REFERENCES

Adams, P. D., Pannu, N. S., Read, R. J., and Brünger, A. T.

(1997) Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement, *Proc. Natl. Acad. Sci. U.S.A. 94,* 5018-5023.

Adman, E. T., Sieker, L. C., and Jensen, L. H.

(1973) The structure of bacterial ferredoxin, *J. Biol. Chem. 248*, 3987-3996.

Anderson, G. W., Zimmermann, J. E., and Callahan, F. M.

(1964) The use of esters of N- hydroxysuccinimide in peptide synthesis, *J. Am. Chem. Soc. 86*, 1839-1842.

Arndt, U. W., and Wonacott, A. J.

(1977) The rotation method in crystallography (Arndt, U. W., & Wonacott, A. J., Ed. North Holland, Amsterdam).

Axup, A. W., Albin, M., Mayo, S. L., Crutchley, R. J., and Gray, H. B.

(1988) Distance dependence of photoinduced long-range electron-transfer in zinc ruthenium-modified myoglobins, *J. Am. Chem. Soc. 110*, 435-439.

Bahadur, R. P., Chakrabati, P., Rodier, F., and Janin, J.

(2003) Dissecting subunit interfaces in homodimers proteins, *PROTEINS: Structure, Function, and Genetics 53*, 708-719.

Bairoch, A., Bucher, P., and Hofmann, K.

(1997) The PROSITE database, its status in 1997, *Nucleic Acids Res. 25*, 217-221.

Bechtold, R., Kuehn, C. L. Lepre, C., and Isied, S. S.

(1986) Directional electron transfer in ruthenium-modified horse heart cytochrome c, *Nature 322*, 286-289.

Beckert, V., and Bernhardt, R.

(1997) Specific aspects of electron transfer from adrenodoxin to cytochromes P450scc and P45011β, *J. Biol. Chem. 272*, 4883-4888.

Beckert, V., Dettmer, R., and Bernhardt, R.
(1994) Mutations of tyrosine 82 in bovine adrenodoxin that affect binding to cytochromes P45011A1 and P45011B1 but not electron transfer, *J. Biol. Chem. 269*, 2568-2573.

Beckert, V., Schrauber, H., Bernhardt, R., Van Dijk, A. A., Kakoschke, C., and Wray, V.
(1995) Mutational effects on the spectroscopic properties and biological activities of oxidized bovine adrenodoxin, and their structural implications, *Eur. J. Biochem. 231*, 226-235.

Beilke, D., Weiss, R., Lohr, F., Pristovsek, P., Hannemann, F., Bernhardt, R., and Ruterjans, H.
(2002) A new electron transport mechanism in mitochondrial steroid hydroxylase systems based on structural changes upon the reduction of adrenodoxin, *Biochemistry 41*, 7969-7978.

Beratan, D. N., Betts, J. N., Onuchic, J. N.
(1991) Protein electron transfer rates set by the bridging secondary and tertiary structure, *Science 252*, 1285-1288.

Beratan, D. N., and Hopfield, J. J.
(1984) Calculation of electron-tunneling matrix-elements in rigid systems - mixed-valence dithiaspirocyclobutane molecules, *J. Chem. Soc. 106*, 1584-1594.

Beratan, D. N., and Onuchic, J. N.
(1991) Electron-transfer - from model compounds to proteins, *Adv. Chem. Ser. 228*, 7.

Beratan, D. N., Onuchic, J. N., Betts, J. N., Bowler, B. E., and Gray, H. B.
(1990) Electron-tunneling pathways in ruthenated proteins, *J. Am. Chem. Soc. 112*, 7915.

Bes, M. T., Parisini, E., Inda, L. A., Saraiva, L., Peleato, M. L., and Sheldrick, G. M.
(1999) Crystal structure determination at 14 Å resolution of ferredoxin from the green algae *Chlorella fusca*, *Structure 7*, 1201-1211.

Binda, C., Coda, A., Aliverti, A., Zanetti, G., and Mattevi, A.
(1998) Structure of the mutant E92K of [2Fe-2S] ferredoxin I from *Spinacia oleracea* at 17 Å resolution, *Acta Crystallogr. D54*, 1353-1358.

Bhasker, C. R., Okamura, T., Simpson, E. R., and Waterman, M. R.
(1987) Mature bovine adrenodoxin contains a 14-amino-acid COOH-terminal extension originally detected by cDNA sequencing, *Eur. J. Biochem. 164*, 21-25.

Bränden, C. I., and Jones, A.
(1990) Between objectivity and subjectivity, *Nature 343*, 687-689.

Brünger, A. T.
(1988) *X-PLOR Reference Manual 2.1* Yale University, New Haven.

Brünger, A. T.
(1992) XPLOR manual, version 3.1. Yale University, New Haven, CT.

Brünger, A. T.
(1992) The free R value: a novel statistical quantity for assessing the accuracy of crystal structures, *Nature 355,* 472-474.

Brünger, A. T., Adams, P. D., and Rice, L. M.
(1997) New application of simulated annealing in X-ray crystallography and solution NMR, *Structure 5*, 325-336.

Bucher, M. H., Evdokimov, A. G., and Waugh, D. S.
(2002) Differential effects of short affinity tags on the crystallization of *Pyrococcus furiosus* maltodextrin-binding protein, *Acta Crystallogr. D58*, 392-397.

Buckley, F., and Harary, F.
(1990) *Distance in Graph*. New York: Addison-Wesley

Burova, T. V., Beckert, V., Uhlmann, H., Ristau, O., Bernhardt, R., and Pfeil, W.
(1996) Conformational stability of adrenodoxin mutants, *Protein Science 5*, 1890-1897.

Cammack, R., Rao, K. K., Hall, D. O., and Johnson, C. E.
(1971) Mössbauer studies of adrenodoxin. The mechanism of electron transfer in a hydroxylase iron-sulphur protein, *Biochem. J. 125*, 849-856.

Capozzi, F., Curly, S., and Luchinat, C.

(1998) Coordination sheer versus protein environment as determinants of electronic and functional-properties of iron-sulfur proteins, *Struct. Bonding 90*, 127-160.

Carlsen, S. A., Schmell, E., Weigel, P. H., and Roseman, S.

(1981) The effect of the method of isolation on the surface properties of isolated rat hepatocytes, *J. Biol. Chem*. *256*, 8058-8062.

Chandra, N., Acharya, K. R. and Moody, P. C. E.

(1999) Analysis and characterization of data from twinned crystals, *Acta Crystallogr. D55*, 1750-1758.

Chang, R., and Weismann, S. I.

(1967) Electron transfer between anion and molecule of hexahelicene, *J. Am. Chem. Soc. 89*, 5968.

Chu, J. W., and Kimura, T.

(1973) Studies on adrenal steroid hydroxylases. Molecular and catalytic properties of adrenodoxin reductase (a flavoprotein), *J. Biol. Chem. 248,* 2089-2094.

Closs, G. L., Calcaterra, L. T., Green, N. J., Penfield, K. W., and Miller, J. R.

