Supporting Information

1. Selected geometric parameters and spin and charge populations

Table S1. Geometric parameters of optimized structures of [NiL] at M06-L/Def2-TZVP level of theory

Complex	Geometric parameter									Ligand field
	Bond length (Å)						Bond Angle			
	Ni-S	Ni-P	Ni-Fe	Ni-H	S-H	H-H	S-Ni-S	P-Ni-P	P-Ni-S	
$Ni^{II}L$	2.190/ 2.177	2.234/ 2.315	4.297	-	-	-	89.1	96.8	86.6	Square planar
$Ni^{I}L^{-}$	2.288/ 2.292	2.202/ 2.202	4.295	-	-	-	88.8	102.5	100.8	Tetrahedral
$[Ni^{III}H^{-}L]$	2.195/ 2.248	2.252/ 2.334	4.215	1.471	-	-	90.5	96.9	103.1	Square pyramidal
$[Ni^{I-}LH]$	2.357/ 2.266	2.237/ 2.230	4.242	-	1.346	-	84.3	104.1	129.9	Tetrahedral
$[Ni^{II}H^{-}L]^{-}$	2.284/ 2.298	2.212/ 2.261	4.183	1.462	-	-	87.9	103.7	124.5	Trigonal bipyramidal
$[Ni^{0-}LH]^{-}$	2.276/ 2.375	2.127/ 2.113	4.136	-	1.353	-	83.1	109.8	113.9	-
$[Ni^{II}H^{-}LH]$	2.335/ 2.308	2.189/ 2.213	4.051	1.452	1.348	-	87.4	111.7	108.5	Trigonal bipyramidal
$[Ni^{IV}H^{-}H^{-}L]$	2.236/ 2.303	2.249/ 2.428	4.312	1.435/ 1.456	-	1.876	89.5	94.5	101.9	Octahedral
$[Ni^{II}L]+H_2$	2.183/ 2.193	2.294/ 2.235	3.832	-	-	0.751	88.9	92.8	88.7	Distorted square planar
Ts1	2.295/ 2.212	2.477/ 2.236	4.288	1.475/ 1.461	1.883	2.031	90.6	94.9	102.7	
Ts2	2.239/ 2.308	2.254/ 2.431	4.335	1.453/ 1.466	-	1.348	88.1	94.2	96.4	

Table S2. Calculated charges for optimized structures at M06-L/Def2-TZVP level of theory.

Complex	CHARGE									
	Mulliken					Löwdin				
	Ni	S	P	Fe	H	Ni	S	P	Fe	H
$[Ni^{II}L]$	0.379	-0.508/ -0.500	0.261/ 0.600	0.864	-	-0.835	0.429/ 0.438	0.877/ 0.866	-0.116	-
$[Ni^{I}L]^{-}$	0.061	-0.650/ -0.648	0.458/ 0.456	0.578	-	-0.859	0.255	0.830/ 0.831	-0.115	-
$[Ni^{III}H^{-}L]$	-0.143	-0.435/ -0.446	0.737/ 0.759	0.680	-0.120	-0.847	0.431/ 0.407	0.878/ 0.897	-0.121	0.014
$[Ni^{I}LH]$	-0.050	-0.200(H)/ -0.558	0.445/ 0.390	0.549	0.153	-0.801	0.596(H)/ 0.300	0.846/ 0.836	0.114	0.064
$[Ni^{II}H^{-}L]^{-}$	-0.119	-0.496/ -0.654	0.666/ 0.761	0.748	-0.166	-0.967	0.267/ 0.336	0.850/ 0.852	-0.118	-0.005
$[Ni^{0}LH]^{-}$	-0.038	-0.248(H)/ -0.673	0.400/ 0.367	0.602	0.108	-0.958	0.563(H)/ 0.214	0.786/ 0.772	-0.116	0.043
$[Ni^{II}H^{-}LH]$	-0.233	-0.188(H)/ -0.493	0.774/ 0.767	0.753	-0.122(Ni)/ 0.151(S)	-0.912	0.611(H)/ 0.373	0.851/ 0.857	-0.111	0.016(Ni)/ 0.066(S)
$[Ni^{IV}H^{-}H^{-}L]$	-0.259	-0.400/ -0.476	0.825/ 0.662	0.681	-0.042/ -0.005	-0.907	0.441/ 0.360	0.903/ 0.886	-0.120	0.040/ 0.066
$[Ni^{II}L]+H_2$	0.007	-0.422/ -0.406	0.659/ 0.538	0.552	0.100/ -0.168	-0.829	0.436/ 0.441	0.864/ 0.874	-0.118	0.004/ 0.006
Ts1	-0.197	-0.336/ -0.461	0.616/ 0.779	0.690	0.059/ -0.072	-0.926	0.491/ 0.374	0.875/ 0.888	-0.122	0.111/ 0.030
Ts2	-0.287	-0.411/ -0.484	0.625/ 0.808	0.681	0.027/ 0.064	-0.928	0.441/ 0.349	0.882/ 0.900	-0.119	0.097/ 0.076
$[Ni^{II}LH]^{+}$	-0.102	-0.085/ -0.394	0.805/ 0.497	0.569	0.195	-0.755	0.724/ 0.466	0.874/ 0.891	-0.111	0.100

Table S3. Calculated spin populations for optimized structures at M06-L\Def2-TZVP level of theory

Complex	SPIN									
	Mulliken					Löwdin				
	Ni	S	P	Fe	H	Ni	S	P	Fe	H
$[Ni^{I}L]^{-}$	0.668	0.102/ 0.101	0.047/ 0.055	0.012	N.A.	0.707	0.078	0.030	0.013	-
$[Ni^{III}H^{-}L]$	0.530	0.105/ 0.130	0.163/ 0.028	0.022	-0.034	0.563	0.109/ 0.087	0.107/ 0.008	0.019	-0.025
$[Ni^{I}LH]$	0.744	0.048(H)/ 0.106	0.070/ 0.014	0.009	-0.004	0.763	0.040(H)/ 0.087	0.039/ 0.017	0.008	-0.001

Table S4. Geometric parameters of optimized structures of [NiL2] at M06-L\Def2-TZVP level of theory

Complex	Geometric parameter								Ligand field
	Bond length (Å)					Bond Angle			
	Ni-S	Ni-P	Ni-H	S-H	H-H	S-Ni-S	P-Ni-P	P-Ni-S	
$[Ni^{II}L2]$	2.181/ 2.177	2.184/ 2.186	-	-	-	90.8	85.9	91.9	Square planar
$[Ni^{I}L2]^{-}$	2.277/ 2.281	2.219/ 2.196	-	-	-	89.2	86.9	106.3	Tetrahedral
$[Ni^{III}H^{-}L2]$	2.200/ 2.224	2.237/ 2.327	1.480	-	-	87.0	96.9	98.9	Square Pyramidal
$[Ni^{II}H^{-}L2]^{-}$	2.217/ 2.201	2.124/ 3.938	1.493	-	-	91.3	-	124.5	Square Planar

Table S5. Calculated charge for optimized structures of [NiL2] at M06-L\Def2-TZVP level of theory

Complex	CHARGE							
	Mulliken				Löwdin			
	Ni	S	P	H	Ni	S	P	H
$[Ni^{II}L2]$	-0.007	-0.501/ -0.493	0.585/ 0.665	-	-0.855	0.387/ 0.390	0.820/ 0.816	-
$[Ni^{I}L2]^{-}$	0.098	-0.662/ -0.648	0.583/ 0.487	-	-0.862	0.233/ 0.236	0.770/ 0.776	-
$[Ni^{III}H^{-}L2]$	-0.065	-0.436/ -0.441	0.678/ 0.609	-0.094	-0.857	0.412/ 0.402	0.828/ 0.828	0.030
$[Ni^{II}H^{-}L2]^{-}$	-0.119	-0.496/ -0.654	0.666/ 0.761	-0.166	-0.967	0.267/ 0.336	0.850/ 0.852	-0.005

Table S6. Calculated spin populations for optimized structures at M06-L\Def2-TZVP level of theory

Complex	SPIN							
	Mulliken				Löwdin			
	Ni	S	P	H	Ni	S	P	H
$[Ni^{I}L2]^{-}$	0.635	0.111/ 0.113	0.074/ 0.055	-	0.667	0.086/0.089	0.036/ 0.040	-
$[Ni^{III}H^{-}L2]$	0.512	0.108/ 0.134	0.169/ 0.047	-0.018	0.552	0.112/ 0.092	0.017/ 0.109	-0.014

2. Relaxed surface scan for [Ni^{II}H^{-}LH]

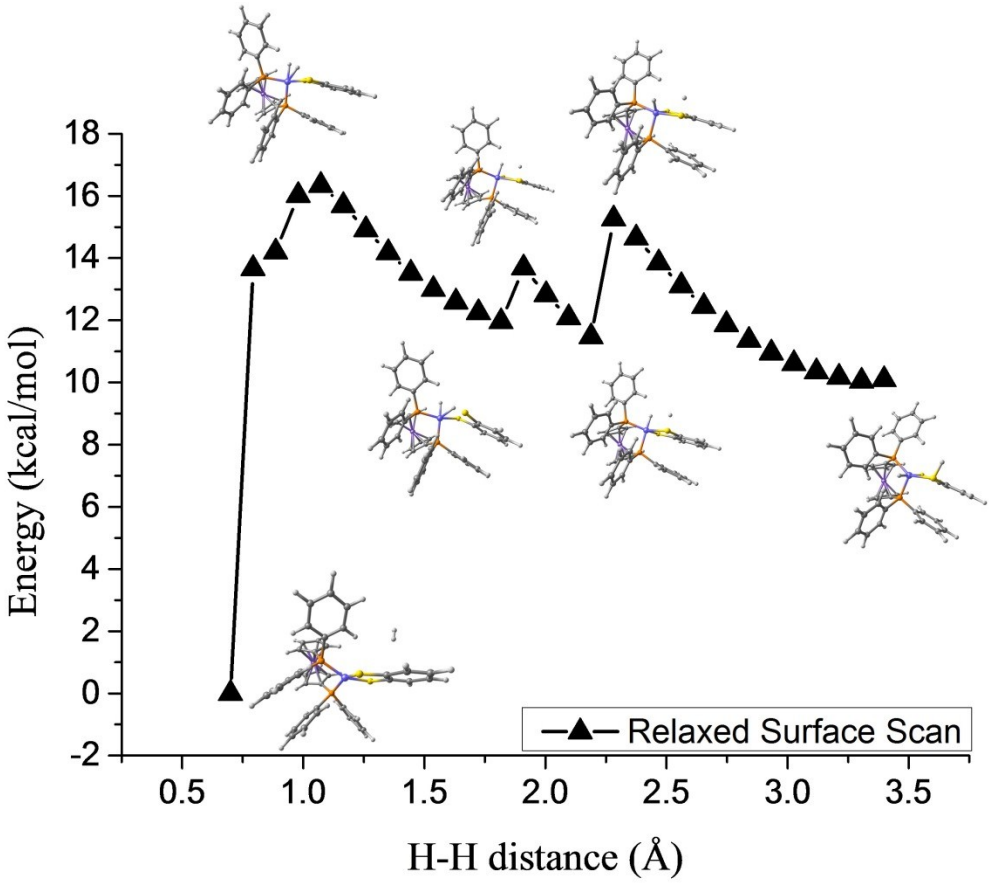
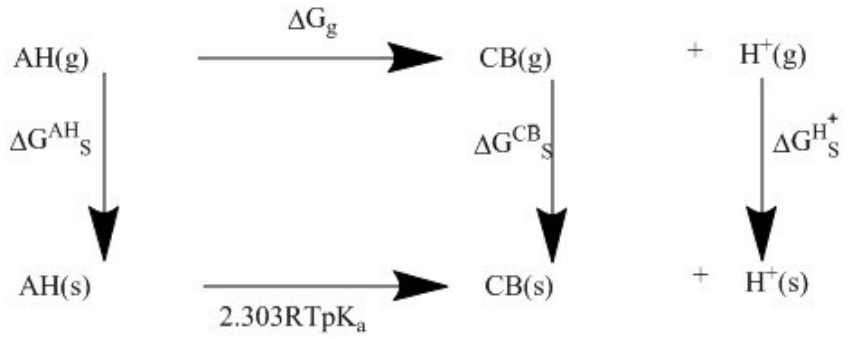


Figure S1. Relaxed surface scan for [Ni^{II}H^{-}LH], performed in order to investigate the possibility of direct H-H bond formation. The figure indicates that a direct H-H bond formation does not occur. Rather, the scan contains two apparent discontinuities that correspond to the S-H bond dissociation and the subsequent interaction of both protons with nickel, at distances smaller than 1.8 Å, before an H-H bond is formed.

3. Calculation of pK_a values and reduction potentials

For the calculation of pKa values, the following thermodynamic cycles for calculation of solvation energy of proton in THF as suggested by Kelly et al[1] have been used.

pKa for neutral acids:



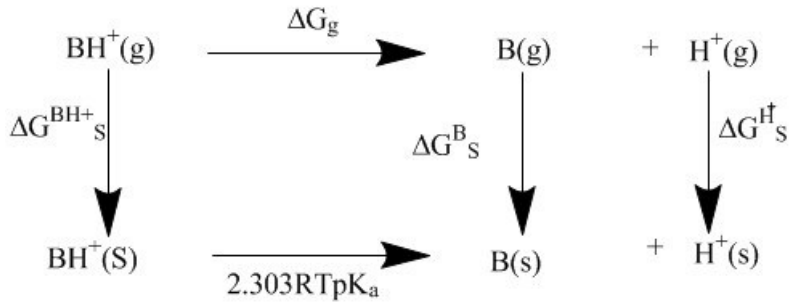
Scheme 1. Thermochemical cycle for neutral Brønsted-Lowry acids

According to the above cycle,

$$2.303RTpK_a + \Delta G_S^{AH} = \Delta G_g + \Delta G_S^{CB} + \Delta G^{H^+}{}_S + \Delta G^{0\rightarrow *} \quad (1)$$

Here ΔG_S^{AH} is the solvation free energy of the acid, ΔG_S^{CB} is the solvation free energy of the conjugated base, ΔG_g is the gas phase free energy change, $\Delta G^{H^+}{}_S$ is the solvation free energy of proton and as suggested by Kelly et al[1] $\Delta G^{0\rightarrow *}$ is the free energy change associated with the moving a solute from standard state gas-phase concentration of 1 atm to standard state solution phase concentration of 1 M at 298K, the latter value equals to 1.9 kcal/mol.[1]

The Gibbs free energy for the formation of proton in gas phase amounts to –6.28 kcal/mol.[2]
pKa for ionic acids:



Scheme 2. Thermochemical cycle for ionic Brønsted-Lowry acids

According to the above cycle,

$$2.303RTpK_a + \Delta G^{BH^+_S} = \Delta G_g + \Delta G^B_S + \Delta G^{H^+_S} + \Delta G^{0\rightarrow *} \quad (2)$$

Here $\Delta G^{BH^+_S}$ is the solvation free energy of the acid, ΔG^B_S is the solvation free energy of conjugated base, ΔG_g is the gas phase free energy change and $\Delta G^{H^+_S}$ and $\Delta G^{0\rightarrow *}$ are as with equation 1.

