Supporting Information

Nuclear Resonance Vibrational Spectroscopy (NRVS) of Rubredoxin and MoFe Protein Crystals

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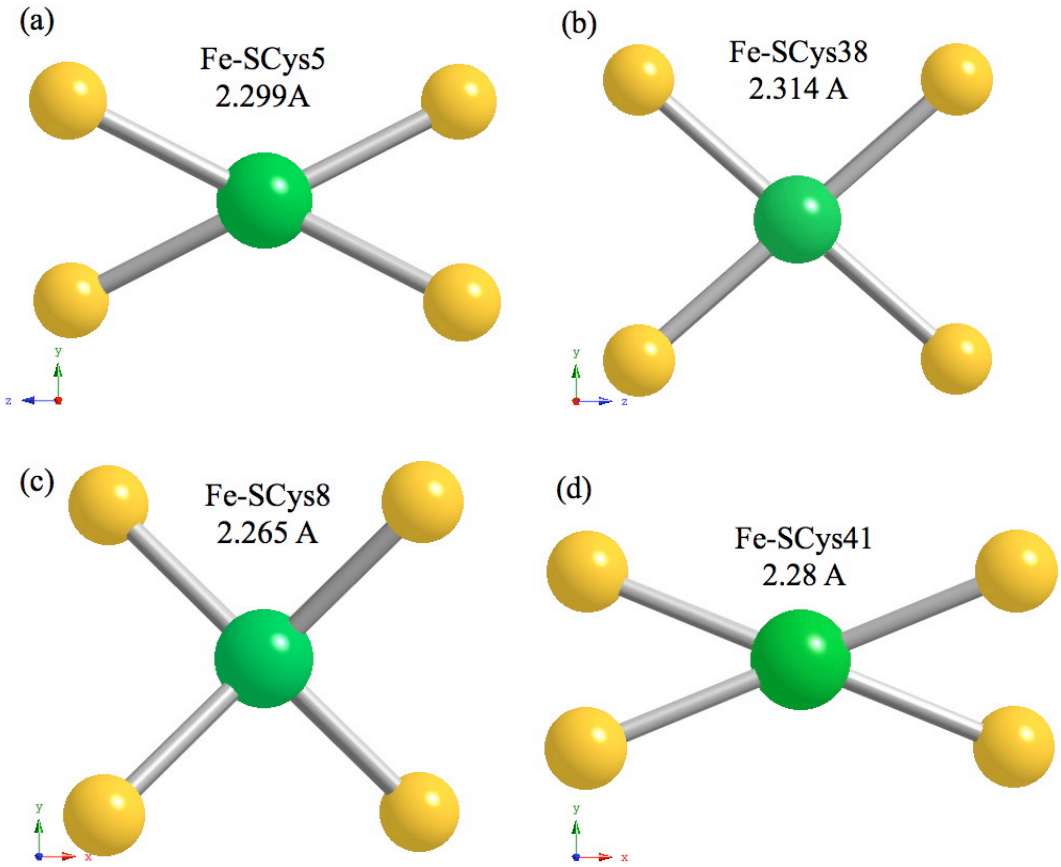

Figure S1. Overlap of individual Fe-S bond in one unit cell of *Pf* Rd extracted from crystal structure of oxidized WT *Pf* Rd at 0.95 Å resolution (PDB Code 1BRF). Crystal axes are indicated at bottom left of each figure as x, y, z, which correspond to crystal *a*-, *b*-, and *c*-axis. Color code: Fe (green), S (yellow).

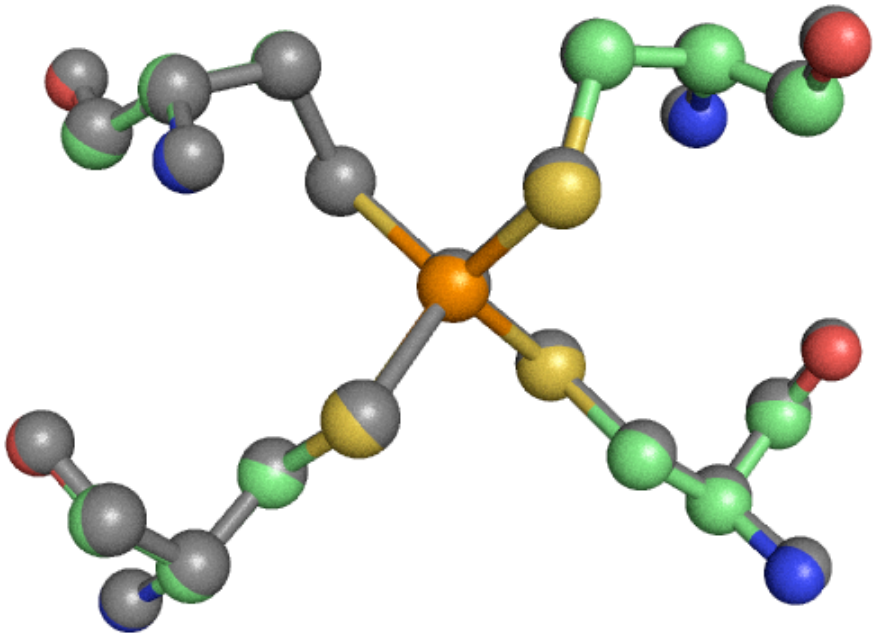

Figure S2. Iron site structure of oxidized WT *Pf* Rd (Color) using crystal structure coordinates (PDB code: 1BRF) compared to that of oxidized *Pf* met-Rd (Grey) using crystal structure coordinates (PDB code: 1BQ8). H atoms are omitted for clarity.

