. Ando and T. Asakura, eds. *Solid State NMR of Polymers*: Elsevier: Amsterdam.
- (57) Etzkorn, M., Seidel, K., Li, L., Martell, S., Geyer, M., Engelhard, M. and Baldus, M. (2010) Complex formation and light activation in membrane-embedded sensory rhodopsin II as seen by solid-state NMR spectroscopy. *Structure*, 18, 293-300.
- (58) Feher, G., Okamura, M. Y. and McElroy, J. D. (1972) Identification of an electron acceptor in reaction centers of *Rhodopseudomonas spheroides* by EPR spectroscopy. *BBA-Bioenergetics*, 267, 222-226.

- (59) Fillingame, R. H. (2000) Getting to the bottom of the F₁ ATPase. *Nat. Struct. Biol.*, 7, 1002-1004.
- (60) Fillingame, R. H., Jiang, W. and Dmitriev, O. Y. (2000) Coupling H⁺ transport to rotary catalysis in F-type ATP synthases: Structure and organization of the transmembrane rotary motor. *J. Exp. Biol.*, 203, 9-17.
- (61) Fischer, M. R., Degroot, H. J. M., Raap, J., Winkel, C., Hoff, A. J. and Lugtenburg, J. (1992) ¹³C Magic angle spinning NMR-study of the light-induced and temperature-dependent changes in *Rhodobacter sphaeroides* R-26 reaction centers enriched in 4'-¹³C tyrosine. *Biochemistry*, 31, 11038-11049.
- (62) Flores, M., Savitsky, A., Paddock, M. L., Abresch, E. C., Dubinskii, A. A., Okamura, M. Y., Lubitz, W. and Moebius, K. (2010) Electron-nuclear and electron-electron double resonance spectroscopies show that the primary quinone acceptor Q(A) in reaction centers from photosynthetic bacteria *Rhodobacter sphaeroides* remains in the same orientation upon light-induced reduction. *J. Phys. Chem. B.*, 114, 16894-16901.
- (63) Fonseca Guerra, C., Snijders, J. G., te Velde, G. and Baerends, E. J. (1998) Towards an order-N DFT method. *Theor. Chem. Acc.*, 99, 391-403-403.
- (64) Förster, T. (1948) Zwischenmolekulare Energiewanderung und Fluoreszenz. *Ann. Phys.*, 437, 55-75.
- (65) Franken, E. M., Shkuropatov, A. Y., Francke, C., Neerken, S., Gast, P., Shuvalov, V. A., Hoff, A. J. and Aartsma, T. J. (1997a) Reaction centers of *Rhodobacter sphaeroides* R-26 with selective replacement of bacteriopheophytin *a* by pheophytin *a*: II. Temperature dependence of the quantum yield of P⁺Q_A⁻ and ³P formation. *BBA-Bioenergetics*, 1321, 1-9.
- (66) Franken, E. M., Shkuropatov, A. Y., Francke, C., Neerken, S., Gast, P., Shuvalov, V. A., Hoff, A. J. and Aartsma, T. J. (1997b) Reaction centers of *Rhodobacter sphaeroides* R-26 with selective replacement of bacteriopheophytin by pheophytin *a* : I. Characterisation of steady-state absorbance and circular dichroism, and of the P⁺Q_A⁻ state. *BBA-Bioenergetics*, 1319, 242-250.
- (67) Frese, R. N., Siebert, C. A., Niederman, R. A., Hunter, C. N., Otto, C. and van Grondelle, R. (2004) The long-range organization of a native photosynthetic membrane. *Proc. Natl. Acad. Sci. U. S. A.*, 101, 17994-17999.
- (68) Friesner, R. and Won, Y. (1989) Spectroscopy and Electron-Transfer Dynamics of the Bacterial Photosynthetic Reaction Center. *Biochim. Biophys. Acta.*, 977, 99-122.
- (69) Ganapathy, S., Oostergetel, G. T., Wawrzyniak, P. K., Reus, M., Gomez Maqueo Chew, A., Buda, F., Boekema, E. J., Bryant, D. A., Holzwarth, A. R. and de Groot, H. J. M. (2009) Alternating syn-anti bacteriochlorophylls form concentric helical nanotubes in chlorosomes. *Proc. Natl. Acad. Sci. U. S. A.*, 106, 8525-8530.
- (70) Gardiennet, C., Loquet, A., Etzkorn, M., Heise, H., Baldus, M. and Bockmann, A. (2008) Structural constraints for the Crh protein from solid-state NMR experiments. *J. Biomol. NMR.*, 40, 239-250.
- (71) Gennis, R. B., Barquera, B., Hacker, B., Vandoren, S. R., Arnaud, S., Crofts, A. R., Davidson, E., Gray, K. A. and Daldal, F. (1993) The bc(1) complexes of *Rhodobacter sphaeroides* and *Rhodobacter capsulatus*. *J. Bioenerg. Biomembr.*, 25, 195-209.

- (72) Goldstein, R. A. and Boxer, S. G. (1987) Effects of nuclear-spin polarization on reaction dynamics in photosynthetic bacterial reaction centers. 51, 937-946.