From this equation we have calculated the solvation free energy of proton in THF ($\Delta G^{H^+_S}$) for a small series of standard acid and base with known pK_a values in THF (Table S7)

Table S7. Solvation free energy of neutral species, ionic species, calculated solvation free energy of proton and pKa values.

Ion	Neutral	pK_a	ΔG_g kcal/mol	ΔG_s (neutral) kcal/mol	ΔG_s (ion) kcal/mol	$\Delta G^{H^+_S}$ kcal/mol
CH_3COO^-	Acetic Acid	22.48[3]	344.6	-6.0	-57.4	-264.5
$C_6H_5COO^-$	Benzoic Acid	25.10[4]	335.4	-6.0	-51.7	-257.4
4-NO_2-$C_6H_5COO^-$	4-Nitro-Benzoic Acid	21.16[4]	324.1	-7.7	-48.0	-257.0
4-Cl-$C_6H_5COO^-$	4-Chloro-Benzoic Acid	23.88[4]	331.0	-6.2	-49.0	-255.9
$C_6H_5O^-$	Phenol	29.23[4]	338.1	-9.1	-48.6	-260.6
2-NO_2- $C_6H_5O^-$	2-Nitro-Phenol	24.41[4]	332.8	-5.3	-45.6	-261.1
4-NO_2- $C_6H_5O^-$	4-Nitro-Phenol	21.13[4]	318.6	-8.8	-42.8	-257.7
4-Cl_2- $C_6H_5O^-$	2-Chloro-Phenol	26.80[4]	335.6	-5.2	-45.3	-261.0
PyridineH^+	Pyridine	8.25[4]	217.1	-3.4	-47.6	-252.0
Average $\Delta G^{H^+_S}$ (kcal/mol)						-258.5

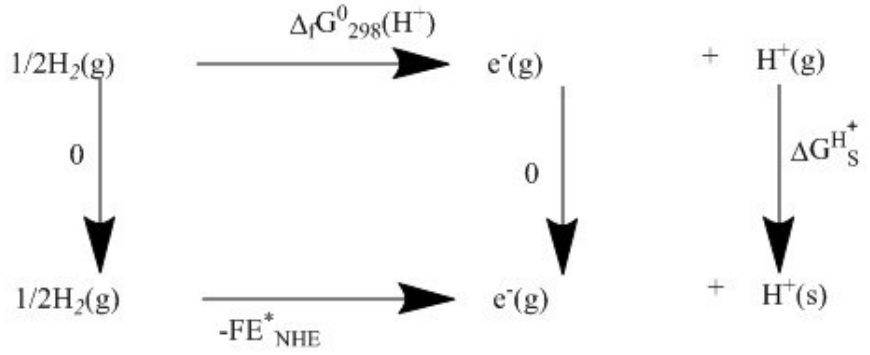
All calculations are performed at M06L/def2-tzvp level of theory, RI approximation and COSMO for solvent effects. The solvent is THF ($\varepsilon_R = 7.25$).

The series of calculations corroborates well with data reported by Kelly at al.[1]

Since only the relative pKa value for the protonation step is of relevance, we have used average ($\Delta G^{H^+_S}$) for our calculations.

Normal hydrogen electrode potential:

Normal hydrogen electrode (NHE) reduction potentials have been calculated using the thermodynamic cycle as given in scheme 3. The calculated solvation free energy of proton ($\Delta G^{H^+}_S$) following the suggestion of Kelly et al.[1]



Scheme 3. Thermochemical cycle for the normal hydrogen electrode potential.

Using the equation for the electromotive force, the reduction potential vs NHE has been calculated using equation 3.[1]

$$E^*_{NHE} = -\frac{\Delta_f G^0_{298}(H^+) + \Delta G^{H^+}_S + \Delta G^{0\rightarrow *}}{F} \qquad (3)$$

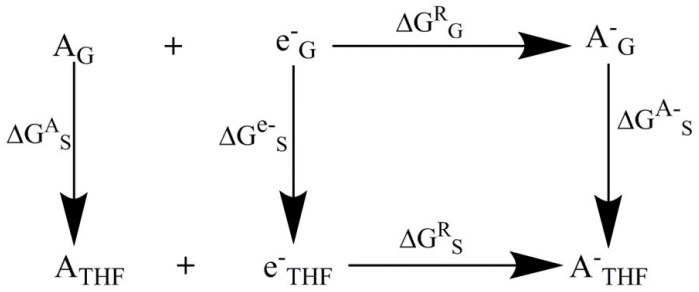
where $\Delta_f G^0_{298}(H^+)$ is the gas phase free energy of formation of a proton, equal to 361.7 kcal/mol at 298K. Using a value of $\Delta G^{H^+}_S = -258.5\ kcal/mol$ (cf. Table S7), $E^*_{NHE} = -4.39\ V$ in THF.

Now converting the NHE potential to SCE potential[5]

$E^*_{SCE} = E^*_{NHE} + 0.241V = -4.15\ V$

Calculation of relative reduction potentials:

Relative reduction potential as well as relative free energy change for the one electron reduction step. Thermodynamic cycle for the free energy of a one-electron reduction process:



Scheme 4. Thermochemical cycle for a one-electron reduction step

This discussion closely follows a procedure outlined by Song, Neese and Ye.[2] According to the above thermodynamic cycle the reaction enthalpy in solution, ΔG_S^R, is calculated as

$$\Delta G_S^R = \Delta G_g^R + \Delta G^{A^-}_S - \Delta G_S^A - \Delta G^{e^-}_S \quad (4)$$

Since it is difficult to calculate the solvation energy of an electron, the relative ΔG_S^R value is calculated with respect to the SCE in THF.

The calculated above the E^*_{SCE} is equals to -4.15V is used in the following equation

$$E^0(SCE)_{THF} = -\frac{\Delta G_S^R}{F} = -\frac{\Delta G_g^R + \Delta G^{A^-}_S - \Delta G_S^A - \Delta G^{e^-}_S}{F} = -\frac{\Delta G_g^R + \Delta G^{A^-}_S - \Delta G_S^A}{F} - 4.15 \quad (5)$$

4. Orbital analysis

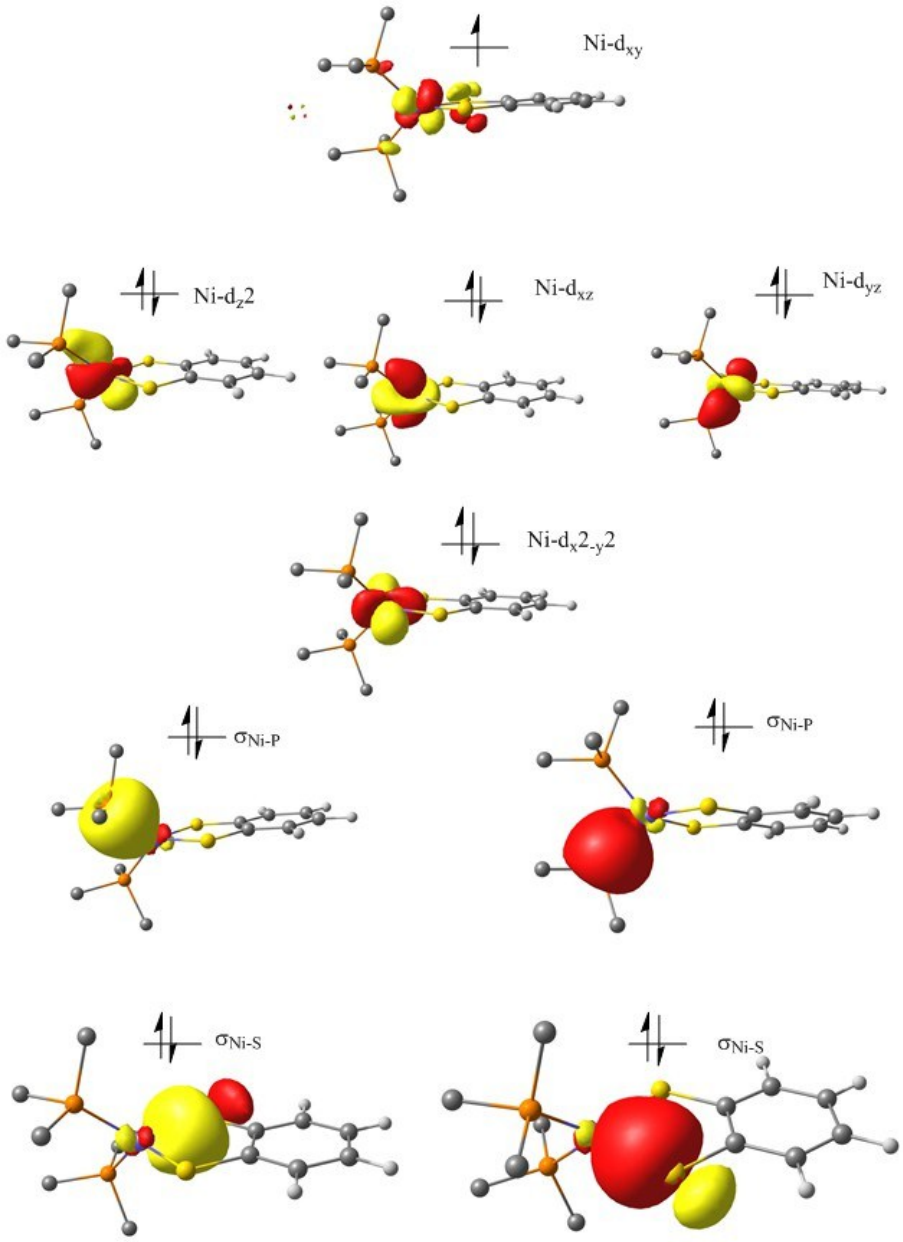


Figure S2. Localized orbitals of $[Ni^{I}L]^{-}$.

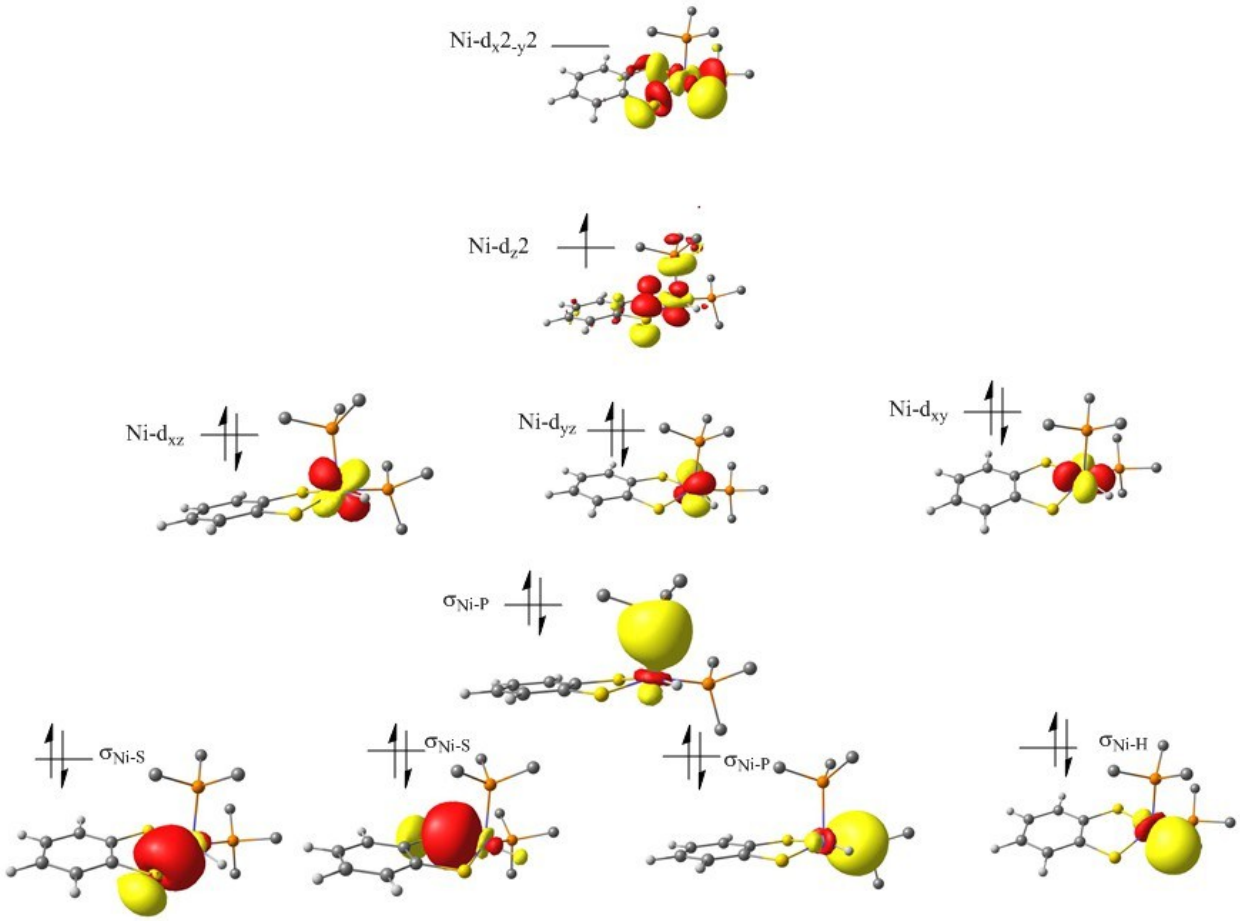


Figure S3. Localized orbitals of $[Ni^{III}H^{-}L]^{-}$.

