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Structural and functional models for [NiFe] hydrogenase

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Raja Angamuthu

Cover-page illustration:

Crystal structure of $[\text{Ni}_6(\text{cpss})_{12}]$ (Chapter 6). Ni, green; S, red; Cl, yellow; C, gray.

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Structural and Functional Models for [NiFe] Hydrogenase

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a.u.	Arbitrary unit
ACN	Acetonitrile
APT	Attached Proton Test
b	Broad
bpy	2,2'-Bipyridine
CoM	Coenzyme M; 2-thioethane sulfonate
COSY	Correlation Spectroscopy
CV	Cyclic voltammetry; cyclic voltammogram
Cys	Cysteine
d	Doublet
dedtc	Diethyldithiocarbamate
DMF	<i>N,N</i> -Dimethylformamide
dpa	Dipicolylamine
dppe	1,2-Bis(diphenylphosphino)ethane
E_{pa}	Anodic potential; oxidation potential
E_{pc}	Cathodic potential; reduction potential
EPPG	Edge plane pyrolytic graphite (electrode)
eq.	Equivalent
ESI-MS	Electrospray ionization mass spectrometry
Et	Ethyl
FTIR	Fourier transform infra red
GC	Glassy carbon
Glu	Glutamic acid
GSH	Glutathione
H ₂ ase	Hydrogenase
H ₂ bdt	Benzene-1,2-dithiol
H ₂ bme*-daco	1,5-bis(mercaptoethyl)-1,5-diazacyclooctane
H ₂ pdt	Propane-1,3-dithiol
H ₂ tpdt	2-Thiopropane-1,3-dithiol
Hacac	Acetylacetone, 2,4-pentanedione
HCp	1,3-Cyclopentadiene
HER	Dihydrogen evolution reaction
HG-GSH	Hemithioacetal
His	Histidine
HS-HPT	<i>N</i> -(7-mercaptoheptanoyl)- <i>O</i> -phospho-L-threonine; coenzyme B

J	Coupling constant
LMCT	Ligand-to-metal charge transfer
m	Multiplet in NMR; medium in IR
m/z	Ratio of mass upon charge
M_d	Distal metal
Me	Methyl
MeCoM	Methyl-coenzyme M; 2-(methylthio)ethanesulfonate
MLCT	Metal-to-ligand charge transfer
M_p	Proximal metal
NMR	Nuclear magnetic resonance
NOESY	Nuclear Overhauser Effect Spectroscopy
OTf^-	Trifluoridomethanesulfonate
PEM	Proton exchange membrane
Ph	Phenyl
PMe_3	Trimethylphosphine
PPh_3	Triphenylphosphine
ppm	Parts per million
ROESY	Rotating-Frame NOE Spectroscopy
s	Singlet in NMR; strong in IR
SCE	Standard calomel electrode
SHE	Standard hydrogen electrode
t	Triplet
^t Bu	<i>tertiary</i> -Butyl
TEA·HCl	Triethylamine hydrochloride
THF	Tetrahydrofuran
TMS	Tetramethylsilane
tmtu	1,1,3,3-tetramethyl-2-thiourea
TOCSY	Total Correlation Spectroscopy
tpa	Tripicolylamine
TsOH·H ₂ O	<i>para</i> -Toluenesulfonic Acid monohydrate
UV-Vis	Ultra violet and visible spectroscopy
Val	Valine
w	Weak
δ	Chemical shift
τ	Trigonality index