- (73) Gordon, S. L. and Wüthrich, K. (1978) Transient proton-proton Overhauser effects in horse ferrocytochrome c. *J. Am. Chem. Soc.*, 100, 7094-7096.
- (74) Griffiths, J. M., Bennett, A. E., Engelhard, M., Siebert, F., Raap, J., Lugtenburg, J., Herzfeld, J. and Griffin, R. G. (2000) Structural investigation of the active site in bacteriorhodopsin: Geometric constraints on the roles of Asp-85 and Asp-212 in the proton-pumping mechanism from solid state NMR. *Biochemistry*, 39, 362-371.
- (75) Grommek, A., Meier, B. H. and Ernst, M. (2006) Distance information from proton-driven spin diffusion under MAS. *Chem. Phys. Lett.*, 427, 404-409.
- (76) Grondelle, R. and Novoderezhkin, V. (2006) Energy transfer in photosynthesis: experimental insights and quantitative models.
- (77) Gullion, T. and Schaefer, J. (1989) Rotational-echo double-resonance NMR. *J. Magn. Reson.*, 81, 196-200.
- (78) Hartmann, S. R. and Hahn, E. L. (1962) Nuclear Double Resonance in the Rotating Frame. *Phys. Rev.*, 128, 2042.
- (79) Heinen, W., Wenzel, C. B., Rosenmoller, C. H., Mulder, F. M., Boender, G. J., Lugtenburg, J., de Groot, H. J. M., van Duin, M. and Klumperman, B. (1998) Solid-state NMR study of miscibility and phase separation in blends and semi-interpenetrating networks of ¹³C-labeled poly(styrene-co-acrylonitrile) and poly(styrene-co-maleic anhydride). *Macromolecules*, 31, 7404-7412.
- (80) Henrichs, P. M. and Linder, M. (1984) Carbon-13 spin diffusion in the determination of intermolecular structure in solids. *J. Magn. Reson.*, 58, 458-461.
- (81) Hiller, M., Krabben, L., Vinothkumar, K. R., Castellani, F., van Rossum, B. J., Kuhlbrandt, W. and Oschkinat, H. (2005) Solid-state magic-angle spinning NMR of outer-membrane protein G from Escherichia coli. *Chembiochem*, 6, 1679-1684.
- (82) Hing, A. W., Vega, S. and Schaefer, J. (1992) Transferred-echo double-resonance NMR. *J. Magn. Reson.*, 96, 205-209.
- (83) Hoff, A. J., Rademaker, H., Vangrondelle, R. and Duysens, L. N. M. (1977) Magnetic-field dependence of yield of triplet-state in reaction centers of photosynthetic bacteria. *Biochim. Biophys. Acta*, 460, 547-554.
- (84) Hoff, A. J. and Deisenhofer, J. (1997) Photophysics of photosynthesis. Structure and spectroscopy of reaction centers of purple bacteria. *Phys. Rep.*, 287, 2-247.
- (85) Hohwy, M., Rienstra, C. M., Jaroniec, C. P. and Griffin, R. G. (1999) Fivefold symmetric homonuclear dipolar recoupling in rotating solids: Application to double quantum spectroscopy. *J. Chem. Phys.*, 110, 7983-7992.
- (86) Holm, H. W. and Vennes, J. W. (1970) Occurrence of Purple Sulfur Bacteria in a Sewage Treatment Lagoon. *Appl. Environ. Microb.*, 19, 988-996.

-
- (87) Holzwarth, A. R. and Muller, M. G. (1996) Energetics and kinetics of radical pairs in reaction centers from *Rhodobacter sphaeroides*. A femtosecond transient absorption study. *Biochemistry*, 35, 11820-11831.
- (88) Hoshino, T., Kubo, A., Imashiro, F. and Terao, T. (1998) Proton two-dimensional multiple pulse NMR experiments on the nematic liquid crystal MBBA. *Mol. Phys.*, 93, 301-313.
- (89) Hu, X. and Schulten, K. (1998) Model for the light-harvesting complex I (B875) of *Rhodobacter sphaeroides*. *Biophys. J.*, 75, 683-694.
- (90) Hu, X. C., Damjanovic, A., Ritz, T. and Schulten, K. (1998) Architecture and mechanism of the light-harvesting apparatus of purple bacteria. *Proc. Natl. Acad. Sci. U. S. A.*, 95, 5935-5941.
- (91) Huber, H., Meyer, M., Scheer, H., Zinth, W. and Wachtveitl, J. (1998) Photosynthesis Research. *SpringerLink*, 55, 153-162.
- (92) Hughes, A. V., Rees, P., Heathcote, P. and Jones, M. R. (2006) Kinetic analysis of the thermal stability of the photosynthetic reaction center from *Rhodobacter sphaeroides*. *Biophys. J.*, 90, 4155-4166.
- (93) Hull, W. E. and Sykes, B. D. (1975) Dipolar nuclear spin relaxation of ^{19}F in multispin systems. Application to ^{19}F labeled proteins. *J. Chem. Phys.*, 63, 867-880.
- (94) Hunter, C. N., Daldal, F., Thurnauer, M. C. and Beatty, J. T., eds. (2008) *The Purple Phototrophic Bacteria*. Dordrecht: Springer.