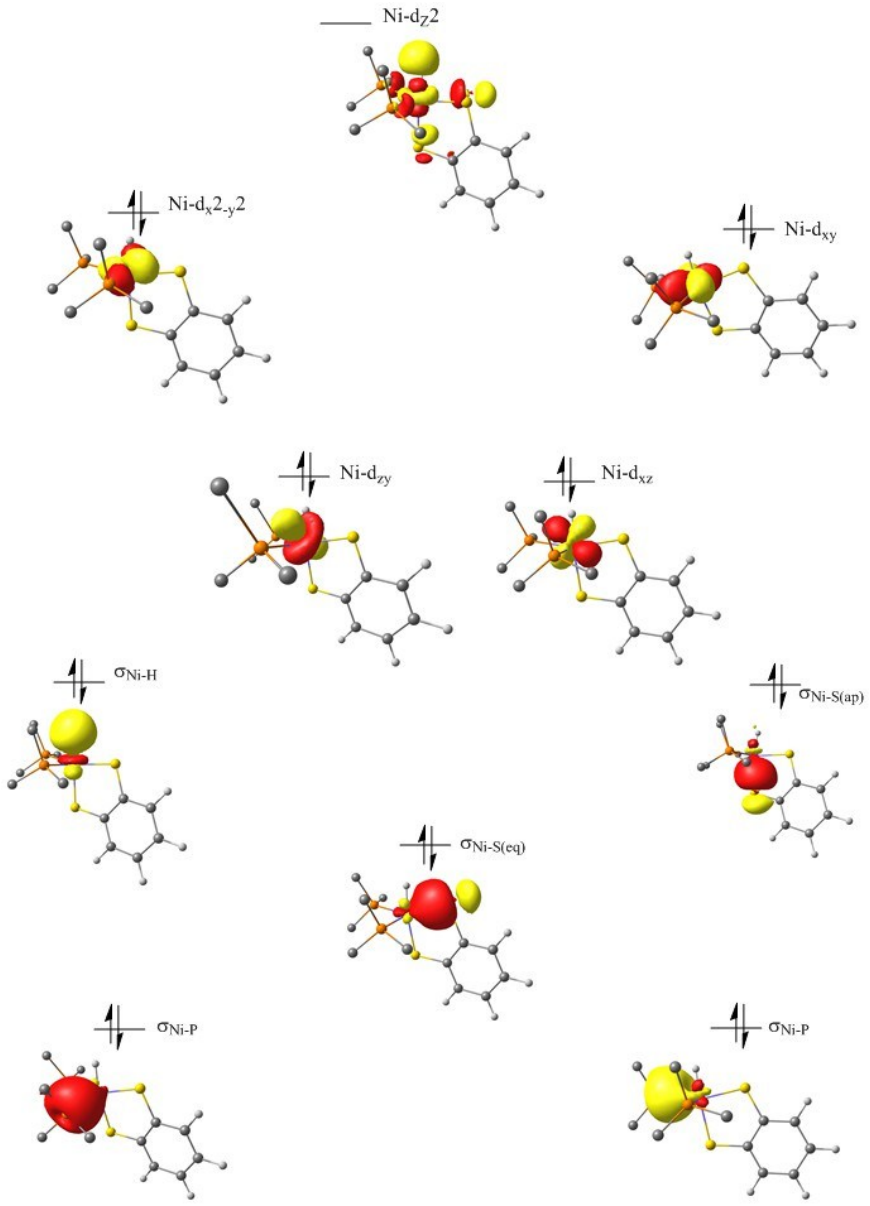


Figure S4. Localized orbitals of $[Ni^{II}H^{-}L]^{-}$.

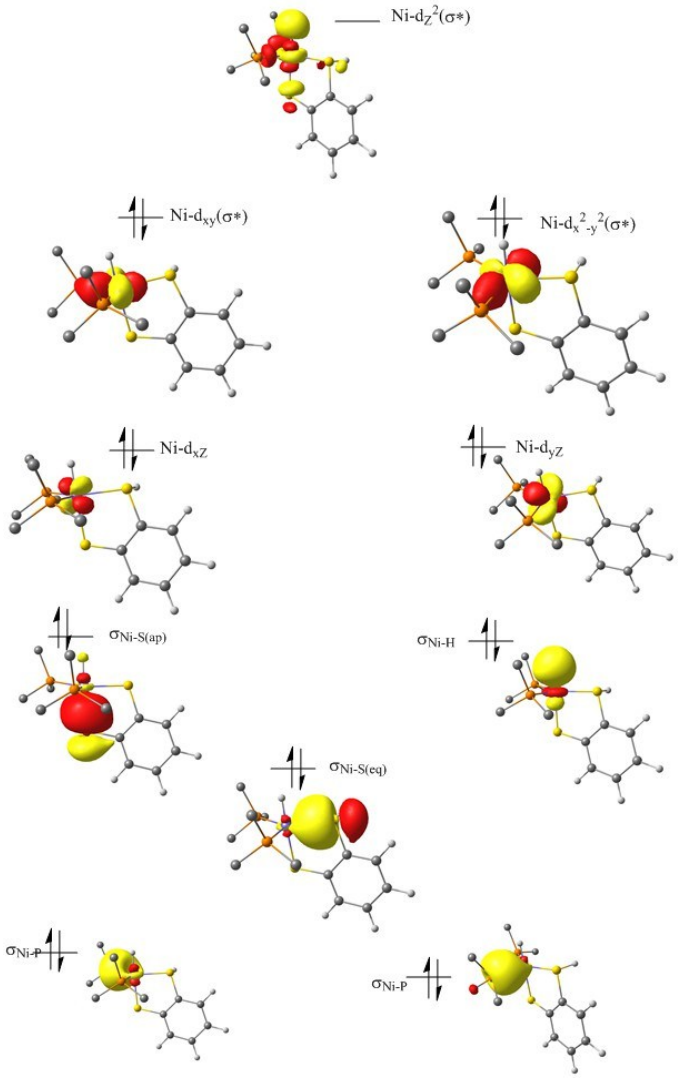


Figure S5. Localized orbitals of [Ni^{II}H^{-}LH].

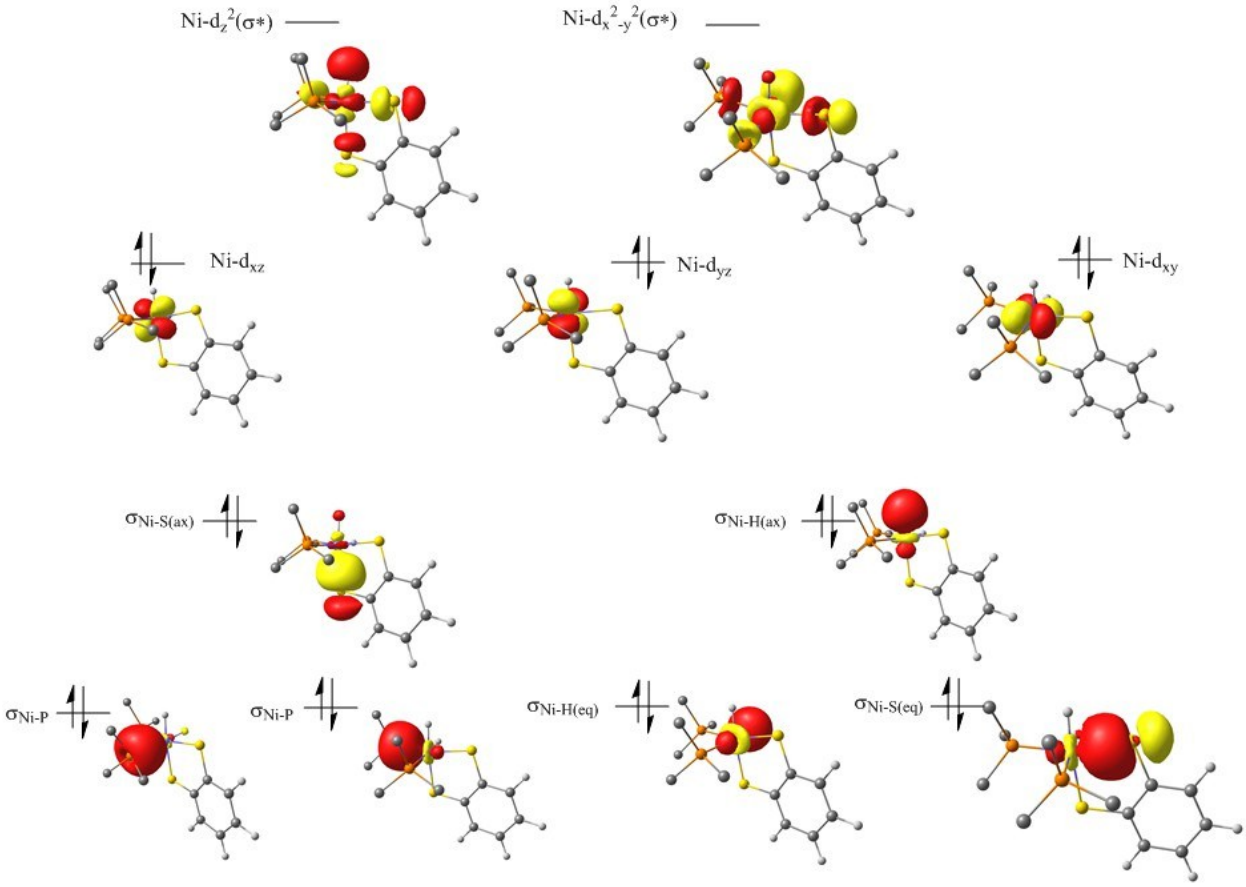


Figure S6. Localized orbitals of [Ni^{IV}H^{-}H^{-}L].

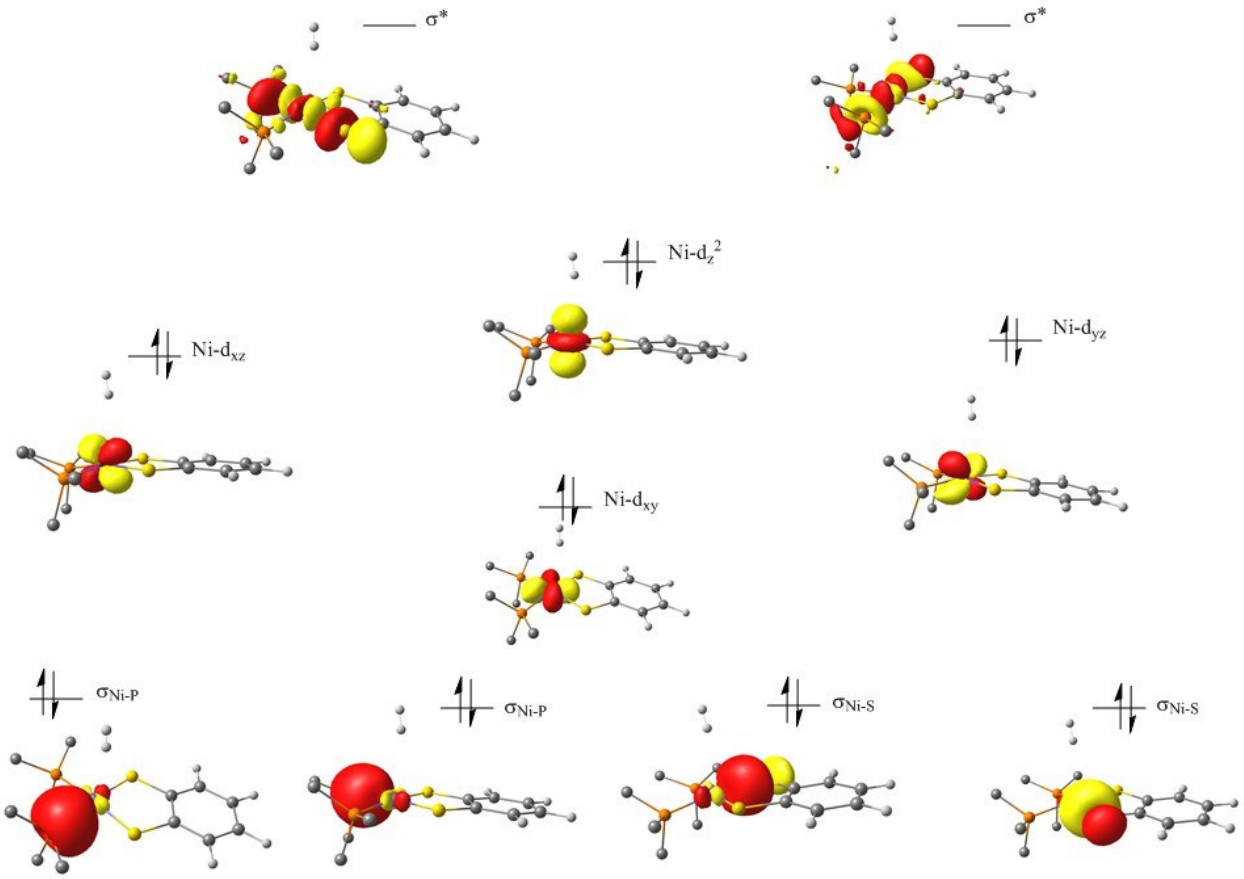


Figure S7. Localized orbitals of $[Ni^{II}L]+H_2$.

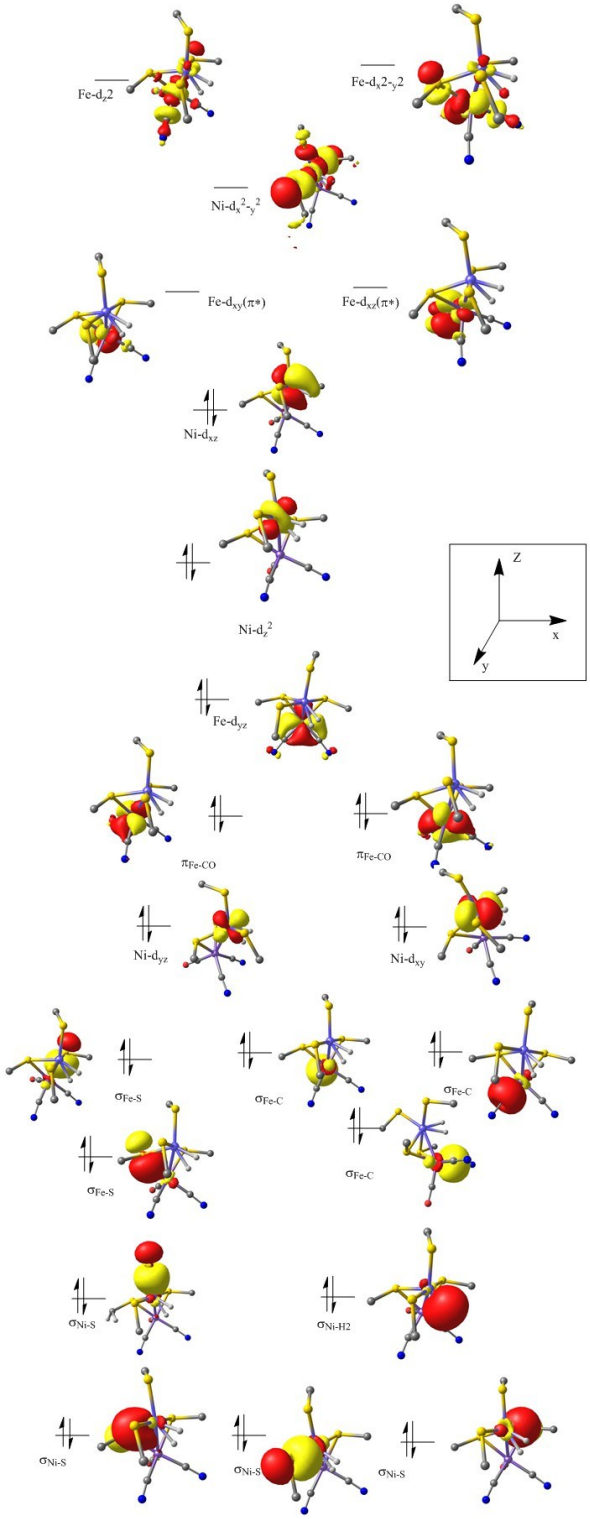


Figure S8. Localized orbitals of Ni-SIa + H_2 for [NiFe] hydrogenase.

