Supporting Information

Lee et al. 10.1073/pnas.1202429109

DNAS Nd



Fig. S1. Stability of cofactor-deficient molybdenum-iron (MoFe) proteins upon europium(II) diethylenetriaminepentaacetate [Eu(II)-DTPA] treatment. Perpendicular-mode EPR spectra of $\Delta nifH$ (1), $\Delta nifB\Delta nifZ$ (2), and $\Delta nifB$ (3) MoFe proteins before (black) and after (red) incubation with Eu(II)-DTPA. Samples were prepared by incubating MoFe proteins with Eu(II)-DTPA, followed by the removal of Eu(II)-DTPA and the addition of Na₂S₂O₄ (see *Materials and Methods*).



Fig. S2. Time-dependent hydrocarbon formation by cofactor-deficient MoFe proteins. (*A*) Formation of CH₄, C_2H_4 , C_2H_6 , C_3H_6 , C_3H_8 , $1-C_4H_8$, $n-C_4H_{10}$, $1-C_5H_{10}$, $n-C_5H_{12}$, and NH₃ from the reduction of CN⁻ by $\Delta nifH(\bullet)$, $\Delta nifB\Delta nifZ$ (\heartsuit), and $\Delta nifB$ (\bigcirc) MoFe proteins. (*B*) Formation of CH₄, C_2H_4 , C_2H_6 , C_3H_6 and C_3H_8 from the reduction of CO by $\Delta nifH(\bullet)$, $\Delta nifB\Delta nifZ$ (\heartsuit), and $\Delta nifB$ (\bigcirc) MoFe proteins.

Products	Activities		
	∆ <i>nifB</i> MoFe protein	∆ <i>nifB∆nifZ</i> MoFe protein	∆ <i>nifH</i> MoFe protein
From H ⁺			
H ₂	20,017 ± 4,014	59,142 ± 6,974	150,626 ± 20,147
From N_2H_4			
NH₃	ND	8,910 ± 967	27,175 ± 2,401
H ₂	9,184 ± 1,011	38,732 ± 4,120	87,306 ± 9,307
From N_3^-			
NH ₃	15,100 ± 2,713	31,407 ± 4,944	118,649 ± 17,049
H ₂	ND	8,727 ± 994	17,799 ± 2,194
From C ₂ H ₂			
C_2H_4	9,185 ± 1,004	36,019 ± 2,984	110,827 ± 10,090
C_2H_6	ND	ND	5,921 ± 713
H ₂	5,152 ± 813	14,179 ± 704	40,008 ± 1,490
From C ₂ H ₄			
C ₂ H ₆	ND	5,149 ± 417	17,174 ± 891
H ₂	16,674 ± 2,097	39,603 ± 3,319	126,521 ± 9,897

Table S1. Substrate-reducing activities of cofactor-deficient MoFe proteins in Eu(II)-DTPA-driven reactions

Activities are expressed in nanomole product/micromole protein per hour. See *Materials and Methods* for assay conditions. ND, not detectable.

PNAS PNAS