- (95) Igumenova, T. I., McDermott, A. E., Zilm, K. W., Martin, R. W., Paulson, E. K. and Wand, A. J. (2004) Assignments of carbon NMR resonances for microcrystalline ubiquitin. *J. Am. Chem. Soc.*, 126, 6720-6727.
- (96) Janssen, G. J., Daviso, E., van Son, M., de Groot, H. J. M., Alia, A. and Matysik, J. (2010) Observation of the solid-state photo-CIDNP effect in entire cells of cyanobacteria *Synechocystis*. *Photosynth. Res.*, 104, 275-282.
- (97) Jentzen, W., Ma, J.-G. and Shelnutt, J. A. (1998) Conservation of the conformation of the porphyrin macrocycle in hemoproteins. *Biophys. J.*, 74, 753-763.
- (98) Jeschke, G. (1997) Electron-electron-nuclear three-spin mixing in spin-correlated radical pairs. *J. Chem. Phys.*, 106, 10072-10086.
- (99) Jeschke, G. (1998) A new mechanism for chemically induced dynamic nuclear polarization in the solid state. *J. Am. Chem. Soc.*, 120, 4425-4429.
- (100) Jeschke, G. and Matysik, J. (2003) A reassessment of the origin of photochemically induced dynamic nuclear polarization effects in solids. *Chem. Phys.*, 294, 239-255.
- (101) Johnson, G. W., Lee, I. J. and Small, G. J. (1991) Excited state spectral line narrowing spectroscopies. In: H. Scheer, ed. *Chlorophylls*: CRC Pr I Llc.
- (102) Jones, B. R. (1956) Studies of pigmented non-sulfur purple bacteria in relation to cannery waste lagoon odors. *Sewage Ind. Wastes*, 28, 883-893.
- (103) Jones, M. R. (2009) The petite purple photosynthetic powerpack. *Biochem. Soc. T.*, 037, 400-407.

- (104) Jordan, P. M. (1991) *In Bio Synthesis of tetrapyrroles*. Amsterdam: Elsevier.
- (105) Jungas, C., Ranck, J. L., Rigaud, J. L., Joliot, P. and Vermeiglio, A. (1999) Supramolecular organization of the photosynthetic apparatus of *Rhodobacter sphaeroides*. *Embo J.*, 18, 534-542.
- (106) Junge, W., Lill, H. and Engelbrecht, S. (1997) ATP synthase: an electrochemical transducer with rotatory mechanics. *Trends Biochem. Sci*, 22, 420-423.
- (107) Kalk, A. and Berendsen, H. J. C. (1976) Proton magnetic relaxation and spin diffusion in proteins. *J. Magn. Reson.*, 24, 343-366.
- (108) Kaptein, R. and Oosterhoff, J. L. (1969) Chemically induced dynamic nuclear polarization II : (Relation with anomalous ESR spectra). *Chem. Phys. Lett.*, 4, 195.
- (109) Kaptein, R. (1971) Simple rules for chemically induced dynamic nuclear polarization. *Chem. Commun.*, 14, 732-733.
- (110) Karrasch, S., Bullough, P. A. and Ghosh, R. (1995) The 8.5-angstrom projection map of the light-harvesting complex from *Rhodospirillum rubrum* reveals a ring composed of 16 subunits. *EMBO J.*, 14, 631-638.
- (111) Kolodziejski, W., Corma, A., Wozniak, K. and Klinowski, J. (1996) $^{13}\text{C} \rightarrow ^1\text{H}$ Cross-polarization NMR in solids at natural ^{13}C abundance. *J. Phys. Chem.*, 100, 7345-7351.
- (112) Kubo, A. and McDowell, C. A. (1988) Spectral spin diffusion in polycrystalline solids under magic-angle spinning. *J. Chem. Soc., Faraday Trans. 1*, 84, 3713 - 3730.
- (113) Kumar, A., Ernst, R. R. and Wüthrich, K. (1980) A two-dimensional nuclear Overhauser enhancement (2D NOE) experiment for the elucidation of complete proton-proton cross-relaxation networks in biological macromolecules. *Biochem. Biophys. Res. Co.*, 95, 1-6.
- (114) Kumar, A., Wagner, G., Ernst, R. R. and Wuethrich, K. (1981) Buildup rates of the nuclear Overhauser effect measured by two-dimensional proton magnetic resonance spectroscopy: implications for studies of protein conformation. *J. Am. Chem. Soc.*, 103, 3654-3658.
- (115) Lee, C. T., Yang, W. T. and Parr, R. G. (1988) Development of the colle-salveti correlation-energy formula into a functional of the electron-density. *Phys. Rev. B*, 37, 785-789.
- (116) Lee, M. and Goldburg, W. I. (1965) Nuclear Magnetic Resonance line narrowing by a rotating rf field. *Phys. Rev.*, 140.
- (117) Lee, Y. K., Kurur, N. D., Helmle, M., Johannessen, O. G., Nielsen, N. C. and Levitt, M. H. (1995) Efficient dipolar recoupling in the NMR of rotating solids - a sevenfold symmetrical radiofrequency pulse sequence. *Chem. Phys. Lett.*, 242, 304-309.
