Structural and functional models for [NiFe] hydrogenase

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Cover-page illustration:

Crystal structure of $[Ni_6(cpss)_{12}]$ (Chapter 6). Ni, green; S, red; Cl, yellow; C, gray.

Printed by:

Ridderprint BV, Ridderkerk, The Netherlands

Structural and Functional Models for [NiFe] Hydrogenase

PROEFSCHRIFT

ter verkrijging van de graad van Doctor aan de Universiteit Leiden,

op gezag van Rector Magnificus prof. mr. P. F. van der Heijden,

volgens besluit van het College voor Promoties

te verdedigen op woensdag 14 oktober 2009

klokke 16.15 uur

door

Raja Angamuthu

geboren te Karur (Tamil Nadu), India in 1980

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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 volammogram
Cys	Cysteine
d	Doublet
dedtc	Diethyldithiocarbamate
DMF	*N,N*-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_2ase	Hydrogenase
H_2bdt	Benzene-1,2-dithiol
H_2bme*-daco	1,5-bis(mercaptoethyl)-1,5-diazacyclooctane
H_2pdt	Propane-1,3-dithiol
H_2tpdt	2-Thiapropane-1,3-dithiol
Hacac	Acetylacetone, 2,4-pentanedione
HCp	1,3-Cyclopentadiene
HER	Dihydrogen evolution reaction
HG-GSH	Hemithioacetal
His	Histidine
HS–HPT	*N*-(7-mercaptoheptanoyl)-*O*-phospho-L-threonie; 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	*tertiary*-Butyl
TEA·HCl	Triethylamine hydrochloride
THF	Tetrahydrofuran
TMS	Tetramethylsilane
tmtu	1,1,3,3-tetramethyl-2-thiourea
TOCSY	Total Correlation Spectroscopy
tpa	Tripicolylamine
$TsOH·H_2O$	*para*-Toluenesulfonic Acid monohydrate
UV-Vis	Ultra violet and visible spectrocopy
Val	Valine
w	Weak
δ	Chemical shift
τ	Trigonality index