(1986) Distance, stereoelectronic effects, and the Marcus inverted region in intramolecular electron-transfer in organic radical-anions, *J. Phys. Chem. 90*, 3673-3683.

Cole, P. A.

(1996) Chaperone-assisted protein expression, *Structure 4*, 239-242.

Contzen, J., Kostka, S., Kraft, R., and Jung, C.

(2002) Intermolecular electron transfer in cytochrome $P450_{cam}$ covalently bound with Tris(2,2′-bipyridyl)ruthenium(II): structural changes detected by FTIR spectroscopy, *J. Inorg. Biochem. 91,* 607-617.

Corpet, F.

(1988) Multiple sequence alignment with hierarchical clustering, *Nucleic Acids Res. 16*, 10881-10890.

Crosby, G. A.

(1975) Spectroscopic investigations of excited states of transition- metal complexes, *Acc. Chem. Res. 8*, 231-238.

Crowther, R., and Blow, R.

(1967) A method of positioning a known molecule in a unknown crystal structure, *Acta Crystallogr. 23*, 544-548.

Crutchley, R. J., Ellis, W. R., Jr., and Gray, H. B.

(1986) *Frontiers in Bioinorganic Chemistry* (Xavier, A. V., Ed.) Verlag Chemie, Weinheim, FRG.

Cupp, J. R., and Vickery, L. E.

(1988) Identification of free and [Fe2S2]-bound cysteine residues of adrenodoxin, *J. Biol. Chem. 263*, 17418-17421. (erratum in *J. Biol. Chem. 264*, 7760, 1989.)

Cupp, J. R., and Vickery, L. E.

(1989) Adrenodoxin with a COOH-terminal deletion (des 116-128) exhibits enhanced activity, *J. Biol. Chem. 264*, 1602-1607.

Curry, W. B., Grabe, M. D., Kurnikov, I. V., Skourtis, S. S., Beratan, D. N., Regan, J. J., Aquino, A. J., Beroza, P., and Onuchic, J. N.

(1995) Pathways, pathway tubes, pathway docking and propagators in electron transfer proteins, *J. Bioenerg. Biomembr. 27,* 285-293.

Cushman, D. W., Tsai, R. L., and Gunsalus, I. C.

(1967) The ferroprotein component of a methylene hydroxylase, *Biochem. Biophys. Res. Commun. 26*, 577-583.

Damrauer, N. H., Cerullo, G., Yeh, A., Boussie, T. R., Shank, C. V., and McCusker, J. K.
(1997) Femtosecond dynamics of excited-state evolution in $[Ru(bpy)_3]^{2+}$, *Science 275*, 54-57.

Dauter, T.
(2003) Twinned crystals and anomalous phasing, *Acta Crystallogr. D59*, 2004-2016.

Debus, R. J., Barry, B. A., Sithole, I., Babcock, G. T., and McIntosh, L.
(1988) Directed mutagenesis indicates that the donor to P 680+ in photosystem II is tyrosine-161 of the D1 polypeptide, *Biochemistry 27*, 9071-9074.

Demas, J. N., and Addington, J. W.
(1976) Luminescence quenching of the tris (2,2`- phenanthroline) ruthenium (II) cations, *J. Am. Chem. Soc. 98*, 5800-5806.

Demas, J. N., and Crosby, G. A.
(1971) Quantum efficiencies on transition metal complexes. II. Charge- transfer luminence, *J. Am. Chem. Soc. 93*, 2841-2847.

Demas, J. N., and Taylor, D. G.
(1979) On the "intersystem crossing" yields in ruthenium (II) and osmium (II) photosensitizers, *Inorg. Chem. 18*, 3177-3179.

DeVault, D.
(1984) Quantum Mechanical Tunneling in Biological Systems. New York: Cambridge Univ. Press. 2nd ed.

Dionisi, H. M., Checa, S. K., Krapp, A. R., Arakaki, A. K., Ceccarelli, E. A., Carrillo, N., and Viale, A. M.
(1998) Cooperation of the DnaK and GroE chaperone systems in the folding pathway of plant ferredoxin-$NADP^+$ reductase expressed in *Escherichia coli, Eur. J. Biochem. 251*, 724-728.

Dodson, E.
(2003) Is it jolly SAD, *Acta Crystallogr. D59*, 1958-1965.

Dodsworth, E. S., Vleck, A. A., and Lever, A. B. P.
(1994) Factorization of ligand-based reduction potentials, *Inorg. Chem. 33*, 1045-1049.

Dumas, P., Ennifar, E. and Walter, P.
(1999) Detection and treatment of twinning: an improvement and new results, *Acta Crystallogr. D55*, 1179-1187.

Dunn, A. R., Dmochowski, I. J., Bilwes, A. M., Gray, H. B., and Crane, B. R.
(2001) Probing the open state of cytochrome $P450_{cam}$ with ruthenium-linker substrates, *Proc. Natl. Acad. Sci. U.S.A. 98,* 12420-12425.

Durham, D., Pan, L. P., Long, J. E., and Millet, F.
(1989) Photoinduced electron-transfer kinetics of singly labeled ruthenium bis(bipyridine) dicarboxybipyridine cytochrome *c* derivatives, *Biochemistry 28,* 8659-8665.

Fu, W., Drozdzewski, P. M., Davies, M. D., Sligar, S.G., and Johnson, M. K.
(1992) Resonance Raman and magnetic circular dichroism studies of reduced [2Fe-2S] proteins, *J. Biol. Chem. 267*, 15502-15510.

Geren, L., Hahm, S., Durham, B., and Millet, F
(1991) Photoinduced electron transfer between cytochrome c peroxidase and yeast cytochrome c labeled at Cys 102 with (4-bromomethyl-4'-methylbipyridine)[bis(bipyridine)]ruthenium2+, *Biochemistry 30*, 9450-9457.

Geren, L. M., O'Brien, P., Stonehuerner, J., and Millett, F.
(1984) Identification of specific carboxylate groups on adrenodoxin that are involved in the interaction with adrenodoxin reductase, *J. Biol. Chem. 259*, 2155-2160.

Grinberg, A. V., and Bernhardt, R.
(1998) Effect of replacing a conserved proline residue on the function and stability of bovine adrenodoxin, *Protein Eng. 11*, 1057-1064.

Grinberg, A. V. and Bernhardt, R.
(2001) Contribution of a salt bridge to the thermostability of adrenodoxin determined by site-direct mutagenesis, *Archiv. Biochem. Biophys. 396*, 25-34.

Grinberg, A. V., Hannemann, F., Schiffler, B., Müller, J. J., Heinemann, U., and Bernhardt, R.

(2000) Adrenodoxin: Structure, stability, and electron transfer properties, *PROTEINS: Structure, Function and Genetics 40*, 590-612.

Gonzáles, A.

(2003) Optimizing data collection for structure determination, *Acta Crystallogr. D59*, 1935-1942.

Hager, G. D., and Crosby, G. A.

