

Corrections

Hydrogen-Induced Structural Changes at the Nickel Site of the Regulatory [NiFe] Hydrogenase from *Ralstonia eutropha* Detected by X-ray Absorption Spectroscopy, by Michael Haumann,* Antje Porthun, Thorsten Buhrke, Peter Liebisch, Wolfram Meyer-Klaucke, Bärbel Friedrich, and Holger Dau, Volume 42, Number 37, September 23, 2003, pages 11004–11015.

Page 11010. Table 2 should have appeared as follows.

Table 2: Simulation Parameters of EXAFS Spectra of the RH^a

state	fit no.	shell	coordination no. N_i , per Ni	distance R_i (Å)	σ (Å)	R_F (%) (1.3–2.5 Å)	BVS
RH ^{ox}	I	O,N	3	2.07	0.06	18.7	1.99
		S	2	2.18	0.04		
	II	O,N	2	2.06	0.05	15.6	2.25
		S	3	2.17	0.04		
	III	S	4	2.18	0.05	22.7	2.07
		O,N	1	2.06	0.03		
	IV	S	4	2.17	0.06	20.7	2.48
		O,N	2	2.06	0.05		
		S	3	2.18	0.04		
		Fe	1	2.73	0.07		
RH ^{+H2}	VIa	O,N	4	2.04	0.12	3.7	2.96
		S	2	2.22	0.06		
	VIb	O,N,(H)	3	2.01	0.11	3.8	nd ^c
		S	2	2.22	0.06		
	VIIa	O,N	3	2.03	0.15	4.0	3.21
		S	3	2.22	0.07		
	VIIb	O,N,(H)	2	1.97	0.14	4.5	nd ^c
		S	3	2.21	0.07		
	VIII	O,N	2	2.05	0.14	9.1	3.44
		S	4	2.20	0.09		
	IX	O,N	4	2.04	0.11	3.0	2.96 ^b
		S	2	2.22	0.06		
		Fe	1	3.00	0.12		
Ni(H ₂ O) ₆	X	O	6	2.03	0.07	10.4	2.13

^a RH^{ox} is the as-isolated, oxidized state of the RH; RH^{+H2} is the RH incubated under hydrogen, thereby yielding the EPR-active Ni–C state of the RH. The filtered R -factor (mean weighted error sum; for further details, see ref 49), R_F , represents the deviation between data and simulation (in percent) for reduced distances here ranging from 1.3 to 2.5 Å. The σ value is the EXAFS Debye–Waller factor. The bond valence sum (BVS, eq 1 in the text) was calculated with a B of 0.37 (50), using R_{0i} values, for Ni(II), of 1.647 Å for Ni–O and 1.937 Å for Ni–S vectors and, for Ni(III), of 1.731 Å for Ni–O and 2.040 Å for Ni–S vectors (data taken from ref 39). The R_i values are derived from the EXAFS analysis. ^b The Fe atom has not been included in the BVS calculations. ^c Simulations where the BVS has not been calculated have been carried out after reduction of the number of (O,N) ligands in the corresponding approaches by one to mimic the presence of a Ni-bound H species (see the text).

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