- (118) Lendzian, F., Huber, M., Isaacson, R. A., Endeward, B., Plato, M., Bonigk, B., Mobius, K., Lubitz, W. and Feher, G. (1993) The electronic-structure of the primary donor cation-radical in *Rhodobacter sphaeroides* R-26 - endor and triple-resonance studies in single-crystals of reaction centers. *Biochim. Biophys. Acta.*, 1183, 139-160.
- (119) Leskes, M., Madhu, P. K. and Vega, S. (2006) Proton line narrowing in solid-state nuclear magnetic resonance: New insights from windowed phase-modulated Lee-Goldburg sequence. *J. Chem. Phys.*, 125, 124506-124518.

-
- (120) Leskes, M., Madhu, P. K. and Vega, S. (2009) Why does PMLG proton decoupling work at 65 kHz MAS? *J. Magn. Reson.*, 199, 208-213.
- (121) Levitt, M. H., Oas, T. G. and Griffin, R. G. (1988) Rotary resonance recoupling in heteronuclear spin pair systems. *Isr.J.Chem.*, 28, 271-282.
- (122) Levitt, M. H., Kolbert, A. C., Bielecki, A. and Ruben, D. J. (1993) High-resolution ^1H NMR in solids with frequency-switched multiple-pulse sequences. *Solid State Nucl. Mag.*, 2, 151-163.
- (123) Levitt, M. H. (2002) Symmetry-based pulse sequences in magic-angle spinning solid-state NMR. In: D. M. Grant and R. K. Harris, eds. *Encyclopedia of Nuclear Magnetic Resonance; Advances in NMR*. Chichester, UK: John Wiley & Sons Ltd., 165-196.
- (124) Linder, M., Henrichs, P. M., Hewitt, J. M. and Massa, D. J. (1985) Use of carbon-carbon nuclear spin diffusion for the study of the miscibility of polymer blends. *J. Chem. Phys.*, 82, 1585-1598.
- (125) Lockhart, D. J. and Boxer, S. G. (1987) Magnitude and direction of the change in dipole moment associated with excitation of the primary electron donor in *Rhodospseudomonas sphaeroides* reaction centers. *Biochemistry*, 26, 664-668.
- (126) Lockhart, D. J. and Boxer, S. G. (1988) Stark effect spectroscopy of *Rhodobacter sphaeroides* and *Rhodospseudomonas viridis* reaction centers. *Proc. Natl. Acad. Sci. U. S. A.*, 85, 107-111.
- (127) Loquet, A., Bardiaux, B., Gardiennet, C., Blanchet, C., Baldus, M., Nilges, M., Malliavin, T. and Bockmann, A. (2008) 3D structure determination of the Crh protein from highly ambiguous solid-state NMR restraints. *J. Am. Chem. Soc.*, 130, 3579-3589.
- (128) Lowe, I. J. (1959) Free induction decays of rotating solids. *Phys. Rev. Lett.*, 2, 285.
- (129) Lubitz, W., Abresch, E. C., Debus, R. J., Isaacson, R. A., Okamura, M. Y. and Feher, G. (1985) Electron nuclear double resonance of semiquinones in reaction centers of *Rhodospseudomonas sphaeroides*. *BBA-Bioenergetics*, 808, 464-469.
- (130) Lubitz, W. and Feher, G. (1999) The primary and secondary accepters in bacterial photosynthesis III. Characterization of the quinone radicals Q_A^- and Q_B^- by EPR and ENDOR. *Appl. Magn. Reson.*, 17, 1-48.
- (131) Lyle, P. A., Kolaczowski, S. V. and Small, G. J. (1993) Photochemical hole-burned spectra of protonated and deuterated reaction centers of *Rhodobacter sphaeroides*. *J. Phys. Chem.*, 97, 6924-6933.
- (132) Madigan, M. T. (1984) A novel photosynthetic purple bacterium isolated from a yellowstone hot spring. *Science*, 225, 313-315.
- (133) Marcus, R. A. (1956a) On the theory of oxidation-reduction reactions involving electron transfer *J. Chem. Phys.*, 24, 966-978.
- (134) Marcus, R. A. (1956b) Electrostatic free energy and other properties of states having nonequilibrium polarization *J. Chem. Phys.*, 24, 979-989.
- (135) Marcus, R. A. (1965) On the theory of electron-transfer reactions. VI. Unified treatment for homogeneous and electrode reactions. *J. Chem. Phys.*, 43, 679-701.

- (136) Marcus, R. A. and Sutin, N. (1985) Electron transfers in chemistry and biology. *Biochim. Biophys. Acta - Reviews on Bioenergetics*, 811, 265-322.
- (137) Martin, J. L., Breton, J., Hoff, A. J., Migus, A. and Antonetti, A. (1986) Femtosecond spectroscopy of electron-transfer in the reaction center of the photosynthetic bacterium *Rhodospseudomonas-sphaeroides* R-26 - direct electron-transfer from the dimeric bacteriochlorophyll primary donor to the bacteriopheophytin acceptor with a time constant 2.8 +/- 0.2 psec. *Proc. Natl. Acad. Sci. U. S. A.*, 83, 957-961.