(1975) Charge-transfer excited states of ruthenium (II) complexes. I. Quantum yield and decay measurements, *J. Am. Chem. Soc. 97*, 7031-7037.

Hannemann, F., Rottmann, M., Schiffler, B., Zapp, J., and Bernhardt, R.

(2001) The loop region covering the iron-sulfur cluster in bovine adrenodoxin comprises a new interaction site for redox partners, *J. Biol. Chem. 276*, 1369-1375.

Hanukoglu, I., and Jefcoate, C. R.

(1980) Mitochondrial cytochrome P-450sec. Mechanism of electron transport by adrenodoxin, *J. Biol. Chem. 255*, 3057-3061.

Hanukoglu, I., Privalle, C. T., and Jefcoate, C. R.

(1981) Mechanisms of ionic activation of adrenal mitochondrial cytochromes P-450_{scc} and P-45011β, *J. Biol. Chem. 256,* 4329-4335.

Hara, T., and Kimura, T.

(1989) Active complex between adrenodoxin reductase and adrenodoxin in the cytochrome P-450scc reduction reaction, *J. Biochem. 105*, 601-605.

Hara, T., and Kimura, T.

(1989) Purification and catalytic properties of a cross-linked complex between adrenodoxin reductase and adrenodoxin, *J. Biochem. 105*, 594-600.

Hara, T., and Miyata, T.
(1991) Identification of a cross-linked peptide of a covalent complex between adrenodoxin reductase and adrenodoxin, *J. Biochem. 110*, 261-266.

Hara, T., and Takeshima, M.
(1994) Conclusive evidence of a quartery cluster model for cholesterol side-chain cleavage reaction catalyzed by cytochrome $P450_{scc}$. In *Cytochrome P450. 8th International Conference* (Lechner, M. C., ed.), 417-420, John Libbey Eurotext, Paris, France.

Harada, Y., Lifchitz, A., and Berthou, J.
(1981) A translation function combining packing and diffraction information: An application to lysozyme (High-temperature form), *Acta Crystallogr. A37*, 398-406.

Hartl, F. U.
(1996) Molecular chaperones in cellular protein folding, *Nature 381*, 571-580.

Hintz, M. J., and Peterson, J. A.
(1980) The kinetics of reduction of cytochrome P-450cam by the dithionite anion monomer, *J. Biol. Chem. 255*, 7317-7325.

Hirasawa, M., Chang, K. T., and Knaff, D. B.
(1991) The interaction of ferredoxin and glutamate synthase: cross-linking and immunological studies, *Arch. Biochem. Biophys. 286*, 171-177.

Hiwatashi, A., Sakihama, N., Shin, M., and Ichikawa, Y.
(1986) Heterogeneity of adrenocortical ferredoxin, *FEBS Lett. 209*, 311-315.

Hooft, R. W. W., Vriend, G., Sander, C., and Abola, E. E.
(1996) Errors in protein structures, *Nature 381*, 272-272.

Hopfield, J. J.
(1974) Electron transfer between biological molecules by thermally activated tunneling, *Proc. Natl. Acad. Sci. U.S.A. 71*, 3640-3644.

Hopfield, J. J.

(1982) *Oxidases and Related Redox Systems*, J. J. Hopfield, Ed., Pergamon Press: Oxford, 3-19.

Horie, S., and Watanabe, T.

(1975) Properties of high spin type P-450 preparations from bovine adrenal cortex mitochondria, *J. Steroid Biochem. 6*, 401-409.

Hornsby, P. J.

(1980) Regulation of cytochrome P-450-supported 11 beta-hydroxylation of deoxycortisol by steroids, oxygen, and antioxidants in adrenocortical cell cultures, *J. Biol. Chem*. *255*, 4020-4027.

Huang, J. J., and Kimura, T.

(1973) Adrenal steroid hydroxylases. Oxidation-reduction properties of adrenal iron-sulfur protein (adrenodoxin), *Biochemistry 12,* 406-409.

Ikemizu, S., Bando, M., Sato, T., Morimoto, Y., Tsukihara, T., and Fukuyama, K.

(1994) Structure of [2Fe-2S] ferredoxin I from *Equisetum avense* at 18 Å resolution, *Acta Crystallogr*. *D50*, 167-174.

Isied, S. S., and Vassilian, A.

(1984) Electron-transfer across polypeptides. 3. oligoproline bridging ligands, *J. Am. Chem. Soc.* 106, 1732-1736.

Isied, S. S., Worosila, G., and Atherton, S. J.

(1982) Electron-transfer across polypeptides .4. intramolecular electron-transfer from ruthenium (II) to iron(III) in histidine-33 modified horse heart cytochrome-*c*, *J. Am. Chem. Soc. 104*, 7659-7661.

Janin, J.

(1995) Principles of protein-protein recognition from structure to thermodynamics, Biochemie 77, 497-505.

Janin, J.

(1997) Specific versus non-specific contacts in protein crystals, *Nat. Struct. Biol. 4*, 973-974.

Janin, J. and Rodier, F.

(1995) Protein-protein interaction at crystal contacts, *Proteins 23*, 580-587.

Jacobson, B. L., Chae, Y. K., Markley, J. L., Rayment, I., and Holden, H. M.

(1993) Molecular structure of the oxidized, recombinant, heterocyst [2Fe-2S] ferredoxin from *Anabaena 7120* determined to 17 Å resolution, *Biochemistry 32*, 6788-6793.

Johnson, C. E., Cammack, R., Rao, K. K., and Hall, D. O.

(1971) The interpretation of the EPR and Mössbauer spectra of two-iron, one-electron, iron-sulphur proteins, *Biochem. Biophys. Res. Commun. 43*, 564-571.

Jones, T. A., Zhou, J.-Y., Cowan, S. W., and Kjeldgaard, M.

(1991) Improved methods for building protein models in electron density maps and the location of errors in these models, *Acta Crystallogr. A47***,** 110-119.

Jortner, J.

(1980) Dynamics of electron transfer in bacterial photosynthesis, *Biochim. Biophys. Acta 594*, 193-230.

Juris, A., Balzani, V., Barigelletti, F., Campagna, S., Belser, P., and Vonzelewsky, A.

(1988) Ru(II) polypyridine complexes: photophysics, photochemistry, electrochemistry, and chemiluminescence, *Coord. Chem. Rev. 84,* 85-277.

Kabsch, W.

(1976) A solution for the best rotation to relate two sets of vectors, *Acta Crystallogr. A32*, 922-923.

Kabsch, W.

(1988) Evaluation of single-crystal X-ray diffraction data from a position-sensitive detector, *J. Appl. Cryst. 21*, 916-924.

Kabsch, W.
(2001) Chapter 25.2.9. *XDS* in *International Tables for Crystallography*, Volume F. Crystallography of Biological Macromolecules, Rossmann, M.G. and Arnold, E. (2001). Editors. Dordrecht: Kluwer Academic Publishers.

Kalyanasundaram, K.
(1982) Photophysics, photochemistry and solar energy conversion with tris(bipyridyl)ruthenium(II) and its analogues, *Coord. Chem. Rev. 46*, 159-244.