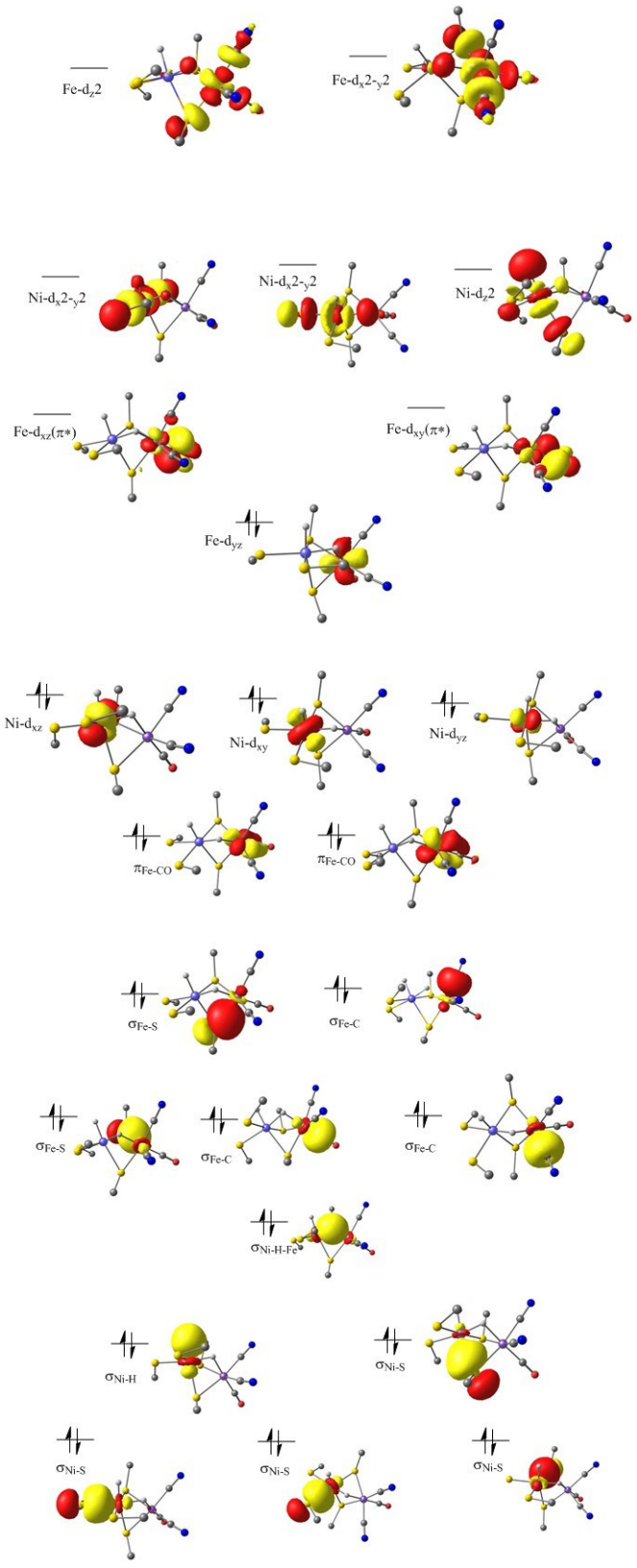


Figure S9. Localized orbitals of the dihydride intermediate in [NiFe] hydrogenase.

5. Coordinates [Angstrom] of all structural models

$Ni^{II}L$:

28	-0.090225000	0.050561000	-0.287664000
26	4.194161000	-0.037709000	0.034307000
16	-1.594137000	1.621457000	-0.549316000
16	-1.503982000	-1.393506000	-1.098153000
15	1.264024000	-1.660364000	0.191850000
15	1.367639000	1.738403000	0.335340000
6	-3.005581000	0.858578000	-1.245567000
6	-2.968879000	-0.516617000	-1.482514000
6	-4.087389000	-1.160306000	-2.015387000
1	-4.051888000	-2.229672000	-2.192298000
6	-5.228703000	-0.434417000	-2.315914000
1	-6.092437000	-0.939337000	-2.731022000
6	-5.263362000	0.939530000	-2.084875000
1	-6.154747000	1.508564000	-2.319500000
6	-4.158251000	1.584527000	-1.553251000
1	-4.179649000	2.652967000	-1.369496000
6	2.942947000	-1.499708000	-0.458854000
6	4.185277000	-2.047689000	0.012251000
1	4.322722000	-2.671635000	0.881057000
6	5.226560000	-1.568896000	-0.825803000
1	6.279679000	-1.770397000	-0.695983000
6	4.652413000	-0.736572000	-1.823627000
1	5.191514000	-0.195438000	-2.586561000
6	3.250543000	-0.694589000	-1.609154000
1	2.526528000	-0.127559000	-2.178360000
6	3.119817000	1.468056000	0.787754000
6	3.657213000	0.646300000	1.841138000
1	3.094916000	0.087412000	2.571543000
6	5.072685000	0.650531000	1.739690000
1	5.747409000	0.095867000	2.374883000
6	5.437124000	1.461994000	0.635626000
1	6.440522000	1.637303000	0.277342000
6	4.250588000	1.969258000	0.047634000
1	4.207239000	2.586550000	-0.835568000
6	1.427103000	-1.849695000	2.002631000
6	2.228748000	-2.840722000	2.575408000
1	2.711609000	-3.580605000	1.947846000
6	2.403766000	-2.893254000	3.949302000
1	3.041268000	-3.655293000	4.381149000
6	1.759625000	-1.974999000	4.771341000
1	1.902126000	-2.016261000	5.844404000
6	0.921466000	-1.019017000	4.216122000
1	0.398748000	-0.314872000	4.852604000
6	0.754591000	-0.959026000	2.838223000
1	0.101096000	-0.208917000	2.399670000
6	0.847121000	-3.357844000	-0.336450000
6	-0.000307000	-4.148974000	0.438971000
1	-0.421268000	-3.751273000	1.355752000
6	-0.294802000	-5.447093000	0.051859000
1	-0.942153000	-6.057505000	0.669351000
6	0.243704000	-5.964537000	-1.119125000
1	0.020015000	-6.981890000	-1.416161000
6	1.071494000	-5.176092000	-1.906630000

1	1.494737000	-5.573849000	-2.820942000
6	1.370931000	-3.878056000	-1.519542000
1	2.026397000	-3.273632000	-2.136092000
6	0.777186000	2.787684000	1.719096000
6	-0.090049000	3.856726000	1.480822000
1	-0.388309000	4.093930000	0.466863000
6	-0.558476000	4.629595000	2.533069000
1	-1.221672000	5.461611000	2.330188000
6	-0.176414000	4.345136000	3.837423000
1	-0.539728000	4.953229000	4.656810000
6	0.680938000	3.282551000	4.084951000
1	0.992872000	3.055442000	5.097552000
6	1.154697000	2.510813000	3.034205000
1	1.834146000	1.696831000	3.249615000
6	1.597323000	2.925038000	-1.035148000
6	1.325849000	2.540592000	-2.344914000
1	0.871066000	1.572601000	-2.532085000
6	1.614421000	3.395760000	-3.400742000
1	1.403045000	3.085983000	-4.416692000
6	2.164727000	4.645061000	-3.152417000
1	2.386868000	5.313668000	-3.975361000
6	2.427262000	5.041557000	-1.846031000
1	2.855538000	6.016519000	-1.647188000
6	2.149762000	4.185186000	-0.792980000
1	2.373988000	4.491201000	0.223329000

$Ni^{I}L^{-}$:

28	-0.085581000	0.335652000	-0.026257000
26	4.199758000	0.551278000	-0.213793000
16	-1.753392000	1.667104000	0.802082000
16	-1.684995000	-1.145774000	-0.732724000
15	1.363989000	0.419026000	1.630295000
15	1.213634000	0.420155000	-1.803160000
6	-3.233983000	0.813829000	0.431554000
6	-3.204386000	-0.428050000	-0.245627000
6	-4.417154000	-1.072672000	-0.522653000
1	-4.388026000	-2.023883000	-1.044201000
6	-5.634543000	-0.525291000	-0.148654000
1	-6.555902000	-1.048586000	-0.377644000
6	-5.663350000	0.696775000	0.519386000
1	-6.607268000	1.138047000	0.818703000
6	-4.474186000	1.349883000	0.802517000
1	-4.488640000	2.301634000	1.323621000
6	3.123180000	0.013989000	1.400109000
6	4.289010000	0.753012000	1.790257000
1	4.286782000	1.698172000	2.312581000
6	5.439659000	0.064662000	1.317455000
1	6.462869000	0.395157000	1.422847000
6	5.005133000	-1.107088000	0.638585000
1	5.640050000	-1.823633000	0.138286000
6	3.584813000	-1.140576000	0.686025000
1	2.948566000	-1.886277000	0.230919000
6	2.941599000	0.986644000	-1.725757000
6	3.359489000	2.178411000	-1.046758000
1	2.702510000	2.866997000	-0.534895000
6	4.775802000	2.271944000	-1.124582000
1	5.385410000	3.043496000	-0.677376000
6	5.251546000	1.142609000	-1.846115000
1	6.286915000	0.905480000	-2.043692000
6	4.129585000	0.353518000	-2.220145000
1	4.165496000	-0.588962000	-2.746239000
6	1.537702000	2.052130000	2.468027000
6	2.066343000	2.195149000	3.751521000
1	2.345573000	1.313997000	4.320389000
6	2.249280000	3.454827000	4.304050000
1	2.664849000	3.552259000	5.300416000
6	1.903223000	4.589638000	3.579914000
1	2.049280000	5.573387000	4.010401000
6	1.361940000	4.458453000	2.308307000
1	1.078934000	5.339374000	1.744082000
6	1.175235000	3.196354000	1.760003000
1	0.733936000	3.079340000	0.773295000
6	0.952277000	-0.694886000	3.032643000
6	-0.395938000	-0.949438000	3.296922000
1	-1.150411000	-0.488664000	2.664762000
6	-0.762765000	-1.789161000	4.338396000
1	-1.812196000	-1.975944000	4.533729000
6	0.209274000	-2.400975000	5.121542000
1	-0.078572000	-3.062842000	5.929785000
6	1.552164000	-2.166771000	4.858220000
1	2.316948000	-2.644630000	5.459946000
6	1.921372000	-1.318474000	3.822774000
1	2.973500000	-1.142139000	3.627004000

6	0.562815000	1.522999000	-3.121139000
6	-0.823205000	1.620080000	-3.270439000
1	-1.463414000	1.041856000	-2.609730000
6	-1.371325000	2.454580000	-4.233145000
1	-2.448033000	2.518813000	-4.338245000
6	-0.546269000	3.217656000	-5.051195000
1	-0.975876000	3.877729000	-5.795391000
6	0.832012000	3.136060000	-4.905327000
1	1.482459000	3.729967000	-5.537254000
6	1.383224000	2.292628000	-3.949695000
1	2.461373000	2.235458000	-3.846515000
6	1.464635000	-1.166402000	-2.705717000
6	1.298799000	-2.357904000	-2.002377000
1	0.943662000	-2.311082000	-0.975867000
6	1.569655000	-3.579561000	-2.604664000
1	1.442023000	-4.498114000	-2.043803000
6	1.996995000	-3.622988000	-3.924942000
1	2.209337000	-4.574817000	-4.397455000
6	2.143249000	-2.442048000	-4.643513000
1	2.468936000	-2.472475000	-5.676936000
6	1.878081000	-1.222466000	-4.037125000
1	2.003150000	-0.302987000	-4.600479000

$[Ni^{III}H^{-}L]$:

28	2.884841000	12.905531000	14.265964000
26	1.638652000	15.863729000	16.998977000
16	3.241460000	12.194386000	12.219699000
16	4.114354000	14.744611000	13.862612000
15	2.934927000	12.736074000	16.510772000
15	0.875637000	14.084636000	14.116625000
6	3.962640000	13.559306000	11.402921000
6	4.365214000	14.686933000	12.138237000
6	4.966823000	15.760795000	11.473069000
1	5.276847000	16.626882000	12.047084000
6	5.161643000	15.720196000	10.104528000
1	5.629242000	16.559238000	9.603415000
6	4.754873000	14.604177000	9.373935000
1	4.901649000	14.571872000	8.301173000
6	4.160682000	13.534432000	10.018274000
1	3.839681000	12.664208000	9.456844000
6	2.784114000	14.266437000	17.460754000
6	1.913010000	14.588299000	18.556188000
1	1.180798000	13.934047000	19.002091000
6	2.182063000	15.921441000	18.958108000
1	1.663312000	16.459094000	19.737781000
6	3.220076000	16.434481000	18.134461000
1	3.625300000	17.434468000	18.173187000
6	3.594403000	15.424280000	17.210835000
1	4.345920000	15.511743000	16.439871000
6	0.693655000	15.532926000	15.204947000
6	-0.250927000	15.701789000	16.275535000
1	-1.006636000	14.987962000	16.568782000
6	-0.045535000	16.977582000	16.866605000
1	-0.596489000	17.379246000	17.703869000
6	1.033025000	17.607092000	16.189043000
1	1.459293000	18.570380000	16.425689000
6	1.506456000	16.717314000	15.186331000
1	2.369347000	16.876894000	14.559216000
6	1.612858000	11.675135000	17.194817000
6	1.855708000	10.328959000	17.474670000
1	2.847943000	9.914811000	17.335839000
6	0.834739000	9.512037000	17.938658000
1	1.040622000	8.471154000	18.157196000
6	-0.441508000	10.025494000	18.131705000
1	-1.234819000	9.387244000	18.501664000
6	-0.694875000	11.359201000	17.846333000
1	-1.689552000	11.768045000	17.980777000
6	0.322627000	12.173737000	17.372259000
1	0.110813000	13.209280000	17.135580000
6	4.449699000	11.992027000	17.201719000
6	5.401004000	11.417033000	16.364190000
1	5.246915000	11.432419000	15.289290000
6	6.539734000	10.829703000	16.902670000
1	7.276066000	10.382173000	16.246682000
6	6.733053000	10.818519000	18.276451000
1	7.621849000	10.362577000	18.695732000
6	5.787882000	11.395224000	19.118202000
1	5.937779000	11.388704000	20.191240000
6	4.650993000	11.979136000	18.584736000

