Electronic supplementary information

Miguel Saggu[1] Christian Teutloff[2] Marcus Ludwig[3]
Marc Brecht[2] Maria-Eirini Pandelia[4] Oliver Lenz[3]
Bärbel Friedrich[3] Wolfgang Lubitz[4] Peter Hildebrandt[1]
Friedhelm Lendzian[1] Robert Bittl[2] ⋆

December 1, 2009

[1]Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin
[2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin
[3]Humboldt-Universität zu Berlin, Chausseestrasse 117, 10115 Berlin
[4]Max-Planck-Institut für Bioanorganische Chemie, Stiftstr. 34-36, 45470 Mühlheim an der Ruhr
⋆Robert.Bittl@physik.fu-berlin.de

D. vulgaris Miyazaki F

The spectrum of the reoxidized *D. vulgaris* Miyazaki F hydrogenase has been simulated to obtain the relative ratio between Ni_r-B and Ni_u-A.

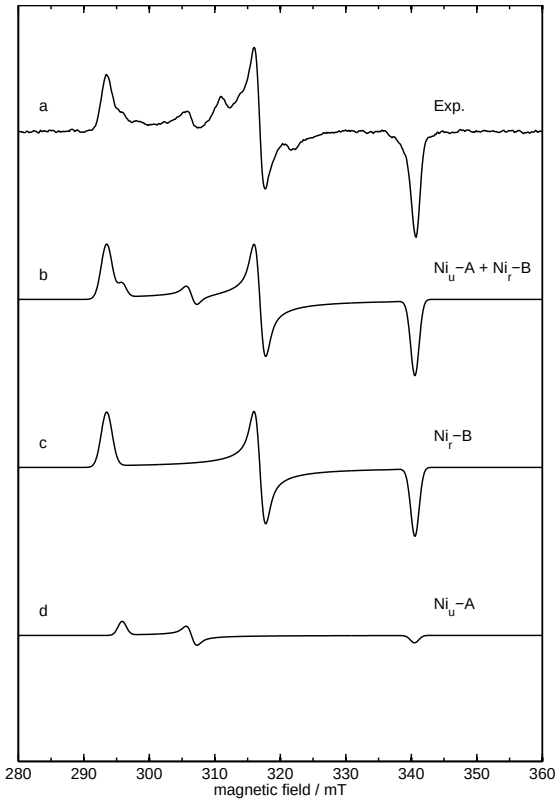

Figure 1: X-Band cw-EPR spectra of reoxidized hydrogenase from *D. vulgaris* Miyazaki F. (a) Experimental spectrum at T = 100K showing mainly signals from Ni_r-B (85%) and minor signals from Ni_u-A (15%). (b) simulation of complete signal to estimate the amount of Ni_r-B. (c) simulation of Ni_r-B. Used parameters: g-values 2.33, 2.16, 2.01 and 1.5mT linewidth (g-strain 0.01, 0.004, 0 for g_x, g_y and g_z). (d) simulation of Ni_u-A. Used parameters: g-values 2.32, 2.24, 2.01 and 1.9mT linewidth. Experimental conditions: T = 100K, 1 mW microwave power; 1 mT modulation amplitude, 12.5 kHz modulation frequency, microwave frequency 9.5GHz.