Kalyanasundaram, K.
(1992) Photochemistry of Polypyridine and Porphyrine Complexes Ch. 6, Academic Press, London,.

Karpishin, T. B., Grinstaff, M. W., Komar-Panuicucci, S., McLendon, G., and Gray, H. B.
(1994) Electron transfer in cytochrome *c* depends upon the structure of the intervening medium, *Structure 2*, 415-422.

Kawatsu, T., Kakitani, T., and Yamato, T.
(2000) A novel method for determining the electron tunneling pathways in protein, *Inorg. Chim. Acta 300-302*, 862-868.

Kawatsu, T., Kakitani, T., and Yamato, T.
(2001) Worm model for electron tunneling in proteins: consolidation of the pathway model and the Dutton plot, *J. Phys. Chem. 105*, 4424-4435.

Keller, P., Moradpour, A., Amouyal, E., and Kagan, H. B.
(1980) Hydrogen-production by visible-light using viologen-dye mediated redox cycles, *Nouv. J. Chim. 4*, 377-384.

Kestenbaum, D.
(1998) New math speeds the search for protein structures, *Science 282*, 30-31.

Kestner, N. R., Logan, J., and Jortner, J.
(1974) Thermal electron transfer reactions in polar solvents, *J. Phys. Chem. 78*, 2148-2166.

Kido, T., and Kimura, T.
(1979) The formation of binary and ternary complexes of cytochrome P-450_{scc} with adrenodoxin and adrenodoxin reductase-adrenodoxin complex. The implication in ACTH function, *J. Biol. Chem. 254,* 11806-11815.

Kimura, T.
Redox components of adrenal steroid hydroxylase. In: biological and chemical aspects of oxygenases, p. 179. *K. Bloch* and *O. Hayaishi,* ed. Tokyo: Maruzen 1966.

Kimura, T.
(1968) Biochemical aspects of iron-sulfur linkage in non-heme iron protein, with special reference to "Adrenodoxin", *Struct. Bonding 5*, 1-40.

Kimura, T., Parcells, J. H., and Wang, H. P.
(1978) Purification of adrenodoxin reductase, adrenodoxin, and cytochrome P-450 from adrenal cortex, *Methods Enzymol. 52*, 132-142.

Kimura, T., and Suzuki, K.
(1965) Enzymatic reduction of non-heme iron protein (adrenodoxin) by reduced nicotinamide adenine dinucleotide phosphate, *Biochem. Biophys. Res. Commun. 20*, 373-379.

Kimura, T., and Suzuki, K.
(1967) Components of the electron transport system in adrenal steroid hydroxylase. Isolation and properties of non-heme iron protein (Adrenodoxin), *J. Biol. Chem. 242*, 485-491.

Kober, E. M., and Meyer, T.
(1984) An electronic structural model for the emitting MLCT excited-state of $Ru(bpy)_3^{2+}$ and $Os(bpy)_3^{2+}$, *J. Inorg. Chem. 23*, 3877-3886.

Koch, E.
(1992) International Tables for Crystallography, Vol. C, edited by A. J. C. Wilson, pp. 10-14. Dordrecht: Kluwer Academic Publishers.

Kostič, N. M., Margalit, R., Che, C.-M., and Gray, H. B.

(1983) Kinetics of long-distance ruthenium-to-copper electron-transfer in [pentaaammineruthenium histidine-83]azurin, *J. Am. Chem. Soc. 105*, 7765-7767.

Krueger, R. J., and Siegel, L. M.

(1982) Spinach siroheme enzymes: Isolation and characterization of ferredoxin-sulfite reductase and comparison of properties with ferredoxin-nitrite reductase, *Biochemistry 21*, 2892-2904.

Koradi, R., Billeter, M., and Wüthrich, K.

(1996) MOLMOL: a program for display and analysis of macromolecular structures *J. Mol. Graphics 14*, 51-55.

Laemmli, U. K.

(1970) Cleavage of structural proteins during the assembly of the head of bacteriophage T4, *Nature 227*, 680-685.

Lambeth, D. O., and Palmer, G.

(1973) The kinetics and mechanism of reduction of electron transfer proteins and other compounds of biological interest by dithionite, *J. Biol. Chem. 248,* 6095-6103.

Lambeth, J. D., and Pember, S. O.

(1983) Cytochrome P-450scc-adrenodoxin complex. Reduction properties of the substrate-associated cytochrome and relation of the reduction states of heme and iron–sulfur centers to association of the proteins, *J. Biol. Chem. 258*, 5596–5602.

Lambeth, J. D., Seybert, D. W., Lancaster, J. R., Salerno, J. C., and Kamin, H.

(1982) Steroidogenic electron transport in adrenal cortex mitochondria, *Mol. Cell. Biochem. 45*, 13-31.

Lapko, A. G., Müller, A., Heese, O., Ruckpaul, K., and Heinemann, U.

(1997) Preparation and crystallization of a cross-linked complex of bovine adrenodoxin and adrenodoxin reductase, *PROTEINS: Structure, Function, and Genetics 28*, 289-292.

Larsson, S.
(1981) Electron-transfer in chemical and biological-systems - orbital rules for non-adiabatic transfer, *J. Am. Chem. Soc. 103*, 4031-4040.

Larsson, S.
(1983) Electron-transfer in proteins, *J. Chem. Soc. Faraday Trans. 2, 79*, 1357-1388.

Laskowski, R. A., MacArthur, M. W., Moss, D. S., and Thornton, J. M.
(1993) PROCHECK: a program to check the stereochemical quality of protein structures. *J. Appl. Cryst. 26*, 283-291.

Lieberman, S., and Lin, Y. Y.
(2001) Reflections on sterol side-chain cleavage process catalyzed by cytochrome $P450_{scc}$, *J. Ster. Biochem. Mol. Biol. 78*, 1-14.

Marcus, R. A.
(1956) On the energy of oxidation-reduction reactions involving electron transfer, *J. Chem. Phys. 24*, 966-978.

Marcus, R. A.
(1965) On the theory of electron-transfer reactions. VI. Unified treatment for homogen electrode reactions, *J. Chem. Phys. 43,* 679-701.

Marcus, R. A.
(1982) The 2nd Robinson,R.A. Memorial Lecture - Electron, Proton and Related Transfers, *Faraday Disc. Chem. Soc. 74,* 7-15.

Marcus, R. A., and Siders, P.
(1982) Theory of highly exothermic electron-transfer reactions, *J. Phys. Chem. 86,* 622-630.

Marcus, R. A., and Sutin, N.
(1985) Electron transfer in chemistry and biology, *Biochim. Biophys. Acta 811*, 265-322.

Martin, J., Mayhew, M., Langer, T., and Hartl, U.
(1993) The reaction cycle of GroEL and GroES in chaperonin-assisted protein folding, *Nature 366*, 228-233.

Mason, J. R., and Cammack, R.
(1992) The electron transport proteins of hydroxylating bacterial dioxygenases, *Annu. Rev. Microbiol. 46*, 277-305.

