Figure S1. Electron density for the C and D clusters. Maps show $2F_o$-F_c density contoured to 1.5 sigma. Clusters are shown as spheres with iron colored brown, sulfur colored yellow, and nickel colored green. A. D-cluster density. B. C-cluster density.

A. B.

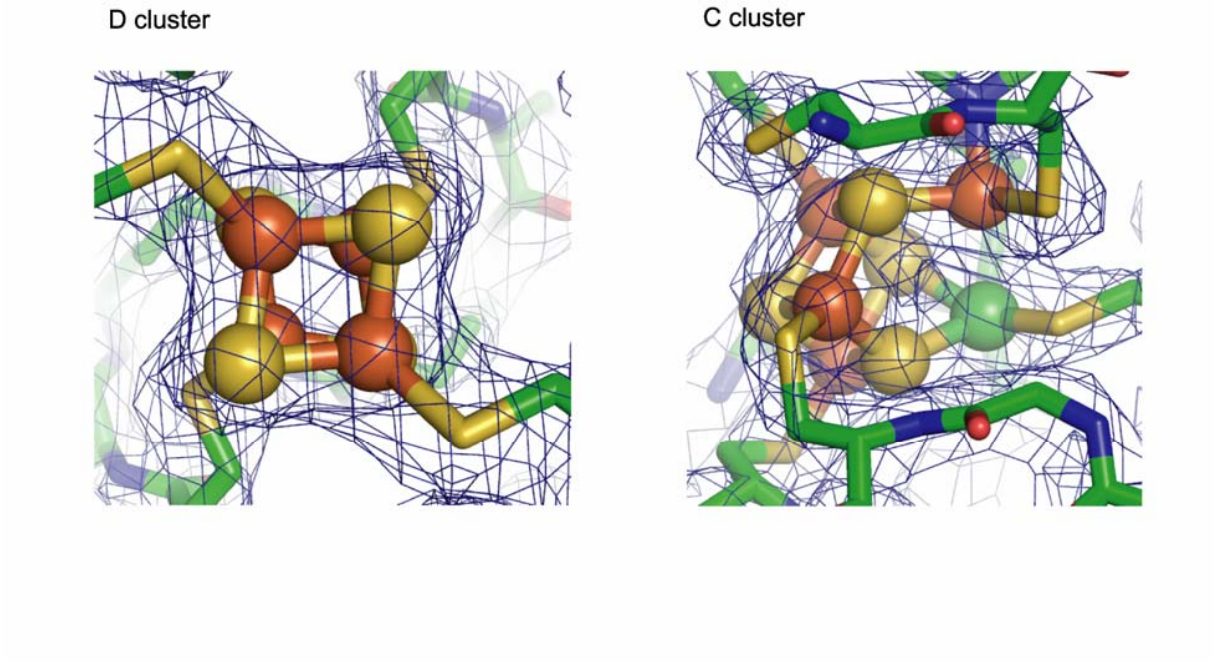

Table S1. Xe binding sites in mtCODH/ACS based on $|Fo_{Xe}|$ -$|Fo_{Native}|$ difference Fourier maps and refinement

Xe sites	Channel 1, Mol 1		Channel 2, Mol 1		Channel 1, Mol 2		Channel 2, Mol 2		Neighboring residues, (atoms, and average distances)
	Occ	B-factor	Occ	B-factor	Occ	B-factor	Occ	B-factor	
1	0.13	32.32	0.15	23.79	0.19	34.46	0.09	13.77	CODH residues: C468(SG-3.3), A590(CB-3.4), T602(CG2-3.6), W595(CD1-3.9), S579(C-4.0), G592(CA-4.0), H603(O-3.9), A578(C-4.5), I591(CG2-4.6)
2	1.00	25.33	1.00	27.34	0.86	29.20	1.00	33.81	CODH residues: P608(CG-3.8), V102(CG2-3.9), A589(O3.9), T593(OG1-3.9), F632(CZ-3.9), I106(CD1-4.7)
3A	0.56	26.65	0.60	30.46	0.48	28.75	0.51	29.28	CODH residues: 3A: I106(CD1-3.7), L620(CD2-3.9), A234(CB-4.0), T593(CG2-4 M148(CE-4.0), E156(OE2-3.7), M182(SD-3.9), F184(CZ-4.7), Y221(CE1-3.7), A222(CA-4.0), I248(CG2-3.8).0), V231(CG1-4.4), V102(CG1-4.6).
B	0.35	25.68	0.19	14.04	0.26	30.93	0.30	33.15	3B: V102(CG1-3.4), A234(CB-3.8), A99(O-4.0), G103(N-4.4), V231(CA-4.4), I106(CD1-4.6), L230(O4.8)
4	0.87	29.88	0.84	30.13	0.69	28.85	0.67	30.30	CODH residues: L620(CD2-3.6), I235(CD1-3.8), V231(CG1-3.9), V596(CG1-4.0), T593(CG2-4.4), F632(CE2-4.2), A624(CB-4.5)
5	1.00	21.32	1.00	24.50	1.00	27.49	0.87	31.68	CODH residues: V228(CG1-4.0), F232(CE1-4.2), I619(CG1-4.4), I623(CG2-3.8), V627(CG2-4.2) ACS residues: T31(CG1-4.0), Y35(CG1-4.6)
6	0.31	27.13	0.30	29.16	0.24	29.10	0.18	30.25	ACS residues: T106(CG2-4.9), A110(CB-4.7), F212(O, 4.2), T213(CG2-4.1), I215(CG2-3.9), V261(CG1-3.4), A265(CB, 4.1), HOH877-3.6, HOH837-4.7
7	1.00	21.87	1.00	24.50	1.00	27.49	0.73	33.0	ACS residues: W107(NE1-4.4), I158(CG2-4.5), L160(CD2-4.8), I215(CG1-4.0), V252(CG2-4.0), A265(O-3.8), A266(CA-4.3), A269(CB-4.3)
8	0.19	25.25			0.14	19.28			ACS residues: M148(CE-4.0), E156(OE2-3.7), M182(SD-3.9), F184(CZ-4.7), Y221(CE1-3.7), A222(CA-4.0), I248(CG2-3.8)
9	0.73	34.79	0.75	30.98	0.45	31.90	0.37	42.27	ACS residues: Cu-3.7, Ni-3.9, G145(C-4.4), I146(N-4.8), V149(CG1-3.8), F229(CD1-3.2), C509(SG-4.2), F512(CB-4.9), C595(CB-4.2), G596(N-4.4), C597(CB-4.1)
10	0.28	24.55	0.41	31.99	0.20	25.94	0.36	35.46	ACS residues: S396(O-3.3), L287(CD1-3.73), A400(CB-3.8), T374(CG2-3.8), Y388(CD1-3.9), A397(N-4.0), I386(CD1-4.1), C350(SG-4.3), I291(CD1-4.45)