- (138) Matysik, J., Alia, Gast, P., van Gorkom, H. J., Hoff, A. J. and de Groot, H. J. M. (2000a) Photochemically induced nuclear spin polarization in reaction centers of photosystem II observed by ¹³C-solid-state NMR reveals a strongly asymmetric electronic structure of the P680.+ primary donor chlorophyll. *Proc. Natl. Acad. Sci. U. S. A.*, 97, 9865-9870.
- (139) Matysik, J., Alia, Holland, J., Egorova-Zachernyuk, T., Gast, P. and de Groot, H. J. M. (2000b) Sample illumination and photo-CIDNP in a magic-angle spinning NMR probe. *Indian J. Biochem. Biophys.*, 37, 418-423.
- (140) Matysik, J., Schulten, E., Alia, Gast, P., Raap, J., Lugtenburg, J., Hoff, A. J. and de Groot, H. J. M. (2001) Photo-CIDNP ¹³C magic angle spinning NMR on bacterial reaction centres: Exploring the electronic structure of the special pair and its surroundings. *Biol. Chem.*, 382, 1271-1276.
- (141) Matysik, J., Diller, A., Roy, E. and Alia, A. (2009) The solid-state photo-CIDNP effect. *Photosynth. Res.*, 102, 427-435.
- (142) McBrierty, V. J. (1979) Heterogeneity in polymers as studied by nuclear magnetic resonance. *Faraday Discuss. Chem. Soc.*, 68, 78-86.
- (143) McDermott, A., Zysmilich, M. G. and Polenova, T. (1998) Solid state NMR studies of photoinduced polarization in photosynthetic reaction centers: mechanism and simulations. *Solid State Nucl. Mag.*, 11, 21-47.
- (144) McDermott, G., Prince, S. M., Freer, A. A., Hawthornthwaitelawless, A. M., Papiz, M. Z., Cogdell, R. J. and Isaacs, N. W. (1995) Crystal-structure of an integral membrane light-harvesting complex from photosynthetic bacteria. *Nature*, 374, 517-521.
- (145) Mehring, M. and Waugh, J. S. (1972) Magic-angle NMR experiments in solids. *Phys. Rev. B*, 5, 3459.
- (146) Moore, L. J., Zhou, H. and Boxer, S. G. (1999) Excited-state electronic asymmetry of the special pair in photosynthetic reaction center mutants: Absorption and Stark spectroscopy. *Biochemistry*, 38, 11949-11960.
- (147) Mulder, F. M., Heinen, W., van Duin, M., Lugtenburg, J. and de Groot, H. J. M. (2000) Cross-linking induced phase separation in SAN/SMA semi-interpenetrating polymer networks observed by solid state NMR and site specific isotope enrichment. *Macromolecules*, 33, 5544-5548.
- (148) Nielsen, N. C., Cruzet, F., Griffin, R. G. and Levitt, M. H. (1992) Enhanced double-quantum nuclear magnetic resonance in spinning solids at rotational resonance. 96, 5668.
- (149) Novoderezhkin, V. I., Yakovlev, A. G., van Grondelle, R. and Shuvalov, V. A. (2004) Coherent nuclear and electronic dynamics in primary charge separation in photosynthetic reaction centers: A redfield theory approach. 108, 7445-7457.

-
- (150) Noy, D., Moser, C. C. and Dutton, P. L. (2006) Design and engineering of photosynthetic light-harvesting and electron transfer using length, time, and energy scales. *BBA - Bioenergetics*, 1757, 90-105.
- (151) Oas, T. G., Griffin, R. G. and Levitt, M. H. (1988) Rotary resonance recoupling of dipolar interactions in solid-state nuclear magnetic resonance spectroscopy. *J. Chem. Phys.*, 89, 692-695.
- (152) Okamura, M. Y., Steiner, L. A. and Feher, G. (1974) Characterization of reaction centers from photosynthetic bacteria. I. Subunit structure of the protein mediating the primary photochemistry in *Rhodopseudomonas spheroides* R-26. *Biochemistry*, 13, 1394-1403.
- (153) Okamura, M. Y., Isaacson, R. A. and Feher, G. (1975) Primary acceptor in bacterial photosynthesis - obligatory role of ubiquinone in photoactive reaction centers of *Rhodopseudomonas-spheroides*. *Proc. Natl. Acad. Sci. U. S. A.*, 72, 3491-3495.
- (154) Palaniappan, V., Martin, P. C., Chynwat, V., Frank, H. A. and Bocian, D. F. (1993) Comprehensive resonance Raman study of photosynthetic reaction centers from *Rhodobacter sphaeroides*. Implications for pigment structure and pigment-protein interactions. *J. Am. Chem. Soc.*, 115, 12035-12049.
- (155) Pandit, A., Buda, F., van Gammeren, A. J., Ganapathy, S. and de Groot, H. J. M. (2010) Selective chemical shift assignment of bacteriochlorophyll *a* in uniformly [¹³C, ¹⁵N]-labeled light-harvesting 1 complexes by solid-state NMR in ultrahigh magnetic field. *J. Phys. Chem. B.*, 114, 6207-6215.