Masui, H., and Lever, A. B. P.
(1993) Correlations between the ligand electrochemical parameter, el(l), and the hammett substituent parameter, sigma, *Inorg. Chem. 32*, 2199-2201.

McGourty, J. L., Peterson-Kennedy, S. E., Ruo, W. Y., and Hoffman, B. M.
(1987) Characterization of long-range electron transfer in mixed-metal [zinc, iron] hybrid hemoglobins, *Biochemistry 26*, 8302-8312.

McPherson, A.
(1990) Current approaches to macromolecular crystallization, *Eur. J. Biochem. 189*, 1-23.

McPherson, A.
(1999) Crystallization of Biological Macromolecules. New York. CSHL Press.

Mikkelsen, K. V., and Ratner, M. A.
(1987) Electron-tunneling in solid-state electron-transfer reactions, *Chem. Rev. 87*, 113-153.

Morris, A. L., MacArthur, M. W., Hutchinson, E. G., and Thornton, J. M.
(1992) Stereochemical quality of protein structure coordinates, *Proteins 12*, 345-364.

Müller, A., Müller, J. J., Muller, Y. A., Uhlmann, H., Bernhardt, R., and Heinemann, U.
(1998) New aspects of electron transfer revealed by the crystal structure of a truncated bovine adrenodoxin, Adx(4-108), *Structure 6*, 269-280.

Müller, E.-Ch., Lapko, A., Otto, A., Müller, J. J., Ruckpaul, K., and Heinemann, U.
(2001) Covalently cross-linked complex of bovine adrenodoxin with adrenodoxin reductase and cytochrome $P450_{scc}$. Mass spectrometry and Edman degradation of complexes of the steroidogenic hydroxylase system, *Eur. J. Biochem. 268,* 1837-1843.

Müller, J. J., Lapko, A., Bourenkov, G., Ruckpaul, K., and Heinemann, U.
(2001) Adrenodoxin reductase-adrenodoxin complex structure suggests electron transfer path in steroid biosynthesis, *J. Biol. Chem. 276,* 2786-2789.

Müller, J. J., Müller, A., Rottmann, M., Bernhardt, R., and Heinemann, U.
(1999) Vertebrate-type and plant-type ferredoxins: crystal structure comparison and electron transfer pathway modeling, *J. Mol. Biol. 294*, 501-513.

Müller, T., Oehlenschläger, F., and Buehner, M.
(1995) Human interleukin-4 and variant R88Q: Phasing X-ray diffraction data by molecular replacement using X-ray and nuclear magnetic resonance models, *J. Mol. Biol. 247*, 360-372.

Mukai, K., Kimura, T., Helbert, J., and Kevan, L.
(1973) Environment of the iron-sulfur chromophore in adrenodoxin studied by EPR and ENDOR spectroscopy, *Biochim. Biophys. Acta 295*, 49-56.

Murray, J. W., and Garman, E.
(2003) Heavy-atom derivatization, *Acta Crystallogr. D59*, 1903-1913.

Murshudov, G. N., Vagin, A. A., and Dodson, E. J.
(1997) Refinement of macromolecular structures by the maximum-likelihood method, *Acta Crystallogr. D53*, 240-255.

Nagai, K., Perutz, M. F., Poyart, C.
(1985) Oxygen binding properties of human mutant hemoglobins synthesized in *Escherichia coli*, *Proc. Natl. Acad. Sci. U.S.A. 82*, 7252-7255.

Navaza, J.
(1987) On the fast rotation function, *Acta Crystallogr. A43*, 645-653.

Navaza, J.
(1990) Accurate computation of the rotation matrices, *Acta Crystallogr. A46*, 619-620.

Navaza, J.
(1993) On the Computation of the Fast Rotation Function, *Acta Crystallogr. D49*, 588-591.

Navaza, J.

(1994) AMoRe: an automated package for Molecular Replacement, *Acta Crystallogr. A50*, 157-163.

Newton, M. D.

(1982) Mechanistic studies of electron exchange kinetics using *ab initio* electronic-structure techniques, *Am. Chem. Soc. Sym. Ser. 198*, 255-279.

Newton, M. D., and Sutin, N.

(1984) Electron-transfer reactions in condensed phases, *Annu. Rev. Phys. Chem. 35,* 437-480.

Okamura, T., John, M. E., Zuber, M. X., Simpson, E. R., and Waterman, M. R.

(1985) Molecular cloning and amino acid sequence of the precursor form of bovine adrenodoxin: Evidence for a previously unidentified COOH-terminal peptide, *Proc. Natl. Acad. Sci. U.S.A. 82*, 5705-5709.

Omura, T., and Sato, R.

(1964) The carbon monoxide-binding pigment of liver microsomes. I. Evidence for its hemoprotein nature, *J. Biol. Chem. 239,* 2370-2378.

Omura, T., Sato, R., Cooper, D. Y., Rosenthal, O., and Estabrook, R. W.

(1965) Function of cytochrome P-450 of microsomes *Fed. Proc. 24*, 1181.

Onuchic, J. N., and Beratan, D. N.

(1987) Molecular bridge effects on distant Charge tunneling, *J. Am. Chem. Soc. 109*, 6771-6778.

Onuchic, J. N., Beratan, D. N., Winkler, J. R., and Gray, H. B.

(1992) Pathway analysis of protein electron-transfer reactions, *Annu. Rev. Biophys. Biomol. Struct. 21*, 349-377.

Otwinowski, Z., and Minor, W.

(1997) Processing of X-ray data diffraction data collected in oscillation mode, *Meth. Enzymol. 276*, 307-326.

Packer, E. L., Sternlicht, H., and Rabinowitz, J.

(1972) The possible role of aromatic residues of *Clostridium* acidi-urici ferredoxin in electron transport, *Proc. Natl. Acad. Sci. U. S. A. 69*, 3278-3282.

Page, C. C., Moser, C. C., Chen, X., and Dutton, L.

(1999) Natural engineering principles of electron tunneling in biological oxidation-reduction, *Nature 402,* 47-52.

Palmer, G., Brinzinger, H., and Estabrook, R. W.

(1967) Spectroscopic studies on spinach ferredoxin and adrenodoxin, *Biochemistry 6*, 1658-1664.

Pan, L. P., Frame, M., Durham, B., Davis, D., and Millet, F.

(1990) Photo-induced electron transfer within complexes between plastocyanin and ruthenium bisbipyridine dicarboxybipyridine cytochrome c derivatives, *Biochemistry 29*, 3231-3236.

Pannu, N. S., and Read, R. J.

(1996) Improved structure refinement through maximum likelihood, *Acta Crystallogr. A52,* 659-668.

Parsons, S.

(2003) Introduction to twinning, *Acta Crystallogr. D59*, 1995-2003.

Pearson, W. R., and Lipman, D. J.

(1998) Improved tools for biological sequence comparison, *Proc. Natl. Acad. Sci. U.S.A. 85*, 2444-2448.

Pikuleva, I. A., Tesh, K., Waterman, M. R., and Kim, Y.