1	3.913332000	12.425870000	19.243618000
6	-0.681691000	13.146515000	14.314172000
6	-0.632732000	11.755616000	14.387117000
1	0.331351000	11.257169000	14.380896000
6	-1.800769000	11.011838000	14.482996000
1	-1.746029000	9.931595000	14.546145000
6	-3.030075000	11.652727000	14.514836000
1	-3.942330000	11.074511000	14.600380000
6	-3.091337000	13.039652000	14.432046000
1	-4.050370000	13.543175000	14.445442000
6	-1.926106000	13.782305000	14.321087000
1	-1.982937000	14.862010000	14.236889000
6	0.730649000	14.691668000	12.397249000
6	0.198681000	13.818943000	11.442881000
1	-0.212076000	12.864243000	11.750956000
6	0.209291000	14.150911000	10.098541000
1	-0.204221000	13.458629000	9.375064000
6	0.753584000	15.358720000	9.680785000
1	0.770470000	15.613516000	8.628126000
6	1.283716000	16.230854000	10.618743000
1	1.720444000	17.171372000	10.305200000
6	1.279807000	15.898204000	11.966404000
1	1.724482000	16.582254000	12.674801000
1	2.369205000	11.542085000	14.467394000

[$Ni^{I}LH$]:

28	-0.070195000	0.356316000	-0.228275000
26	4.166814000	0.564463000	-0.204246000
16	-1.792332000	1.865280000	0.334249000
16	-1.772417000	-1.078614000	-0.651134000
15	1.298925000	0.480694000	1.536446000
15	1.296423000	0.460754000	-1.988437000
6	-3.191835000	0.840642000	0.730045000
6	-3.157812000	-0.469016000	0.230670000
6	-4.277230000	-1.278020000	0.469759000
1	-4.274199000	-2.292396000	0.087880000
6	-5.361235000	-0.805721000	1.188283000
1	-6.208647000	-1.457266000	1.365286000
6	-5.368721000	0.496216000	1.682024000
1	-6.214813000	0.866690000	2.246658000
6	-4.285336000	1.325649000	1.438403000
1	-4.285457000	2.348426000	1.797142000
6	3.034963000	0.010334000	1.360901000
6	4.212526000	0.695547000	1.808830000
1	4.226904000	1.619789000	2.367869000
6	5.348197000	-0.019930000	1.342375000
1	6.379084000	0.268217000	1.486483000
6	4.891836000	-1.149955000	0.610507000
1	5.514787000	-1.870322000	0.101318000
6	3.471507000	-1.134898000	0.615520000
1	2.821896000	-1.842153000	0.118814000
6	3.007149000	1.031983000	-1.777344000
6	3.369782000	2.210905000	-1.045565000
1	2.678404000	2.888595000	-0.567339000
6	4.785533000	2.317639000	-1.031370000
1	5.356798000	3.083381000	-0.527810000
6	5.316710000	1.212853000	-1.749659000
1	6.364457000	0.989049000	-1.886679000
6	4.231039000	0.422536000	-2.213668000
1	4.313160000	-0.505383000	-2.759455000
6	1.445071000	2.110717000	2.362905000
6	1.878719000	2.235794000	3.683421000
1	2.091769000	1.345976000	4.267059000
6	2.048543000	3.489747000	4.251843000
1	2.391559000	3.574910000	5.275939000
6	1.783409000	4.634270000	3.509253000
1	1.920404000	5.612815000	3.953388000
6	1.336929000	4.521624000	2.199791000
1	1.121328000	5.410167000	1.618626000
6	1.164748000	3.265721000	1.633816000
1	0.808691000	3.171760000	0.611123000
6	0.725084000	-0.630160000	2.872996000
6	-0.652276000	-0.778496000	3.051063000
1	-1.335231000	-0.240375000	2.401376000
6	-1.150622000	-1.623441000	4.030126000
1	-2.222101000	-1.730162000	4.153930000
6	-0.277867000	-2.342616000	4.837747000
1	-0.665744000	-3.011940000	5.595985000
6	1.093110000	-2.208284000	4.664464000
1	1.777484000	-2.770752000	5.288426000
6	1.593742000	-1.356424000	3.688839000

1	2.666266000	-1.261665000	3.558544000
6	0.723616000	1.537089000	-3.358797000
6	-0.635794000	1.524631000	-3.679437000
1	-1.312789000	0.903609000	-3.098164000
6	-1.118926000	2.294503000	-4.726914000
1	-2.174511000	2.272070000	-4.969574000
6	-0.253406000	3.097506000	-5.460446000
1	-0.630992000	3.701749000	-6.276466000
6	1.097309000	3.125658000	-5.142083000
1	1.777410000	3.750132000	-5.709623000
6	1.584420000	2.349724000	-4.098792000
1	2.642800000	2.373304000	-3.864302000
6	1.582419000	-1.128978000	-2.865873000
6	1.276921000	-2.326719000	-2.223540000
1	0.815540000	-2.295977000	-1.239817000
6	1.548436000	-3.544645000	-2.834561000
1	1.309499000	-4.469700000	-2.324005000
6	2.121092000	-3.574799000	-4.098287000
1	2.334542000	-4.523501000	-4.575906000
6	2.413532000	-2.385087000	-4.755428000
1	2.854919000	-2.404590000	-5.744937000
6	2.142824000	-1.170638000	-4.144353000
1	2.375667000	-0.245174000	-4.661397000
1	-1.779683000	2.582506000	1.474215000

$[Ni^{II}H^{-}L]^{-}$:

28	2.543547000	12.774731000	14.192401000
26	1.610149000	15.775241000	16.953356000
16	3.497346000	11.663838000	12.438692000
16	3.890452000	14.566093000	13.684507000
15	2.897416000	12.615657000	16.370612000
15	0.684656000	14.053336000	14.041439000
6	4.422997000	12.878432000	11.578482000
6	4.580281000	14.167648000	12.123618000
6	5.310102000	15.123484000	11.410954000
1	5.419967000	16.116567000	11.834574000
6	5.888945000	14.823640000	10.185432000
1	6.447256000	15.584317000	9.651963000
6	5.743231000	13.547855000	9.650687000
1	6.189930000	13.298007000	8.695085000
6	5.016197000	12.590413000	10.344781000
1	4.894763000	11.594727000	9.930550000
6	2.775776000	14.151870000	17.341979000
6	1.934533000	14.458875000	18.460544000
1	1.201430000	13.797238000	18.897265000
6	2.214727000	15.786479000	18.884091000
1	1.717753000	16.312837000	19.686114000
6	3.229371000	16.313836000	18.037451000
1	3.636464000	17.313405000	18.082285000
6	3.571092000	15.315993000	17.084015000
1	4.289240000	15.411613000	16.281782000
6	0.551559000	15.447049000	15.216119000
6	-0.313778000	15.602489000	16.349480000
1	-1.035757000	14.876815000	16.696798000
6	-0.076680000	16.879492000	16.932346000
1	-0.568187000	17.276730000	17.808491000
6	0.951663000	17.517587000	16.183027000
1	1.383978000	18.484832000	16.393456000
6	1.350161000	16.633822000	15.142245000
1	2.129184000	16.801981000	14.412162000
6	1.690294000	11.572739000	17.266013000
6	2.008406000	10.393618000	17.939987000
1	3.039432000	10.065392000	18.004058000
6	1.012948000	9.628996000	18.537560000
1	1.280124000	8.716042000	19.057273000
6	-0.315126000	10.028636000	18.475621000
1	-1.087461000	9.432162000	18.946534000
6	-0.645577000	11.199006000	17.801641000
1	-1.679138000	11.521362000	17.737276000
6	0.346653000	11.954160000	17.199344000
1	0.083698000	12.864154000	16.670081000
6	4.510741000	11.993790000	16.982238000
6	5.386320000	11.415045000	16.066598000
1	5.087550000	11.362068000	15.021620000
6	6.621149000	10.932515000	16.485215000
1	7.298184000	10.485586000	15.766865000
6	6.990511000	11.029696000	17.819584000
1	7.955021000	10.658099000	18.145317000
6	6.124281000	11.611157000	18.739572000
1	6.411809000	11.691012000	19.781721000
6	4.892729000	12.091518000	18.322564000

1	4.218299000	12.547227000	19.041106000
6	-1.011618000	13.327047000	14.166390000
6	-1.146813000	11.940244000	14.137089000
1	-0.250155000	11.331977000	14.069798000
6	-2.398351000	11.342871000	14.213506000
1	-2.481094000	10.262322000	14.195267000
6	-3.537122000	12.127143000	14.325573000
1	-4.514537000	11.663899000	14.393334000
6	-3.418608000	13.512131000	14.352189000
1	-4.303715000	14.131711000	14.439113000
6	-2.167721000	14.105573000	14.268705000
1	-2.090131000	15.186861000	14.293540000
6	0.549731000	14.970325000	12.448026000
6	1.201878000	14.425034000	11.343118000
1	1.775495000	13.511297000	11.472217000
6	1.145057000	15.053254000	10.107036000
1	1.671144000	14.622423000	9.262378000
6	0.432627000	16.235889000	9.959406000
1	0.393064000	16.732791000	8.997165000
6	-0.222308000	16.787457000	11.054277000
1	-0.776250000	17.713088000	10.946661000
6	-0.162024000	16.160773000	12.291258000
1	-0.658646000	16.613932000	13.142596000
1	1.748229000	11.563327000	14.386326000

[$Ni^{II}H^{-}LH$]:

28	0.238170000	0.149990000	0.313816000
26	4.281152000	-0.081440000	0.203083000
16	-1.870228000	1.090973000	-0.038324000
16	0.863809000	1.042504000	-1.720715000
15	1.224452000	-1.798328000	0.152727000
15	1.489595000	1.615845000	1.401713000
6	-1.596368000	2.257308000	-1.370533000
6	-0.384598000	2.207301000	-2.070972000
6	-0.202129000	3.140216000	-3.104761000
1	0.729086000	3.124364000	-3.659368000
6	-1.178496000	4.069103000	-3.411401000
1	-1.003561000	4.778422000	-4.212183000
6	-2.371959000	4.108635000	-2.695635000
1	-3.131977000	4.843311000	-2.928574000
6	-2.573343000	3.200008000	-1.669080000
1	-3.490473000	3.215852000	-1.091763000
6	3.015779000	-1.643024000	-0.151027000
6	4.113099000	-2.049440000	0.675139000
1	4.037438000	-2.471286000	1.665632000
6	5.320310000	-1.802026000	-0.032656000
1	6.318515000	-1.976619000	0.341007000
6	4.985414000	-1.241763000	-1.296145000
1	5.685019000	-0.912119000	-2.049941000
6	3.570610000	-1.132564000	-1.369520000
1	3.002051000	-0.731643000	-2.196593000
6	3.263512000	1.521069000	1.011006000
6	4.277328000	1.029704000	1.901075000
1	4.108568000	0.672521000	2.906763000
6	5.535416000	1.112030000	1.244999000
1	6.484863000	0.804136000	1.657186000
6	5.315487000	1.626572000	-0.062129000
1	6.068161000	1.774338000	-0.822249000
6	3.919886000	1.853900000	-0.220565000
1	3.426944000	2.175563000	-1.124706000
6	1.214282000	-2.767254000	1.702953000
6	0.672108000	-4.045501000	1.817678000
1	0.259146000	-4.542016000	0.947623000
6	0.651825000	-4.694549000	3.046815000
1	0.224578000	-5.687658000	3.119387000
6	1.175081000	-4.078558000	4.174234000
1	1.160248000	-4.588053000	5.129975000
6	1.715070000	-2.801340000	4.071417000
1	2.122995000	-2.308881000	4.946542000
6	1.727523000	-2.151587000	2.848392000
1	2.141138000	-1.149315000	2.773735000
6	0.803765000	-3.026709000	-1.137856000
6	-0.335811000	-2.843473000	-1.916086000
1	-0.952567000	-1.965464000	-1.749885000
6	-0.669131000	-3.764147000	-2.902605000
1	-1.555697000	-3.612091000	-3.506224000
6	0.135820000	-4.873765000	-3.116910000
1	-0.122440000	-5.591546000	-3.886232000
6	1.279427000	-5.062189000	-2.348135000
1	1.911829000	-5.925895000	-2.515909000
6	1.613713000	-4.142305000	-1.367701000

1	2.510032000	-4.288371000	-0.773112000
6	1.519501000	1.705186000	3.236941000
6	0.686081000	0.899360000	4.006517000
1	0.036303000	0.185071000	3.511400000
6	0.684610000	1.000147000	5.392921000
1	0.032597000	0.362290000	5.977895000
6	1.515900000	1.913345000	6.023161000
1	1.517246000	1.991962000	7.103709000
6	2.346206000	2.731640000	5.264104000
1	2.993629000	3.450893000	5.751281000
6	2.344960000	2.630745000	3.882791000
1	2.992074000	3.274169000	3.295658000
6	0.925738000	3.310579000	1.006926000
6	-0.274810000	3.705836000	1.608457000
1	-0.738430000	3.063251000	2.351543000
6	-0.886101000	4.897417000	1.258513000
1	-1.817402000	5.182624000	1.733594000
6	-0.312850000	5.715609000	0.291687000
1	-0.796616000	6.641437000	0.004932000
6	0.879064000	5.336094000	-0.306302000
1	1.333164000	5.967367000	-1.061219000
6	1.497699000	4.142900000	0.047603000
1	2.423573000	3.863956000	-0.436137000
1	-0.196134000	-0.370395000	1.598920000
1	-2.595624000	0.198178000	-0.741985000

TS1:

28	-0.004279000	0.101395000	-0.085786000
26	4.281764000	-0.011081000	0.005528000
16	-1.878717000	1.267095000	-0.236736000
16	0.838830000	1.168760000	-1.934440000
15	1.273953000	-1.728117000	0.051242000
15	1.470246000	1.497648000	1.333449000
6	-1.537641000	2.471837000	-1.474598000
6	-0.354797000	2.414284000	-2.222008000
6	-0.138342000	3.381110000	-3.207902000
1	0.775081000	3.338303000	-3.790664000
6	-1.058419000	4.393818000	-3.426263000
1	-0.860510000	5.141780000	-4.184716000
6	-2.224818000	4.451302000	-2.671732000
1	-2.946409000	5.242491000	-2.833777000
6	-2.465676000	3.487557000	-1.704856000
1	-3.372667000	3.521684000	-1.111532000
6	3.026508000	-1.545118000	-0.360856000
6	4.191650000	-2.010691000	0.339537000
1	4.204940000	-2.515682000	1.292392000
6	5.332796000	-1.693284000	-0.440981000
1	6.358149000	-1.884989000	-0.161337000
6	4.895139000	-1.045933000	-1.627763000
1	5.530211000	-0.651108000	-2.406495000
6	3.480223000	-0.951167000	-1.586183000
1	2.848804000	-0.494400000	-2.334423000
6	3.246669000	1.502657000	0.934265000
6	4.303021000	0.998023000	1.767509000
1	4.181031000	0.588067000	2.759753000
6	5.538119000	1.154391000	1.081881000
1	6.507359000	0.854872000	1.451707000
6	5.266036000	1.738089000	-0.184708000
1	5.991018000	1.952067000	-0.955626000
6	3.861166000	1.932575000	-0.290605000
1	3.334180000	2.286699000	-1.162708000
6	1.277815000	-2.427103000	1.736721000
6	0.332851000	-3.390646000	2.096082000
1	-0.358726000	-3.774279000	1.354276000
6	0.274338000	-3.866530000	3.397000000
1	-0.461020000	-4.617253000	3.659681000
6	1.157923000	-3.389149000	4.358029000
1	1.113882000	-3.766877000	5.372406000
6	2.091670000	-2.424078000	4.012816000
1	2.775103000	-2.032075000	4.757154000
6	2.143847000	-1.939252000	2.713517000
1	2.859505000	-1.166370000	2.461266000
6	0.837640000	-3.153678000	-1.002485000
6	-0.042055000	-3.014211000	-2.070792000
1	-0.519017000	-2.056117000	-2.248964000
6	-0.301292000	-4.093826000	-2.906888000
1	-0.986687000	-3.977927000	-3.737311000
6	0.313360000	-5.315842000	-2.676835000
1	0.107565000	-6.157979000	-3.326485000
6	1.195636000	-5.461113000	-1.611749000
1	1.678429000	-6.413564000	-1.429064000
6	1.461465000	-4.385132000	-0.781978000

1	2.153684000	-4.500617000	0.045896000
6	1.437676000	1.388776000	3.163062000
6	0.500717000	0.558837000	3.774443000
1	-0.152553000	-0.050687000	3.157005000
6	0.409455000	0.493810000	5.158964000
1	-0.319096000	-0.162405000	5.619971000
6	1.260683000	1.254524000	5.945927000
1	1.197748000	1.198986000	7.026149000
6	2.195291000	2.092656000	5.346656000
1	2.855974000	2.694942000	5.958733000
6	2.277492000	2.166604000	3.965246000
1	2.999213000	2.832687000	3.504615000
6	0.861786000	3.199053000	1.083387000
6	-0.331632000	3.531742000	1.733356000
1	-0.776430000	2.832101000	2.432855000
6	-0.953851000	4.745278000	1.490181000
1	-1.879065000	4.984413000	2.000842000
6	-0.399236000	5.644210000	0.588797000
1	-0.890561000	6.588807000	0.389561000
6	0.786392000	5.325631000	-0.056630000
1	1.227943000	6.021511000	-0.759854000
6	1.411913000	4.110308000	0.184224000
1	2.330891000	3.879714000	-0.335560000
1	-0.628492000	-0.555044000	1.060962000
1	-1.157950000	-0.345362000	-0.889439000

[$Ni^{IV}H^{-}H^{-}L$]:

28	-0.071256000	0.025670000	-0.092899000
26	4.240540000	0.003864000	-0.038767000
16	-1.859329000	1.368132000	-0.121494000
16	0.696049000	1.036975000	-2.014671000
15	1.286841000	-1.760243000	0.069759000
15	1.360491000	1.478446000	1.225465000
6	-1.490586000	2.566736000	-1.351390000
6	-0.388055000	2.403941000	-2.200698000
6	-0.143518000	3.359068000	-3.188640000
1	0.712584000	3.231084000	-3.841960000
6	-0.965456000	4.468147000	-3.323240000
1	-0.750938000	5.205022000	-4.087972000
6	-2.052452000	4.632589000	-2.473310000
1	-2.694770000	5.500049000	-2.564976000
6	-2.312849000	3.685309000	-1.494279000
1	-3.155312000	3.810371000	-0.823056000
6	3.028142000	-1.557231000	-0.359828000
6	4.206635000	-1.986513000	0.342806000
1	4.236528000	-2.471471000	1.305489000
6	5.334492000	-1.661887000	-0.453367000
1	6.365396000	-1.825718000	-0.176682000
6	4.875694000	-1.051845000	-1.651787000
1	5.497632000	-0.662272000	-2.443550000
6	3.459432000	-0.986225000	-1.604733000
1	2.814271000	-0.557221000	-2.357455000
6	3.144616000	1.490561000	0.837367000
6	4.210390000	1.049626000	1.696014000
1	4.094782000	0.655064000	2.694699000
6	5.446612000	1.237676000	1.020779000
1	6.421450000	0.983223000	1.409108000
6	5.168272000	1.781562000	-0.261859000
1	5.893671000	2.003459000	-1.030026000
6	3.758811000	1.919494000	-0.388614000
1	3.232549000	2.226009000	-1.278890000
6	1.285184000	-2.425481000	1.765505000
6	0.328609000	-3.373607000	2.135474000
1	-0.371562000	-3.752853000	1.399440000
6	0.273692000	-3.841656000	3.439144000
1	-0.469018000	-4.581536000	3.711215000
6	1.171906000	-3.371529000	4.390051000
1	1.131337000	-3.744305000	5.406372000
6	2.115185000	-2.419508000	4.034160000
1	2.808848000	-2.033368000	4.771757000
6	2.163947000	-1.940732000	2.732785000
1	2.884657000	-1.175401000	2.472880000
6	0.875787000	-3.202987000	-0.970507000
6	0.056063000	-3.086449000	-2.088115000
1	-0.415364000	-2.135761000	-2.312957000
6	-0.149593000	-4.181577000	-2.918387000
1	-0.790016000	-4.083298000	-3.785947000
6	0.461326000	-5.394638000	-2.637010000
1	0.297697000	-6.248223000	-3.283500000
6	1.287037000	-5.515398000	-1.525083000
1	1.768434000	-6.459867000	-1.302384000
6	1.498948000	-4.424733000	-0.698844000

1	2.149516000	-4.521895000	0.164156000
6	1.313570000	1.328344000	3.051036000
6	0.378533000	0.490318000	3.653098000
1	-0.274906000	-0.113069000	3.030682000
6	0.286502000	0.411036000	5.036730000
1	-0.440836000	-0.251961000	5.489621000
6	1.133857000	1.166405000	5.832593000
1	1.070116000	1.099287000	6.912090000
6	2.063999000	2.015957000	5.242801000
1	2.720450000	2.616579000	5.860847000
6	2.146526000	2.104639000	3.862552000
1	2.861243000	2.783531000	3.410299000
6	0.804267000	3.207976000	1.018756000
6	-0.253601000	3.651049000	1.818125000
1	-0.657404000	3.005428000	2.589202000
6	-0.795634000	4.913125000	1.634446000
1	-1.614278000	5.239724000	2.264394000
6	-0.295904000	5.750618000	0.646399000
1	-0.723186000	6.735340000	0.500042000
6	0.748057000	5.317473000	-0.156928000
1	1.139765000	5.958241000	-0.937563000
6	1.289838000	4.052806000	0.022465000
1	2.087065000	3.728741000	-0.630101000
1	-0.705670000	-0.577076000	1.071003000
1	-0.981503000	-0.858756000	-0.763822000

TS2:

28	-0.088413000	-0.002922000	-0.055188000
26	4.246561000	0.026835000	-0.044194000
16	-1.847603000	1.379055000	-0.153644000
16	0.637868000	0.901328000	-2.051319000
15	1.322348000	-1.756143000	0.072658000
15	1.347133000	1.476390000	1.233989000
6	-1.441353000	2.561051000	-1.384328000
6	-0.359408000	2.333808000	-2.243437000
6	-0.082165000	3.262353000	-3.247386000
1	0.756006000	3.084777000	-3.912429000
6	-0.857389000	4.404772000	-3.388621000
1	-0.622181000	5.118862000	-4.168795000
6	-1.924772000	4.631447000	-2.528013000
1	-2.529587000	5.524688000	-2.627143000
6	-2.213368000	3.713429000	-1.528741000
1	-3.039855000	3.885075000	-0.847917000
6	3.061311000	-1.555709000	-0.353648000
6	4.237982000	-1.957069000	0.368923000
1	4.264098000	-2.428381000	1.338365000
6	5.369335000	-1.628915000	-0.420477000
1	6.399291000	-1.774526000	-0.130573000
6	4.914910000	-1.044854000	-1.633430000
1	5.539485000	-0.659833000	-2.425320000
6	3.497696000	-0.998511000	-1.603097000
1	2.854725000	-0.588974000	-2.368167000
6	3.126809000	1.503403000	0.828599000
6	4.213957000	1.099200000	1.676291000
1	4.120192000	0.715025000	2.681460000
6	5.435596000	1.304089000	0.978775000
1	6.421975000	1.077554000	1.355025000
6	5.125244000	1.820950000	-0.308205000
1	5.833501000	2.046866000	-1.091095000
6	3.710608000	1.923040000	-0.414909000
1	3.160695000	2.202199000	-1.300529000
6	1.311906000	-2.431772000	1.763639000
6	0.364142000	-3.393387000	2.121601000
1	-0.324412000	-3.779436000	1.378098000
6	0.302547000	-3.866373000	3.423405000
1	-0.433561000	-4.616181000	3.686132000
6	1.186095000	-3.388673000	4.383865000
1	1.141021000	-3.765726000	5.398406000
6	2.120366000	-2.422972000	4.040264000
1	2.801898000	-2.030941000	4.785904000
6	2.174312000	-1.937771000	2.741843000
1	2.885526000	-1.159719000	2.492190000
6	0.879074000	-3.180157000	-0.976956000
6	0.010783000	-3.037121000	-2.054714000
1	-0.456468000	-2.075138000	-2.241373000
6	-0.244548000	-4.119202000	-2.889026000
1	-0.920679000	-4.003395000	-3.726912000
6	0.362108000	-5.343383000	-2.648651000
1	0.158189000	-6.186933000	-3.297082000
6	1.234181000	-5.489724000	-1.575492000
1	1.710509000	-6.443863000	-1.385051000
6	1.497651000	-4.412413000	-0.746620000

1	2.181676000	-4.528527000	0.087866000
6	1.306981000	1.328269000	3.059905000
6	0.375082000	0.483705000	3.658301000
1	-0.272331000	-0.123100000	3.032573000
6	0.278209000	0.402528000	5.041333000
1	-0.447110000	-0.264863000	5.491098000
6	1.118493000	1.162280000	5.840557000
1	1.050961000	1.094452000	6.919762000
6	2.045991000	2.017381000	5.254662000
1	2.696392000	2.621447000	5.875675000
6	2.132844000	2.107992000	3.874671000
1	2.844514000	2.791988000	3.425257000
6	0.788617000	3.207364000	1.032428000
6	-0.304602000	3.622531000	1.799277000
1	-0.732786000	2.953393000	2.536541000
6	-0.848506000	4.885187000	1.627082000
1	-1.693952000	5.190031000	2.232138000
6	-0.317031000	5.751480000	0.681054000
1	-0.746748000	6.736218000	0.542254000
6	0.760983000	5.346011000	-0.090821000
1	1.178752000	6.009877000	-0.837957000
6	1.306523000	4.081190000	0.078822000
1	2.137903000	3.783927000	-0.543167000
1	-0.828615000	-0.689341000	1.008787000
1	-1.099267000	-1.025097000	-0.268726000

$[Ni^{II}L] + H_2$:

28	0.557408000	0.704344000	-0.462042000
26	4.337628000	0.544077000	0.146899000
16	-0.049101000	2.678287000	-1.172449000
16	-0.014554000	-0.128866000	-2.408916000
15	1.511519000	-1.314244000	0.065599000
15	1.345035000	1.687418000	1.384348000
6	-0.567332000	2.490116000	-2.833005000
6	-0.548352000	1.213117000	-3.395765000
6	-0.965435000	1.031808000	-4.716291000
1	-0.948877000	0.037025000	-5.147963000
6	-1.395882000	2.115944000	-5.464285000
1	-1.717160000	1.967831000	-6.488122000
6	-1.415382000	3.390627000	-4.901251000
1	-1.751599000	4.238880000	-5.484870000
6	-1.003623000	3.577990000	-3.591447000
1	-1.016375000	4.566683000	-3.145913000
6	3.250180000	-1.075024000	-0.374390000
6	4.458307000	-1.485436000	0.282206000
1	4.526614000	-2.076763000	1.181720000
6	5.557724000	-0.973792000	-0.453307000
1	6.598003000	-1.087481000	-0.186594000
6	5.052149000	-0.258537000	-1.572680000
1	5.640879000	0.273817000	-2.304307000
6	3.634834000	-0.313056000	-1.530232000
1	2.943997000	0.152854000	-2.218501000
6	3.143556000	1.807053000	1.191906000
6	4.247359000	1.374782000	1.999989000
1	4.184252000	0.859071000	2.946727000
6	5.451526000	1.748662000	1.344018000
1	6.450179000	1.535914000	1.695408000
6	5.111299000	2.415976000	0.136026000
1	5.806930000	2.792321000	-0.598583000
6	3.695672000	2.445661000	0.030714000
1	3.110905000	2.852165000	-0.783374000
6	1.556716000	-2.079631000	1.743973000
6	0.627456000	-3.060816000	2.098050000
1	-0.107525000	-3.405000000	1.381856000
6	0.634573000	-3.620296000	3.368045000
1	-0.093532000	-4.382653000	3.617552000
6	1.569084000	-3.214168000	4.309534000
1	1.576486000	-3.656674000	5.298482000
6	2.489952000	-2.231375000	3.975093000
1	3.219061000	-1.894276000	4.702813000
6	2.477274000	-1.666722000	2.709066000
1	3.187054000	-0.887723000	2.471137000
6	0.983005000	-2.768992000	-0.903915000
6	-0.379451000	-3.027453000	-1.059395000
1	-1.106993000	-2.313376000	-0.687219000
6	-0.804929000	-4.190732000	-1.682786000
1	-1.864787000	-4.385203000	-1.791986000
6	0.126105000	-5.100040000	-2.167671000
1	-0.205929000	-6.008267000	-2.655916000
6	1.483378000	-4.843841000	-2.026181000
1	2.212915000	-5.550187000	-2.403531000
6	1.912094000	-3.685400000	-1.393318000