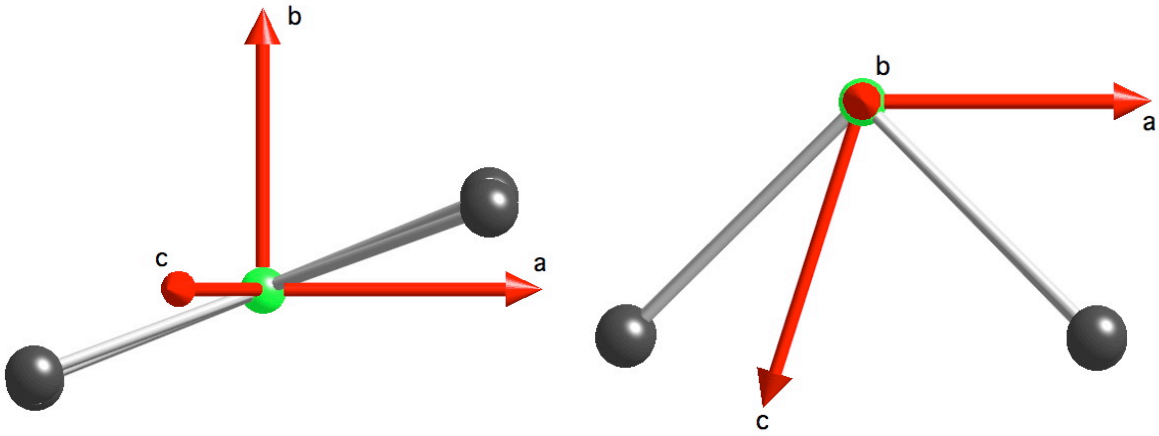

Figure S3. Illustration of the MoFe vector (C_3 axis of the FeMo-co) geometry in the MoFe protein crystal unit cell by overlapping 4 FeMoco MoFe vectors to Fe atom using the crystal structure 1M1N. The red arrows represent the crystal axes. Color code: Fe (green), Mo (black).

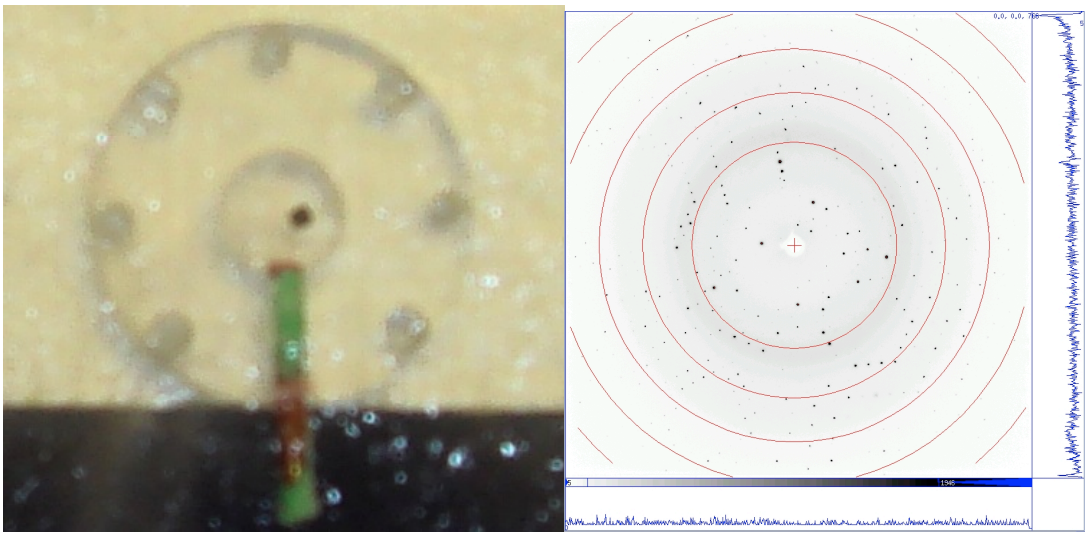

Figure S4. (Left) The picture of the *c*-axis oriented *Pf* Rd crystal when placing in the custom made Lucite disc NRVS cell; (Right) the diffraction pattern of the same crystal.

Table S1. EXAFS Curve Fitting Parameters for the *Pf* Rd crystals with *a*-axis and *c*-axis aligned along X-ray polarization vector [a]

	a-axis aligned crystal			*c*-axis aligned crystal		
	N	*R*(Å)	σ^2 (Å^2)	*N*	*R*(Å)	σ^2 (Å^2)
Fe-S	4	2.263	0.00226	4	2.283	0.00194
ΔE_0 (eV)		-10.82			-11.20	
F		0.203			0.192	

[a] *N* = number of backscattering atoms; *R* = distance; σ^2 = Debye-Waller factor; ΔE_0 = threshold energy; *F* = fit quality defined as $\sqrt{[\Sigma(\chi_o-\chi_c)^2k^6/\Sigma\chi_o^2k^6]}$ (χ_o = observed EXAFS; χ_c = calculated EXAFS). The backscattering numbers (*N*) were fixed to the values expected for the models while *R*, σ^2 and ΔE_0 were floated. The estimated uncertainties in *R*, σ^2 and ΔE_0 were less than ±0.01 Å, ±0.0001 Å^2, and ±0.4 eV, respectively. Phase and amplitude functions were calculated using FEFF 7.0.