(2000) The tertiary structure of full-length bovine adrenodoxin suggests functional dimers, *Arch. Biochem. Biophys. 373,* 44-55.

Pochapsky, T. C., Lyons, T. A., Kazanis, S., Arakaki, T., and Rasnaswamy, G.

(1996) A structure-based model for cytochrome P450cam-putidaredoxin interactions, *Biochemie 78*, 723-733.

Ponstingl, H., Henrick, K., and Thornton, J. M.
(2000) Discriminating between homodimeric and monomeric proteins in the crystalline state, Proteins 41, 47-57.

Privalle, L. S., Privalle, C. T., Leonardy, N. J., and Kamin, H.
(1995) Interactions between spinach ferredoxin-nitrite reductase and its substrates. Evidence for the specificity of ferredoxin, *J. Biol. Chem. 260*, 14344-14350.

Read, R. J.
(1986) Improved Fourier coefficients for maps using phases from partial structures with errors, *Acta Crystallogr. A42*, 140-149.

Read, R. J.
(2003) New way of looking at experimental phasing, *Acta Crystallogr. D59*, 1891-1902.

Rossmann, M. G., and Blow, D. M.
(1962) The detection of subunits within the crystallographic asymmetric unit, *Acta Crystallogr. 15*, 24-31.

Rypniewski, W. R., Breiter, D. R., Benning, M. M., Wesenberg, G., Oh, B. H., Markley, J. L., Rayment, I., and Holden, H. M.
(1991) Crystallization and structure determination to 25-Å resolution of the oxidized [2Fe-2S] ferredoxin isolated from *Anabaena 7120*, *Biochemistry 30*, 4126-4131.

Sagara, Y., Wada, A., Takata, Y., Waterman, M. R., Sekimizu, K., and Horiuchi, T.
(1993) Direct expression of adrenodoxin reductase in *E. coli* and the functional characterization, *Biol. Pharm. Bull. 16*, 627-630.

Schiffler, B., Kiefer, M., Wilken, A., Hannemann, F., Adolph, H. W., and Bernhardt, R.
(2001) The interaction of bovine adrenodoxin with CYP11A1 (Cytochrome $P450_{scc}$) and CYP11B1 (Cytochrome $P450_{11}\beta$). ACCELERATION OF REDUCTION AND SUBSTRATE CONVERSION BY SITE-DIRECTED MUTAGENESIS OF ADRENODOXIN, *J. Biol. Chem. 276*, 36225-36232.

Schiltz, M., Prangé, T., and Fourme, R.
(1994) On the preparation and X-ray data-collection of isomorphous Xenon derivatives, *J. Appl. Cryst. 27*, 950-960.

Schwarz, D., Richter, W., Kruger, V., Chernogolov, A., Usanov, S., and Stier, A.
(1994) Direct visualization of a cardiolipin-dependent cytochrome $P450_{scc}$-induced vesicle aggregation, *J. Struct. Biol. 113,* 207-215.

Scott, J. R., Willie, A., McLean, M., Stayton, P. S., Sligar, S. G., Durham, B., and Millett, F.
(1993) Intramolecular electron transfer in cytochrome b5 labeled with ruthenium(II) polypyridine complexes: rate measurements in the Marcus inverted region, *J. Am. Chem. Soc. 115,* 6820-6824.

Shimada, H., Nagano, S., Ariga, Y., Unno, M., Egawa, T., Hishiki, T., Ishimura, Y., Masuya, F., Obata, T., and Hori, H.
(1999) Putidaredoxin-cytochrome $P450_{cam}$ interaction. Spin state of the heme iron modulates putidaredoxin structure, *J. Biol. Chem. 274,* 9363-9369.

Siders, P. and Marcus, R. A.
(1981) Quantum effects for electron-transfer reactions in the inverted region, *J. Am. Chem. Soc. 103*, 748-752.

Sligar, S. G., and Gunsalus, I. C.
(1976) A thermodynamic model of regulation: modulation of redox equilibria in camphor monooxygenase, *Proc. Natl. Acad. Sci. U.S.A. 73,* 1078-1082.

Soltis, S. M., Stowell, M. H. B., Wiener, M. C., Phillips Jr., G., N., and Rees, D. C.
(1997) Successful flash-cooling of xenon-derivatized myoglobin crystals, *J. Appl. Cryst. 30*, 190-194.

Stryer, L.
(1995) *Biochemistry*, 3rd edn., Freeman, San Francisco

Suhara, K., Gomi, T., Sato, H., Itagaki, E., Takemori, S., and Katagiri, M.
(1978) Purification and immunochemical characterization of the two adrenal cortex mitochondrial cytochrome *P*-450-proteins, *Arch. Biochem. Biophys. 190*, 290-299.

Sun, J., Wishart, J. F., van Eldik, R., Shalders, R. D., and Swaddle, T. W.
(1995) Pressure tuning voltammetry. Reaction volumes for electron transfer in cytochrome *c* and ruthenium-modified cytochromes *c*, *J. Am. Chem. Soc. 117,* 2600-2605.

Sussman, J. L., Shoham, M., and Harel, M.
(1989) Protein adaptation to extreme salinity: the crystal structure of 2Fe-2S ferredoxin from *Halobacterium marismortui*, *Prog. Clin. Biol. Res. 289*, 171-187.

Sutin, N., Brunschwig, B. S. Creutz, C., and Winkler, J. R.
(1988) Nuclear reorganization barriers to electron-transfer, *Pure Appl. Chem. 60*, 1817-1829.

Sutin, N., and Creutz, C.
(1978) Properties and reactivity of the luminescent excited states of polypyridine complexes of ruthenium (II) and osmium (II), *Adv. Chem. Ser. 168*, 1-27.

Suzuki, K., and Kimura, T.
(1965) An iron protein as a component of steroid 11 β-hydroxylase complex. *Biochem. Biophys. Res. Commun. 19*, 340-345.

Szoke, A.
(1993) Holographic methods in X-ray crystallography. II. Detailed theory and connection to other methods of crystallography, *Acta Crystallogr. A49,* 853-866.

Takeuchi, K., Tsubaki, M., Futagawa, J., Masuya, F., and Hori, H.
(2001) Adrenodoxin-cytochrome P450scc interaction as revealed by EPR spectroscopy: Comparison with putidaredoxin-cytochrome P450cam system, *J. Biochem. 130*, 789-797.

Tanaka, M., Haniu, M., Yasunobu, K., and Kimura, T.
(1973) The amino acid sequence of bovine adrenodoxin, *J. Biol. Chem. 248*, 1141-1157.

Taniguchi, T., and Kimura, T.
(1975) NO_2-Tyr^{82} and NH_2-Tyr^{82} derivatives of adrenodoxin. Effects of chemical modification on electron transferring activity, *Biochemistry 14*, 5573-5578.

Taniguchi, T., and Kimura, T.
(1976) Studies on nitrotyrosine-82 and aminotyrosine-82 derivatives of adrenodoxin. Effects of chemical modification on the complex formation with adrenodoxin reductase, *Biochemistry 15*, 2849-2853.