1	2.973668000	-3.500288000	-1.274516000
6	0.992434000	0.991825000	3.038707000
6	-0.094291000	0.135523000	3.200623000
1	-0.659031000	-0.180256000	2.328622000
6	-0.442679000	-0.325594000	4.462029000
1	-1.284956000	-0.997066000	4.576608000
6	0.294844000	0.064377000	5.571488000
1	0.029215000	-0.302159000	6.555939000
6	1.370571000	0.930865000	5.420212000
1	1.940279000	1.247349000	6.285732000
6	1.711394000	1.403494000	4.162195000
1	2.531290000	2.105641000	4.057918000
6	0.855828000	3.410775000	1.769209000
6	-0.502526000	3.660915000	1.973891000
1	-1.226113000	2.868534000	1.807973000
6	-0.929293000	4.909853000	2.392821000
1	-1.985013000	5.091976000	2.552312000
6	-0.004067000	5.924185000	2.611746000
1	-0.336692000	6.899815000	2.944495000
6	1.346210000	5.683244000	2.405916000
1	2.072339000	6.468310000	2.579249000
6	1.777821000	4.431196000	1.985532000
1	2.836585000	4.252859000	1.840138000
1	-2.686894000	0.156568000	0.671659000
1	-2.030368000	0.314068000	0.340862000

[Ni^{II}L2]:

28	2.428714000	12.607655000	13.801308000
16	1.857954000	12.072570000	11.769362000
16	4.210190000	11.356532000	13.665521000
15	2.784584000	13.016387000	15.919620000
15	0.806695000	14.062840000	13.953896000
6	3.108866000	10.983510000	11.202998000
6	4.153423000	10.637654000	12.067076000
6	5.136326000	9.742307000	11.637960000
1	5.940355000	9.473932000	12.314299000
6	5.085506000	9.207211000	10.361049000
1	5.854072000	8.515524000	10.037998000
6	4.050396000	9.559550000	9.497200000
1	4.007538000	9.143449000	8.497943000
6	3.068942000	10.443153000	9.915352000
1	2.258559000	10.719833000	9.249937000
6	1.742643000	14.443282000	16.454285000
6	0.411541000	14.317923000	15.735801000
6	2.180023000	11.691782000	17.014067000
6	2.186817000	11.856387000	18.402332000
1	2.616832000	12.749756000	18.843379000
6	1.650784000	10.878276000	19.223712000
1	1.661517000	11.012611000	20.298566000
6	1.098446000	9.729723000	18.667650000
1	0.675414000	8.968509000	19.311966000
6	1.088976000	9.558804000	17.290903000
1	0.660076000	8.664160000	16.857020000
6	1.630081000	10.535884000	16.464676000
1	1.632144000	10.410723000	15.385532000
6	4.450693000	13.443582000	16.498507000
6	5.230202000	12.562086000	17.245881000
1	4.834165000	11.593364000	17.528107000
6	6.511678000	12.924891000	17.638004000
1	7.107126000	12.236670000	18.225232000
6	7.026880000	14.163624000	17.283509000
1	8.024376000	14.446699000	17.596311000
6	6.262910000	15.039655000	16.521945000
1	6.662601000	16.004996000	16.236397000
6	4.985841000	14.679140000	16.124851000
1	4.401908000	15.364673000	15.518886000
6	-0.803991000	13.774083000	13.172949000
6	-1.260061000	14.528674000	12.093814000
1	-0.654200000	15.336813000	11.701367000
6	-2.494919000	14.252980000	11.522545000
1	-2.844025000	14.849295000	10.688627000
6	-3.278964000	13.221324000	12.018438000
1	-4.244029000	13.011405000	11.573851000
6	-2.822382000	12.453207000	13.082909000
1	-3.427237000	11.641595000	13.468125000
6	-1.588821000	12.722207000	13.652564000
1	-1.232225000	12.107172000	14.473052000
6	1.339199000	15.736179000	13.467136000
6	2.624478000	15.925170000	12.962933000
1	3.260404000	15.059478000	12.797874000
6	3.085707000	17.204851000	12.681157000
1	4.087602000	17.342714000	12.293901000

6	2.263657000	18.301641000	12.895991000
1	2.622673000	19.300127000	12.677583000
6	0.977352000	18.121553000	13.392564000
1	0.333321000	18.976589000	13.558606000
6	0.517213000	16.846754000	13.680618000
1	-0.487101000	16.715689000	14.069994000
1	1.637645000	14.449542000	17.539792000
1	-0.149233000	13.450501000	16.091345000
1	2.249631000	15.367430000	16.168420000
1	-0.221323000	15.196630000	15.868245000

$[Ni^{I}L2]^{-}$:

28	2.450596000	12.551349000	13.737928000
16	1.656806000	10.924961000	12.355093000
16	4.533534000	12.240425000	12.860488000
15	2.792559000	12.889569000	15.874756000
15	0.874444000	14.075584000	13.868587000
6	3.055717000	10.391172000	11.448707000
6	4.324480000	10.980850000	11.663245000
6	5.413375000	10.529271000	10.906153000
1	6.383675000	10.984363000	11.076674000
6	5.275948000	9.525205000	9.960704000
1	6.137974000	9.197589000	9.390817000
6	4.027561000	8.943757000	9.750717000
1	3.903613000	8.157180000	9.015006000
6	2.937891000	9.376770000	10.489403000
1	1.962155000	8.929559000	10.329127000
6	1.756485000	14.327314000	16.432197000
6	0.448610000	14.277231000	15.664867000
6	2.182194000	11.602122000	17.036127000
6	2.199126000	11.774872000	18.423015000
1	2.650972000	12.664048000	18.851752000
6	1.644656000	10.819693000	19.261038000
1	1.661807000	10.967226000	20.334780000
6	1.064453000	9.676276000	18.722816000
1	0.628103000	8.931667000	19.378221000
6	1.043480000	9.493346000	17.347242000
1	0.591652000	8.603602000	16.924980000
6	1.598224000	10.452498000	16.507831000
1	1.577313000	10.327407000	15.426498000
6	4.432436000	13.350251000	16.531939000
6	5.209763000	12.518854000	17.339116000
1	4.814520000	11.565510000	17.671344000
6	6.486649000	12.902074000	17.729747000
1	7.072987000	12.245605000	18.362078000
6	7.010731000	14.119444000	17.318105000
1	8.004265000	14.419454000	17.628471000
6	6.254575000	14.947631000	16.496279000
1	6.658332000	15.895298000	16.159293000
6	4.984801000	14.561449000	16.100352000
1	4.413843000	15.203521000	15.435730000
6	-0.787846000	13.908411000	13.134209000
6	-1.288428000	14.742317000	12.133622000
1	-0.697858000	15.581823000	11.784978000
6	-2.542202000	14.513211000	11.581538000
1	-2.916622000	15.175637000	10.809698000
6	-3.315497000	13.446206000	12.017101000
1	-4.295723000	13.272084000	11.589944000
6	-2.819359000	12.596051000	12.999167000
1	-3.410070000	11.752986000	13.337698000
6	-1.565411000	12.819358000	13.543410000
1	-1.175052000	12.132630000	14.289305000
6	1.370942000	15.809895000	13.503649000
6	2.662491000	16.042553000	13.033665000
1	3.303497000	15.187711000	12.825683000
6	3.127793000	17.339784000	12.853020000
1	4.135483000	17.505447000	12.490498000

6	2.305467000	18.419916000	13.141952000
1	2.668423000	19.432251000	13.008858000
6	1.013039000	18.201009000	13.605984000
1	0.367092000	19.041562000	13.832468000
6	0.550407000	16.906101000	13.785352000
1	-0.459879000	16.747106000	14.149380000
1	1.607687000	14.307277000	17.513473000
1	-0.144929000	13.410148000	15.965428000
1	2.299878000	15.245183000	16.193999000
1	-0.162537000	15.167372000	15.828174000

[$Ni^{III}H^{-}L2$]:

28	2.069720000	12.064834000	13.996705000
16	1.477103000	10.667051000	12.403578000
16	4.124467000	12.180569000	13.153226000
15	2.527429000	12.648800000	16.107563000
15	0.788386000	14.003463000	13.863973000
6	2.883984000	10.512830000	11.384156000
6	4.065170000	11.197785000	11.714247000
6	5.191201000	11.057502000	10.893891000
1	6.101235000	11.586516000	11.153344000
6	5.147505000	10.248305000	9.773243000
1	6.027805000	10.145372000	9.150574000
6	3.974260000	9.567035000	9.447549000
1	3.937712000	8.932788000	8.570241000
6	2.852769000	9.699722000	10.245267000
1	1.937197000	9.173721000	9.999494000
6	1.482365000	14.125681000	16.505144000
6	0.249914000	14.170592000	15.619097000
6	2.118076000	11.450263000	17.414010000
6	2.154338000	11.827020000	18.760208000
1	2.453575000	12.832461000	19.037716000
6	1.812170000	10.920271000	19.750319000
1	1.837693000	11.223705000	20.789938000
6	1.434970000	9.626826000	19.407989000
1	1.164705000	8.919946000	20.183126000
6	1.403585000	9.242877000	18.075172000
1	1.109760000	8.235998000	17.805924000
6	1.743082000	10.151116000	17.080806000
1	1.710461000	9.858301000	16.036383000
6	4.205878000	13.238940000	16.488610000
6	5.058495000	12.607120000	17.392167000
1	4.726986000	11.729171000	17.933580000
6	6.335302000	13.106526000	17.614001000
1	6.985163000	12.614583000	18.327524000
6	6.776310000	14.230617000	16.930528000
1	7.771234000	14.619577000	17.109324000
6	5.939908000	14.853494000	16.011976000
1	6.281213000	15.725534000	15.467237000
6	4.666631000	14.357410000	15.787975000
1	4.023314000	14.839987000	15.056687000
6	-0.794159000	13.975769000	12.969843000
6	-1.221172000	15.015899000	12.144634000
1	-0.594849000	15.887764000	11.998432000
6	-2.455444000	14.946051000	11.512710000
1	-2.778860000	15.763538000	10.879823000
6	-3.272503000	13.839537000	11.694218000
1	-4.236579000	13.789806000	11.203078000
6	-2.847689000	12.792231000	12.503227000
1	-3.477274000	11.921892000	12.642191000
6	-1.614149000	12.854920000	13.130683000
1	-1.279606000	12.027833000	13.749213000
6	1.547664000	15.623299000	13.513887000
6	2.726736000	15.662694000	12.768762000
1	3.154765000	14.733933000	12.403428000
6	3.365688000	16.871565000	12.526025000
1	4.283797000	16.888872000	11.951571000

6	2.834743000	18.051317000	13.027879000
1	3.336791000	18.993769000	12.845643000
6	1.658306000	18.023808000	13.767522000
1	1.239949000	18.942867000	14.159799000
6	1.016755000	16.818826000	14.008072000
1	0.096048000	16.813481000	14.580966000
1	1.224419000	14.116118000	17.564932000
1	-0.418496000	13.331838000	15.824317000
1	2.101712000	15.009347000	16.335970000
1	-0.322309000	15.085811000	15.776559000
1	0.849291000	11.604246000	14.697004000

$[Ni^{II}H^{-}L2]^{-}$:

28	1.804766000	10.755123000	14.455358000
16	0.669703000	9.465682000	13.117798000
16	3.427389000	10.942997000	12.980169000
15	2.387085000	12.081232000	16.009374000
15	1.600357000	14.625021000	13.754420000
6	1.655902000	9.319124000	11.676958000
6	2.895216000	9.980922000	11.618884000
6	3.683314000	9.844690000	10.471255000
1	4.641481000	10.352431000	10.432162000
6	3.259727000	9.072696000	9.400991000
1	3.888724000	8.976765000	8.523642000
6	2.029310000	8.420976000	9.459211000
1	1.690103000	7.813808000	8.628104000
6	1.237653000	8.547291000	10.589727000
1	0.280047000	8.039736000	10.646321000
6	1.081136000	13.373928000	16.253171000
6	0.432122000	13.815163000	14.951331000
6	2.490063000	11.455638000	17.738762000
6	2.911955000	12.304795000	18.765901000
1	3.220029000	13.319963000	18.536535000
6	2.947876000	11.864505000	20.079830000
1	3.273865000	12.536732000	20.865287000
6	2.569420000	10.562799000	20.386368000
1	2.601557000	10.216699000	21.412799000
6	2.155325000	9.709269000	19.373383000
1	1.862855000	8.692792000	19.608369000
6	2.114539000	10.153394000	18.056389000
1	1.787206000	9.493045000	17.259926000
6	3.986443000	12.984150000	15.943636000
6	5.133979000	12.218725000	15.725609000
1	5.035680000	11.150160000	15.561726000
6	6.389338000	12.808329000	15.709693000
1	7.268580000	12.197297000	15.543760000
6	6.519072000	14.178474000	15.900437000
1	7.498500000	14.641623000	15.884303000
6	5.385746000	14.951856000	16.109098000
1	5.474685000	16.022467000	16.255965000
6	4.130707000	14.357953000	16.134363000
1	3.263241000	14.983996000	16.308496000
6	0.496962000	14.609599000	12.296183000
6	-0.042282000	15.737750000	11.680348000
1	0.155851000	16.723965000	12.086009000
6	-0.843995000	15.609093000	10.552006000
1	-1.261533000	16.495502000	10.088368000
6	-1.116683000	14.354401000	10.025405000
1	-1.746806000	14.256750000	9.149623000
6	-0.573081000	13.223392000	10.625656000
1	-0.773536000	12.237907000	10.220363000
6	0.234262000	13.349126000	11.744024000
1	0.668454000	12.460032000	12.200772000
6	1.586601000	16.377209000	14.313308000
6	2.801748000	17.065133000	14.266556000
1	3.682737000	16.551754000	13.894216000
6	2.900218000	18.380945000	14.699375000
1	3.853639000	18.894569000	14.657238000

6	1.778267000	19.032428000	15.192366000
1	1.851295000	20.057165000	15.537178000
6	0.560467000	18.364421000	15.244054000
1	-0.318713000	18.870422000	15.625861000
6	0.466480000	17.050065000	14.808396000
1	-0.493746000	16.546944000	14.849557000
1	0.334078000	12.885856000	16.883213000
1	0.063335000	12.926474000	14.429945000
1	1.463272000	14.216445000	16.835167000
1	-0.431538000	14.456185000	15.144509000
1	0.694197000	10.615564000	15.443680000

