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.

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Structural and Functional Models for [NiFe] Hydrogenase

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Table of Contents

▪	List of Abbreviations	i
1	General Introduction	001
2	Ligand Design, Synthetic Procedures and Experimental Methods	033
3	$[Ni(S_4)Fe(C_5H_5)(CO)](PF_6)$ Complexes Containing Tetradentate $S_2S'_2$-donor Ligands: Synthesis, Characterization and Electrocatalytic Dihydrogen Production	051
4	Synthesis, Characterization and Electrocatalytic Properties of $[Ni(S_4)Fe(C_5H_5)(CO)](PF_6)$ Complexes Containing Bidentate SS'-donor Ligands	071
5	Heterodinuclear [NiRu] Complexes Comprising Ruthenium Bis-Bipyridine: Synthesis, Characterisation and Electrocatalytic Dihydrogen Production	087
6	Hexanuclear (Ni_6-)Metallacrown as Functional Model of [NiFe] Hydrogenase	103
7	A Molecular Cage of Ni(II) and Cu(I) Resembling the Active Site of Ni-Containing Enzymes	121
8	Light-Induced C–S Bond Cleavage in a Nickel Thiolate Complex: Relevance to the Function of Methyl Coenzyme M Reductase (MCR)	131
9	Summary, Conclusions and Future Perspectives	143
▪	Samenvatting (Summary in Dutch)	151
▪	Curriculum Vitae (English)	156
▪	Curriculum Vitae (Tamil)	157
▪	Publications	158
▪	Nawoord (Afterword)	160

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