Tembe, B. L., Friedman, H. L. and Newton, M. D.
(1982) The theory of the Fe2+-Fe3+ electron exchange in water, *J. Chem. Phys. 76*, 1490-1507.

Terwilliger, T. C.
(2000) Maximum likelihood density modification, *Acta Crystallogr*. *D56*, 965-972.

Terwilliger, T. C.
(2002) Automated main-chain model-building by templatematching and iterative fragment extension, *Acta Crystallogr*. *D59*, 34-44.

Terwilliger, T. C., and Berendzen, J.
(1999) Automated MAD and MIR structure solution, *Acta Crystallogr. D55*, 849-861.

Terwisscha van Scheltinga, A. C., Valegård, K., Hjadu, J., and Andresson, I.
(2003) MIR phasing using merohedrally twinned crystals, *Acta Crystallogr. D59*, 2017-2022.

Thornton, S. T., and Rex, A.
(1993) Modern Physics for Scientists and Engineers, Saunders College Publishing.

Tokel-Takvoryan, N. E., Hemingway, R. E., and Bard, A. J.
(1973) Electrogenerated chemiluminescence. XIII. Electrochemical and electrogenerated chemiluminescence studies of ruthenium chelates, *J. Am. Chem. Soc. 95*, 6582-6589.

Tong, L.
(1996) Combined molecular replacement, *Acta Crystallogr. A52*, 782-784.

Tsubaki, M., Hiwatashi, A., and Ichikawa, Y.
(1989) Conformational change of the heme moiety of ferrous cytochrome P-450$_{scc}$-phenyl isocyanide complex upon binding of reduced adrenodoxin, *Biochemistry 28*, 9777-9784.

Tsukihara, T., Fukuyama, K., Mitsushima, M., Harioka, T., Kusunoki, M., Katsube, Y., Hase, T., and Matsubara, H.
(1990) Structure of the [2Fe-2S] ferredoxin I form the blue green algae *Aphanothece sacrum* at 22 Å resolution, *J. Mol. Biol. 216*, 339-410.

Tsukihara, T., Fukuyama, K., Nakamura, M., Katsube, Y., Tanaka, N., Kakudo, M., Wada, K., Hase, T., and Matsubara, H.
(1981) X-ray analysis of a [2Fe-2S] ferredoxin from *Spirulina platensis*. Main chain fold and location of side chains at 25 Å resolution, *J. Biochem*. *90*, 1763-1773.

Tuckey, R. C., McKinley, A. J., and Headlam, M. J.
(2001) Oxidized adrenodoxin acts as a competitive inhibitor of cytochrome P450$_{scc}$ in mitochondria from the human placenta, *Eur. J. Biochem. 268,* 2338-2343.

Tyson, C. A., Lipscomp, J. D., and Gunsalus, I. C.
(1972) The roles of putidaredoxin and P450cam in methylene hydroxylation, *J. Biol. Chem. 247*, 5777-5784.

Uhlmann, H., Beckert, V., Schwarz, D., and Bernhardt, R.
(1992) Expression of bovine adrenodoxin in *E. coli* and site-directed mutagenesis of [2Fe-2S] cluster ligands, *Biochem. Biophys. Res. Commun. 188*, 1131-1138.

Uhlmann, H., and Bernhardt, R.
(1995) The role of threonine 54 in adrenodoxin for the properties of its iron–sulfur cluster and its electron transfer function, *J. Biol. Chem. 270*, 29959-29966.

Uhlmann, H., Kraft, R., and Bernhardt, R.
(1994) C-terminal region of adrenodoxin affects its structural integrity and determines differences in its electron transfer function to cytochrome P-450, *J. Biol. Chem. 269*, 22557-22564.

Ulstrup, J., and Jortner, J.
(1975) The effect of intramolecular quantum modes on free energy relationships for electron transfer reactions, *J. Phys. Chem. 63*, 4358-4368.

Usanov, S. A., Turko, I. V., Chashchin, V. L., and Akhrem, A. A.
(1985) Cross-linking studies of steroidogenic electron transfer: covalent complex of adrenodoxin reductase with adrenodoxin, *Biochim. Biophys. Acta 832*, 288-296.

Valdar, S. J., and Thornton, J. M.
(2001) Conservation helps to identify biologically relevant crystal contacts, J. Mol. Biol. 313, 399-416.

Vallee, B. L., and Ulmer, D. D.
(1965) Optical rotatory dispersion of iron proteins. In: Non-heme iron proteins, p. 43; A. San Pietro, ed. Yellow Springs, Ohio: Antioch Press.

Vonrhein, C., Schmidt, U., Ziegler, G. A., Schweiger, S., Hanukoglu, I., and Schulz, G. E.
(1999) Chaperone-assisted expression of authentic bovine adrenodoxin reductase in Escherichia coli, *FEBS Letters 443*, 167-169.

Vriend, G.
(1990) WHATIF: a molecular modeling and drug design program, *J. Mol. Graph. 8*, 52-56.

Warshel, A.
(1982) Dynamics of reactions in polar-solvents - semi-classical trajectory studies of electron-transfer and proton-transfer reactions *J. Phys. Chem. 86,* 2218-2224.

Watari, H, and Kimura, T.
(1966) Study of the adrenal non-heme iron protein (adrenodoxin) by electron spin resonance, *Biochem. Biophys. Res. Commun. 24*, 106-112.

Winkler, J. R., Nocera, D. G., Yocom, K. M., Bordignon, E., and Gray, H. B.
(1982) Electron-transfer kinetics of pentaammineruthenium(III)(histidine-33)-ferricytochrome-C - measurement of the rate of intramolecular electron-transfer between redox centers separated by 15-a in a protein, *J. Am. Chem. Soc. 104*, 5798-5800.

Xia, B., Volkman, B. F., and Markley, J. L.
(1998) Evidence for oxidation-state-dependent conformational changes in human ferredoxin from multinuclear, multidimensional NMR spectroscopy, *Biochemistry 37*, 3965–3973.

Yeates, T. O.
(1997) Detecting and overcoming crystal twinning, *Methods Enzymol. 276*, 344-358.

Yeates, T. O., and Fam, B. C.
(1999) Protein crystals and their evil twins, *Structure 7*, R25-R29.

Yeh, A. T., Shank, C. V., and McCusker, J. K.
(2000) Ultrafast electron localization dynamics following photo-induced charge transfer, *Science 289*, 935-938.

Young, R. C., Meyer, T. J., and Whitten, D. G.
(1976) Electron transfer quenching of excited states of metal complexes, *J. Am. Chem. Soc. 98*, 286-287.

ACKNOWLEDGEMENTS

My post-graduate experience at the Max-Delbrück-Center (MDC) for Molecular Medicine, Berlin-Buch has been rewarding on many levels and I would like to thank those who have supported me with advice and friendship along the way.