- (156) Pines, A., Gibby, M. G. and Waugh, J. S. (1973) Proton-enhanced NMR of dilute spins in solids. *J. Chem. Phys.*, 59, 569-590.
- (157) Polenova, T. and McDermott, A. E. (1999) A coherent mixing mechanism explains the photoinduced nuclear polarization in photosynthetic reaction centers. *J. Phys. Chem. B*, 103, 535-548.
- (158) Potter, J., Fyfe, P., Frolov, D., Wakeham, M., van Grondelle, R., Robert, B. and JONES, M. (2005) Strong effects of an individual water molecule on the rate of light-driven charge separation in the *Rhodobacter sphaeroides* reaction center. *J. Biol. Chem.*, 280, 27155-27164.
- (159) Prakash, S., Alia, Gast, P., de Groot, H. J. M., Jeschke, G. and Matysik, J. (2005) Magnetic field dependence of photo-CIDNP MAS NMR on photosynthetic reaction centers of *Rhodobacter sphaeroides* WT. *J. Am. Chem. Soc.*, 127, 14290-14298.
- (160) Prakash, S., Alia, Gast, P., de Groot, H. J. M., Matysik, J. and Jeschke, G. (2006) Photo-CIDNP MAS NMR in intact cells of *Rhodobacter sphaeroides* R-26: Molecular and atomic resolution at nanomolar concentration. *J. Am. Chem. Soc.*, 128, 12794-12799.
- (161) Prakash, S., Alia, A., Gast, P., de Groot, H. J. M., Jeschke, G. and Matysik, J. (2007) ¹³C chemical shift map of the active cofactors in photosynthetic reaction centers of *Rhodobacter sphaeroides* revealed by photo-CIDNP MAS NMR. *Biochemistry*, 46, 8953-8960.
- (162) Purchase, R. and Völker, S. (2009) Spectral hole burning: examples from photosynthesis. *Photosynth. Res.*, 101, 245-266-266.
- (163) Qian, P., Hunter, C. N. and Bullough, P. A. (2005) The 8.5 angstrom projection structure of the core RC-LH1-PufX dimer of *Rhodobacter sphaeroides*. *J. Mol. Biol.*, 349, 948-960.

- (164) Reddy, N. R. S., Lyle, P. A. and Small, G. J. (1992) Applications of spectral hole burning spectroscopies to antenna and reaction center complexes. *Photosynth. Res.*, 31, 167-194.
- (165) Reddy, N. R. S., Kolaczowski, S. V. and Small, G. J. (1993) A Photoinduced Persistent Structural Transformation of the Special Pair of a Bacterial Reaction Center. *Science*, 260, 68-71.
- (166) Rohmer, M. (1999) The discovery of a mevalonate-independent pathway for isoprenoid biosynthesis in bacteria, algae and higher plants. *Nat. Prod. Rep.*, 16, 565-574.
- (167) Roy, E., Alia, Gast, P., van Gorkom, H., de Groot, H. J. M., Jeschke, G. and Matysik, J. (2007) Photochemically induced dynamic nuclear polarization in the reaction center of the green sulphur bacterium *Chlorobium tepidum* observed by ^{13}C MAS NMR. *BBA-Bioenergetics.*, 1767, 610-615.
- (168) Roy, E., Rohmer, T., Gast, P., Jeschke, G., Alia, A. and Matysik, J. (2008) Characterization of the primary radical pair in reaction centers of *Heliobacillus mobilis* by ^{13}C Photo-CIDNP MAS NMR. *Biochemistry*, 47, 4629-4635.
- (169) Sarles, L. R. and Cotts, R. M. (1958) Double nuclear magnetic resonance and the dipole interaction in solids. *Phys. Rev.*, 111, 853.
- (170) Scheuring, S., Sturgis, J. N., Prima, V., Bernadac, A., Levy, D. and Rigaud, J. L. (2004) Watching the photosynthetic apparatus in native membranes. *Proc. Natl. Acad. Sci. U. S. A.*, 101, 11293-11297.
- (171) Scheuring, S. and Sturgis, J. N. (2005) Chromatic adaptation of photosynthetic membranes. *Science*, 309, 484-487.
- (172) Scheuring, S., Levy, D. and Rigaud, J. L. (2005) Watching the components of photosynthetic bacterial membranes and their in situ organisation by atomic force microscopy. *BBA-Biomembranes*, 1712, 109-127.
- (173) Schmidt-Rohr, K. and Spiess, H. W. (1994) *Multidimensional solid state NMR and polymers*. London, United Kingdom: Academic Press Ltd.
- (174) Schmidt, S., Arlt, T., Hamm, P., Huber, H., Nägele, T., Wachtveitl, J., Meyer, M., Scheer, H. and Zinth, W. (1994) Energetics of the primary electron transfer reaction revealed by ultrafast spectroscopy on modified bacterial reaction centers. *Chem. Phys. Lett.*, 223, 116-120.
- (175) Scholz, I., Huber, M., Manolikas, T., Meier, B. H. and Ernst, M. (2008) MIRROR recoupling and its application to spin diffusion under fast magic-angle spinning. *Chem. Phys. Lett.*, 460, 278-283.
- (176) Schulten, E. A. M., Matysik, J., Alia, Kiihne, S., Raap, J., Lugtenburg, J., Gast, P., Hoff, A. J. and de Groot, H. J. M. (2002) ^{13}C MAS NMR and photo-CIDNP reveal a pronounced asymmetry in the electronic ground state of the special pair of *Rhodobacter sphaeroides* reaction centers. *Biochemistry*, 41, 8708-8717.
- (177) Shelnutt, J. A., Song, X. Z., Ma, J. G., Jia, S. L., Jentzen, W. and Medforth, C. J. (1998) Nonplanar porphyrins and their significance in proteins. *Chem. Soc. Rev.*, 27, 31-41.
- (178) Shkuropatov, A. Y. and Shuvalov, V. A. (1993) Electron transfer in pheophytin a-modified reaction centers from *Rhodobacter sphaeroides* R-26. *FEBS Lett.*, 322, 168-172.

- (179) Shochat, S., Arlt, T., Francke, C., Gast, P., Vannoort, P. I., Otte, S. C. M., Schelvis, H. P. M., Schmidt, S., Vijgenboom, E., Vrieze, J., Zinth, W. and Hoff, A. J. (1994) Spectroscopic characterization of reaction centers of the (M)Y210W mutant of the photosynthetic bacterium *Rhodobacter sphaeroides*. *Photosynth. Res.*, 40, 55-66.
- (180) Shuvalov, V. and Yakovlev, A. (2003) Coupling of nuclear wavepacket motion and charge separation in bacterial reaction centers. 540, 26-34.
- (181) Siebert, C. A., Qian, P., Fotiadis, D., Engel, A., Hunter, C. N. and Bullough, P. A. (2004) Molecular architecture of photosynthetic membranes in *Rhodobacter sphaeroides*: the role of PufX. *Embo J.*, 23, 690-700.
- (182) Siefert, E., Irgens, R. L. and Pfennig, N. (1978) Phototrophic purple and green bacteria in a sewage treatment plant. *Appl. Environ. Microbiol.*, 35, 38-44.
- (183) Stejskal, E. O., Schaefer, J. and Waugh, J. S. (1977) Magic-angle spinning and polarization transfer in proton-enhanced NMR. *J. Magn. Reson.*, 28, 105-112.
- (184) Stejskal, E. O., Schaefer, J. and McKay, R. A. (1984) Analysis of double cross-polarization rates in solid proteins. *J. Magn. Reson.*, 57, 471-485.
- (185) Suter, D. and Ernst, R. R. (1982) Spectral spin diffusion in the presence of an extraneous dipolar reservoir. *Phys. Rev. B*, 25, 6038.
- (186) Szeverenyi, N. M., Sullivan, M. J. and Maciel, G. E. (1982) Observation of spin exchange by two-dimensional fourier-transform ^{13}C cross polarization-magic-angle spinning. *J. Magn. Reson.*, 47, 462-475.
- (187) Takegoshi, K., Nakamura, S. and Terao, T. (2001) ^{13}C - ^1H dipolar-assisted rotational resonance in magic angle spinning NMR. *Chem. Phys. Lett.*, 344, 631-637.
- (188) Takegoshi, K. and Terao, T. (2002) ^{13}C nuclear Overhauser polarization nuclear magnetic resonance in rotating solids: Replacement of cross polarization in uniformly ^{13}C labeled molecules with methyl groups. *J. Chem. Phys.*, 117, 1700-1707.
- (189) Takegoshi, K., Nakamura, S. and Terao, T. (2003) ^{13}C - ^1H dipolar-driven ^{13}C - ^{13}C recoupling without ^{13}C rf irradiation in nuclear magnetic resonance of rotating solids. *J. Chem. Phys.*, 118, 2325-2341.
- (190) Takegoshi, K. (2008) Homonuclear shift-correlation experiment in solids. In: G. A. Webb, ed. *Modern Magnetic Resonance*: Springer.
- (191) te Velde, G., Bickelhaupt, F. M., Baerends, E. J., Fonseca Guerra, C., van Gisbergen, S. J. A., Snijders, J. G. and Ziegler, T. (2001) Chemistry with ADF. *J. Comput. Chem.*, 22, 931-967.
- (192) Tycko, R. and Dabbagh, G. (1990) Measurement of nuclear magnetic dipole-dipole couplings in magic angle spinning NMR. *Chem. Phys. Lett.*, 173, 461-465.
- (193) Valesco, F. J. and Crofts, A. R. (1991) Complexes or super complexes - inhibitor titrations show that electron-transfer in chromatophores from *Rhodobacter sphaeroides* involves a dimeric ubiquinol: cytochrome *c* oxidoreductase, and is delocalized. *Biochem. Soc. Trans.*, 19, 588-593.