First, I would like to thank my scientific advisors of past and present. I thank Dr. Anna G. Lapko for generating a stimulating and exciting working environment during my study at the International Sakharov Environmental University (ISEU) in Minsk. Dr. Lapko is a model of kindness and an inspiration for me in science. Perhaps most importantly, she has patiently taught me independent thinking and problem solving. Her never-ending enthusiasm for science made working in the lab an addictive activity not only for me, but also for other students. Mrs. Lapko together with Prof. Dr. Klaus Ruckpaul were people who helped to bring me from a graduate student to a member of the Crystallography Group of Prof. Dr. Udo Heinemann at the MDC. I thank Prof. Heinemann for allowing me to work in his lab and to write my thesis. He was also the first person who introduced me the theory of crystallography of biomolecules, giving lectures for PhD students during my stay at MDC. I also would like to thank a person from that group, namely, Dr. Jürgen J. Müller from whom I learned much about the analysis of 3D structures of biomolecules. I thank Dr. Christiane Jung from the Protein Dynamics Group at MDC who has taken a tremendous amount of time to teach me the details of the electron-transfer theory, and much more. Collectively, my advisors have presented me the beautiful gift of knowledge, which I hope to pass on to the next generation with the same enthusiasm as it was given to me.

I would like to thank other past and present members of the Crystallography Group. Anette Feske was actually the first person, which I met when I came to the lab first time early October morning 2001. She made my life in the lab easy, helping with orders, lab stuff and more. I also thank Gisela Sklenar who worked the next bench to me and helped me always with a good advice. I thank Birgit Cloos who is the friendliest secretary I know. I do not want to forget to thank Andreas Knespel for his willingness to help me not only in the group, but also in my old-day life in Berlin.

Katja Fälber, Yvette Roske, Dheeraj Khare, Erik Werner, Ralf Bienert were previous PhD-students of the Crystallography Group who helped me to learn more about lab techniques and crystallization of biomolecules. They are also people who made social life of the group interesting, visiting cinemas and having nice time in Berlin. Some of the PhD students whom I

met four years ago are still in the group. Sarbani Bhattacharrya, Ravi Kumar Lokareddy, Klaas Max are the people who continue to make a working atmosphere in the lab for new coming PhD students Bettina König, Kerstin Böhm, and Daniel Kümmel. New people of the lab, I also thank you for maintaining a friendly atmosphere in the group.

I thank people of the Jung's group, especially Jörg Contzen and Matthias Gerhardt for their help when I was working on my thesis. Sometimes they all were joking that I can even become a member of the Protein Dynamics Group, because I was quite often upstairs doing my experiments. From these people I learned much about the electron transfer in biological systems.

Of course, I would like to thank Dr. Eva-Christina Müller, Jürgen J. Müller's wife, and Dr. Albrecht Otto for their wish to help me to answer the questions what proteins I had purified. They were always open to carry some new additional mass spectrometry and Edman degradation experiments. I thank Drs. Heinz Welfle and Dr. Lubomír Dostál for allowing me to carry photoreduction experiments using argon ion laser with constant switching off the light in the lab when all other members were working there. The EPR basis was provided by Dr. Friedhelm Lendzian and Dr. Marcus Galander from the Technical University in Berlin. I thank you too.

During my stay at the Saarland University in August 2002 I met people who are also working on the proteins of the mitochondrial steroid hydroxylase system. My special thanks go to Prof. Dr. Rita Bernhardt and Dr. Frank Hannemann for their reception in the group and help.

My acknowledgements would be incomplete if I did not mention Mrs. Regina Rahm and Prof. Dr. Friedrich Körber – people who together with Prof. Dr. Ruckpaul and Dr. Lapko understood my wish to be in Berlin as a holder of scholarship of the Berliner Senate.

My thanks I would like also to address to Dr. Tatjana Schmidt for her help and friendship at MDC. It was nice with you to have lunch time in our Mensa during my last months at MDC.

I spent four years in Berlin, living in the Internationales Studienzenrum Berlin. This is a nice house where you can meet such different people that can make your life unforgettable. This was possible due to the management of Mrs. Petra Fritsche and Mrs. Emanuela Ebel whom my many thanks go to.

I must not forget people who were together with me during my study in Minsk. These are Dr. A. G. Lapko, **Prof. Dr. A. A. Milytin**, Dr. V. D. Svirid, Dr. V. V. Selyavko, Dr. Y. Rogov, Dr. I. Veyalkin, Mrs. J. N. Petrovskaya, Katja Torbaschevich, Lena Smirnova, Olesya Ivashkevich, Ira Kalatskaya, Natasha Prokopenko, Vadim Pasjukov, and Sergey Odintsov. Dear colleagues and friends, I thank you for the support that was given to me. I also remember my

schoolmate Olya Gurskaya who stayed with me in contact four years, bringing news from my school friends.

My thanks go to Dr. Ilona Cesniene and Aleksander Miroshnik who makes me look forward to every new day during my first year in Berlin.

I thank my near relations, my sister Natasha, and my Mom and Dad who have given me their love and support over the years.

Thank You All!

PUBLICATIONS

Conferences

The 6th Heart of Europe Bio-Crystallography Meeting (HEC6), 25-27 September, 2003, Wittenberg, Germany.

The 7th Heart of Europe Bio-Crystallography Meeting (HEC7), 30 September-2 October 2004, Krzyżowa, Poland.

XX Congress of the International Union of Crystallography, 23-31 August, 2005, Florence, Italy.

The results of the present thesis in the form of the manuscript "Light-Induced Reduction of Bovine Adrenodoxin(1-108) *via* Covalently Bound Ruthenium(II) Bipyridyl Complex: Intramolecular Electron Transfer and Crystal Structure" were submitted to *Biochemistry* on June 1st, 2005. The manuscript was received for a revision on July 22nd, 2005. The revised manuscript was submitted on September 21st, 2005. Second revision on November 16th, 2005. Accepted on November 19th, 2005.

Hiermit erkläre ich, dass ich diese Doktorarbeit selbständig verfasst und keine anderen als die von mir angegebenen Quellen und Hilfsmittel benutzt habe.

Jörg Contzen hat den Ruthenium(II) Bipyridyl Komplex synthesiert.

Prof. Dr. Christiane Jung hat $P450_{cam}$ zur Verfügung gestellt.

Dr. Anna G. Lapko hat die Palsmiden für die Expression von Adx(WT) und AR zur Verfügung gestellt.

Dr. Frank Hannemann hat die Adx(N-6×His tag/Xa/1-108) Mutante kloniert.

Dr. Eva-Christina Müller hat die ES-TOF-MS-Messungen durchgeführt.

Dr. Katja Fälber hat die X-ray-Daten (SLS, Villigen, Schweiz) gesammelt.

Dr. Jürgen J. Müller hat die X-ray-Daten mit XDS prozessiert und die Elektronendichte des Ruthenium(II) Komplexes und Cys95 anhand des EDEN-Programms verbessert.

Dr. Marcus Galander hat die EPR-Messungen durchgeführt.

Datum, ort 14-Dec-2005, Berlin

Andrei Halavaty