- (194) van Gammeren, A. J., Buda, F., Hulsbergen, F. B., Kiihne, S., Hollander, J. G., Egorova-Zachernyuk, T. A., Fraser, N. J., Cogdell, R. J. and de Groot, H. J. M. (2005) Selective

- chemical shift assignment of B800 and B850 bacteriochlorophylls in uniformly [^{13}C , ^{15}N]-labeled light-harvesting complexes by solid-state NMR spectroscopy at ultra-high magnetic field. *J. Am. Chem. Soc.*, 127, 3213-3219.
- (195) van Niel, C. B. (1944) The culture, general physiology, morphology, and classification of the non-sulfur purple and brown bacteria. *Microbiol. Mol. Biol. Rev.*, 8, 1-118.
- (196) van Rossum, B. J., de Groot, C. P., Ladizhansky, V., Vega, S. and de Groot, H. J. M. (2000) A method for measuring heteronuclear (^1H - ^{13}C) distances in high speed MAS NMR. *J. Am. Chem. Soc.*, 122, 3465-3472.
- (197) Vinogradov, E., Madhu, P. K. and Vega, S. (2002) Proton spectroscopy in solid state nuclear magnetic resonance with windowed phase modulated Lee-Goldburg decoupling sequences. *Chem. Phys. Lett.*, 354, 193-202.
- (198) Vinogradov, E., Madhu, P. K. and Vega, S. (2005) Strategies for High-Resolution Proton Spectroscopy in Solid-State NMR. In: J. Klinowski, ed. *New Techniques in Solid-State NMR*. Germany: Springer.
- (199) Wawrzyniak, P. K., Beerepoot, M., de Groot, H. J. M. and Buda, F. (2011) Acetyl group orientation modulates the electronic ground-state asymmetry of the special pair in purple bacterial reaction centers. *Phys. Chem. Chem. Phys.*, 13, 10270-10279.
- (200) Wawrzyniak, P. K. (2011) Ab initio modeling of primary processes in photosynthesis : protein induced activation of bacteriochlorophylls for efficient light harvesting and charge separation SSNMR: Leiden University, 150.
- (201) Woodbury, N. W. T. and Parson, W. W. (1984) Nanosecond fluorescence from isolated photosynthetic reaction centers of *Rhodospseudomonas sphaeroides*. *BBA - Bioenergetics*, 767, 345-361.
- (202) Xia, D., Yu, C. A., Kim, H., Xian, J. Z., Kachurin, A. M., Zhang, L., Yu, L. and Deisenhofer, J. (1997) Crystal structure of the cytochrome bc_1 complex from bovine heart mitochondria. *Science*, 277, 60-66.
- (203) Yakovlev, A., Vasilieva, L., Khmel'nitskaya, T., Shkuropatova, V., Shkuropatov, A. and Shuvalov, V. (2010a) Primary electron transfer in reaction centers of YM210L and YM210L/HL168L mutants of *Rhodobacter sphaeroides*. *Biochemistry (Moscow)*, 75, 832-840.
- (204) Yakovlev, A. G., Shkuropatov, A. Y. and Shuvalov, V. A. (2002) Nuclear Wave Packet Motion between P^* and $\text{P}+\text{BA}^-$ Potential Surfaces with a Subsequent Electron Transfer to HA in Bacterial Reaction Centers at 90 K. Electron Transfer Pathway. *Biochemistry*, 41, 14019-14027.
- (205) Yakovlev, A. G., Vasilieva, L. G., Khmel'nitskaya, T. I., Shkuropatova, V. A., Shkuropatov, A. Y. and Shuvalov, V. A. (2010b) Primary electron transfer in reaction centers of YM210L and YM210L/HL168L mutants of *Rhodobacter sphaeroides*. 75, 832-840.
- (206) Yamasaki, H., Takano, Y. and Nakamura, H. (2008) Theoretical Investigation of the Electronic Asymmetry of the Special Pair Cation Radical in the Photosynthetic Type-II Reaction Center. *J. Phys. Chem. B*, 112, 13923-13933.
- (207) Yeates, T. O., Komiya, H., Rees, D. C., Allen, J. P. and Feher, G. (1987) Structure of the reaction center from *Rhodobacter sphaeroides* R-26 membrane-protein interactions. *Proc. Natl. Acad. Sci. U. S. A.*, 84, 6438-6442.

- (208) Yeates, T. O., Komiya, H., Chirino, A., Rees, D. C., Allen, J. P. and Feher, G. (1988) Structure of the reaction center from *Rhodobacter-sphaeroides* r-26 and 2.4.1-protein-cofactor (bacteriochlorophyll, bacteriopheophytin, and carotenoid) interactions .4. *Proc. Natl. Acad. Sci. U. S. A.*, 85, 7993-7997.
- (209) Zheng, L., Fishbein, K. W., Griffin, R. G. and Herzfeld, J. (1993) Two-dimensional solid-state proton NMR and proton exchange. *J. Am. Chem. Soc.*, 115, 6254-6261.
- (210) Zysmilich, M. G. and McDermott, A. (1994) Photochemically induced dynamic nuclear-polarization in the solid-state ^{15}N spectra of reaction centers from photosynthetic bacteria *Rhodobacter sphaeroides* R-26. *J. Am. Chem. Soc.*, 116, 8362-8363.