Ni-SIa + H_2:

28	57.901551000	47.769961000	85.189003000
26	57.812178000	49.775728000	86.804224000
1	56.744597000	47.838236000	86.318126000
6	56.067251000	49.985257000	87.427770000
7	54.987902000	50.068967000	87.900242000
6	58.189258000	49.024224000	88.480239000
7	58.299724000	48.559572000	89.560270000
6	58.307618000	51.389518000	87.137544000
8	58.692304000	52.475659000	87.327402000
16	58.417130000	47.036521000	83.070129000
6	58.939776000	48.513185000	82.108746000
1	59.658289000	49.076196000	82.720859000
1	58.074542000	49.173267000	81.956911000
6	59.537213000	48.120340000	80.773552000
1	59.864856000	49.007035000	80.216443000
1	60.403551000	47.458589000	80.894750000
1	58.802854000	47.591538000	80.152974000
16	58.610183000	45.738306000	85.848190000
6	57.936585000	45.557674000	87.543584000
1	58.087562000	46.489756000	88.104355000
1	56.852979000	45.392563000	87.482860000
6	58.608105000	44.405924000	88.262945000
1	58.193402000	44.283572000	89.272322000
1	58.475581000	43.458329000	87.726322000
1	59.686960000	44.577908000	88.364615000
16	59.769946000	49.055588000	85.810973000
6	60.853708000	48.008142000	86.850758000
1	61.340277000	48.651307000	87.592526000
1	60.224329000	47.294447000	87.393231000
6	61.844344000	47.305363000	85.947388000
1	62.496077000	48.020117000	85.430258000
1	61.309828000	46.719294000	85.190589000
1	62.481242000	46.621047000	86.522244000
16	57.184978000	49.844960000	84.532431000
6	55.358856000	49.707747000	84.317721000
1	54.915661000	50.598520000	84.778505000
1	54.991814000	48.840195000	84.876683000
6	54.935578000	49.635836000	82.865712000
1	55.316323000	50.508900000	82.311603000
1	53.838715000	49.695368000	82.832655000
7	55.335498000	48.402792000	82.203580000
1	56.091525000	47.853621000	82.620146000
6	54.740232000	48.029534000	81.044277000
8	53.884416000	48.726603000	80.495190000
6	55.048758000	46.651296000	80.469731000
1	54.865345000	46.699290000	79.391672000
1	54.263288000	45.991791000	80.880073000
7	56.364117000	46.092865000	80.694401000
1	56.883948000	46.336068000	81.545005000
6	56.896353000	45.140588000	79.880787000
8	56.327447000	44.730827000	78.867790000
6	58.257595000	44.612391000	80.308041000
1	58.980635000	44.810941000	79.509484000
1	58.192586000	43.525158000	80.418096000
1	58.625032000	45.051765000	81.240456000
8	52.314571000	48.211302000	84.431865000

8	52.708803000	46.131753000	83.659527000
6	52.168528000	47.271670000	83.595953000
6	51.273427000	47.542422000	82.391291000
1	51.876249000	47.989404000	81.590594000
1	50.478894000	48.252849000	82.640158000
1	50.840757000	46.614372000	82.005476000
1	53.225400000	47.837562000	85.794205000
7	53.744037000	47.589036000	86.675097000
1	54.127703000	48.340705000	87.247237000
6	53.903503000	46.310602000	86.992160000
7	53.432916000	45.372957000	86.163084000
1	53.178241000	45.654043000	85.181471000
1	53.697576000	44.414111000	86.325267000
7	54.507676000	45.941230000	88.139020000
1	54.580442000	44.950754000	88.313803000
6	55.110286000	46.848392000	89.103162000
1	55.789909000	46.249578000	89.721405000
1	55.751942000	47.572970000	88.575115000
6	54.097529000	47.580871000	89.966688000
1	53.499675000	46.851739000	90.533788000
1	53.385997000	48.103714000	89.311628000
6	54.734301000	48.591178000	90.912028000
1	55.230520000	48.076997000	91.746888000
1	55.531774000	49.136130000	90.376225000
6	53.720381000	49.590540000	91.442975000
1	54.170611000	50.233576000	92.215058000
1	52.877306000	49.081946000	91.933077000
7	53.197562000	50.387759000	90.353921000
1	53.764578000	50.459087000	89.503438000
6	51.975018000	50.954033000	90.378785000
8	51.201027000	50.888864000	91.334248000
6	51.535825000	51.580494000	89.056713000
1	50.725158000	52.282023000	89.312325000
6	51.053982000	50.514847000	88.066170000
1	51.707992000	49.632430000	88.141706000
1	50.031217000	50.186159000	88.276417000
6	51.235304000	51.170312000	86.705019000
1	51.273302000	50.447528000	85.881871000
1	50.410051000	51.867892000	86.506359000
6	52.546283000	51.926479000	86.865545000
1	53.400683000	51.278117000	86.625100000
1	52.606661000	52.822297000	86.234721000
7	52.574468000	52.280471000	88.290587000
6	53.304930000	53.274058000	88.873338000
8	53.175379000	53.527793000	90.073502000
6	54.226539000	54.094270000	87.980195000
1	54.595311000	54.899259000	88.626636000
1	53.605127000	54.580339000	87.212044000
6	55.408228000	53.392999000	87.314974000
1	56.018658000	52.861192000	88.054620000
1	55.112923000	52.654078000	86.563603000
1	56.058854000	54.127379000	86.826766000
1	57.325975000	47.248638000	90.873979000
8	57.315965000	46.549419000	91.551386000
6	58.658284000	46.473143000	91.991801000
1	58.823768000	45.469431000	92.404354000
1	59.345242000	46.587625000	91.135640000

6	58.998912000	47.491052000	93.065976000
1	60.034742000	47.322140000	93.402282000
1	58.362804000	47.338090000	93.948801000
7	58.819980000	48.856043000	92.609104000
1	58.734553000	49.017416000	91.603498000
6	58.653036000	49.874951000	93.485124000
8	58.720955000	49.733399000	94.705376000
6	58.214461000	51.210847000	92.881263000
1	58.481938000	51.977457000	93.623356000
6	56.707274000	51.188436000	92.592698000
1	56.115409000	51.464889000	93.471275000
1	56.420653000	50.165055000	92.312583000
6	56.526187000	52.115056000	91.398371000
1	56.496828000	53.164149000	91.724340000
1	55.599100000	51.926229000	90.842965000
6	57.773968000	51.850088000	90.569887000
1	57.633794000	50.987533000	89.901824000
1	58.064983000	52.702381000	89.946807000
7	58.800722000	51.559836000	91.582459000
6	60.134798000	51.849965000	91.519892000
8	60.844955000	51.741479000	92.522766000
6	60.715213000	52.234758000	90.170969000
1	60.050843000	52.899200000	89.603034000
1	61.633232000	52.799512000	90.386964000
6	61.067511000	51.011191000	89.302295000
1	60.122664000	50.539116000	88.989061000
6	61.839043000	49.990961000	90.128120000
1	62.163363000	49.141094000	89.514703000
1	62.735023000	50.437614000	90.580373000
1	61.230676000	49.586673000	90.945533000
6	61.814511000	51.438694000	88.034553000
1	62.760224000	51.942972000	88.280861000
1	62.055031000	50.580965000	87.394639000
1	61.210390000	52.137045000	87.445085000
6	58.796475000	55.619253000	90.256873000
1	58.985021000	56.669812000	90.514069000
1	58.029896000	55.245896000	90.946459000
1	59.718512000	55.063869000	90.469787000
6	58.353053000	55.467891000	88.796835000
1	57.387675000	55.978928000	88.660810000
1	58.158010000	54.408903000	88.575227000
6	59.342311000	56.005900000	87.740433000
1	59.507680000	57.077458000	87.952836000
6	60.704788000	55.295204000	87.792925000
1	60.576711000	54.222130000	87.602423000
1	61.381668000	55.685641000	87.023007000
1	61.201097000	55.408889000	88.764775000
6	58.740818000	55.882551000	86.330769000
1	59.416401000	56.289205000	85.569233000
1	57.780111000	56.408070000	86.252302000
1	58.570940000	54.828475000	86.071861000
6	59.231587000	54.500050000	82.117655000
1	59.966220000	54.733203000	81.331638000
1	58.471314000	53.869570000	81.637712000
6	59.900357000	53.710516000	83.195733000
7	60.959438000	54.209381000	83.916125000
6	61.289905000	53.257721000	84.766012000

1	62.095025000	53.303066000	85.494579000
7	60.500074000	52.164655000	84.628210000
1	60.538238000	51.293297000	85.156612000
6	59.598698000	52.435912000	83.631168000
1	58.839296000	51.716582000	83.341227000
6	58.602650000	55.796772000	82.608505000
1	58.140701000	56.357509000	81.787793000
1	57.830069000	55.604034000	83.362504000
1	59.357414000	56.440799000	83.074189000
1	56.459395000	47.311311000	85.660520000

TS:

28	57.898410000	47.792186000	85.190639000
26	57.803462000	49.768260000	86.798728000
1	56.923341000	47.978412000	86.397398000
6	56.066163000	49.998576000	87.436426000
7	54.990273000	50.087738000	87.914725000
6	58.197139000	49.029216000	88.476439000
7	58.314020000	48.569319000	89.557450000
6	58.314010000	51.382418000	87.131478000
8	58.698055000	52.466976000	87.324328000
16	58.434711000	47.055626000	83.088005000
6	58.956468000	48.524585000	82.113594000
1	59.684376000	49.085321000	82.716429000
1	58.092790000	49.187611000	81.967822000
6	59.537213000	48.120340000	80.773552000
1	59.862519000	49.002680000	80.208554000
1	60.401920000	47.455419000	80.888626000
1	58.793093000	47.592003000	80.164317000
16	58.573370000	45.755608000	85.862810000
6	57.918900000	45.559610000	87.564066000
1	58.072514000	46.487145000	88.130770000
1	56.836571000	45.388118000	87.513409000
6	58.608105000	44.405924000	88.262945000
1	58.208812000	44.273969000	89.277232000
1	58.473465000	43.461573000	87.721163000
1	59.687285000	44.583837000	88.350588000
16	59.803985000	49.101177000	85.797294000
6	60.853403000	48.021585000	86.839827000
1	61.342670000	48.644142000	87.597354000
1	60.202611000	47.313374000	87.364218000
6	61.844344000	47.305363000	85.947388000
1	62.515577000	48.010353000	85.441779000
1	61.310352000	46.731867000	85.180369000
1	62.461555000	46.607716000	86.527820000
16	57.181149000	49.866230000	84.527508000
6	55.355429000	49.723199000	84.320131000
1	54.909572000	50.613679000	84.779042000
1	54.997708000	48.854995000	84.883676000
6	54.927792000	49.644359000	82.870079000
1	55.302836000	50.516752000	82.311107000
1	53.830574000	49.698595000	82.839906000
7	55.332808000	48.410884000	82.211785000
1	56.080195000	47.858663000	82.638107000
6	54.741430000	48.033914000	81.051947000
8	53.888294000	48.730171000	80.497658000
6	55.051222000	46.654484000	80.481787000
1	54.868029000	46.699833000	79.403680000
1	54.266753000	45.995315000	80.893803000
7	56.367292000	46.096258000	80.705723000
1	56.886932000	46.337345000	81.556274000
6	56.896574000	45.145497000	79.887745000
8	56.324087000	44.740573000	78.874985000
6	58.257595000	44.612391000	80.308041000
1	58.978676000	44.812184000	79.508118000
1	58.190418000	43.525051000	80.415017000
1	58.629397000	45.047261000	81.241091000

8	52.320964000	48.211045000	84.428367000
8	52.735525000	46.141292000	83.640107000
6	52.180590000	47.274669000	83.587787000
6	51.273427000	47.542422000	82.391291000
1	51.866675000	47.997213000	81.587796000
1	50.474721000	48.244946000	82.649032000
1	50.845819000	46.612188000	82.005021000
1	53.245810000	47.846906000	85.786284000
7	53.764419000	47.598512000	86.666665000
1	54.142621000	48.348858000	87.243592000
6	53.917392000	46.319576000	86.984127000
7	53.452983000	45.384040000	86.149193000
1	53.206387000	45.665728000	85.166152000
1	53.712280000	44.424144000	86.313461000
7	54.504921000	45.947721000	88.138758000
1	54.578574000	44.956801000	88.310561000
6	55.108756000	46.852481000	89.104367000
1	55.785738000	46.251640000	89.723527000
1	55.752976000	47.575832000	88.577727000
6	54.097042000	47.587033000	89.967019000
1	53.495685000	46.859446000	90.532373000
1	53.388552000	48.113405000	89.311486000
6	54.737116000	48.593285000	90.914353000
1	55.233268000	48.075617000	91.747248000
1	55.535168000	49.137690000	90.378778000
6	53.726356000	49.594004000	91.448990000
1	54.180374000	50.236130000	92.219610000
1	52.883989000	49.086685000	91.941564000
7	53.201465000	50.392103000	90.361667000
1	53.768572000	50.466064000	89.511302000
6	51.977534000	50.954948000	90.386733000
8	51.203205000	50.887447000	91.341863000
6	51.536242000	51.579750000	89.064499000
1	50.725425000	52.281036000	89.320334000
6	51.053240000	50.512123000	88.076587000
1	51.708114000	49.630283000	88.152162000
1	50.031156000	50.183003000	88.289406000
6	51.231643000	51.165325000	86.713987000
1	51.268540000	50.441004000	85.892177000
1	50.405698000	51.862151000	86.515531000
6	52.542636000	51.922192000	86.870974000
1	53.396783000	51.273278000	86.630832000
1	52.602216000	52.816513000	86.237956000
7	52.572797000	52.279346000	88.295088000
6	53.305552000	53.273104000	88.874733000
8	53.179923000	53.528161000	90.075004000
6	54.224078000	54.092619000	87.977642000
1	54.590248000	54.901735000	88.620415000
1	53.600841000	54.573005000	87.207436000
6	55.408229000	53.392999000	87.314974000
1	56.024035000	52.871318000	88.057443000
1	55.115042000	52.646114000	86.570635000
1	56.052480000	54.127570000	86.818610000
1	57.341789000	47.249120000	90.860411000
8	57.335875000	46.543140000	91.530716000
6	58.677640000	46.471418000	91.972926000
1	58.846678000	45.466620000	92.381373000

1	59.365735000	46.592569000	91.118518000
6	59.012663000	47.485763000	93.052383000
1	60.047681000	47.317265000	93.391459000
1	58.373746000	47.327941000	93.932334000
7	58.833383000	48.852395000	92.600501000
1	58.747394000	49.017055000	91.595369000
6	58.665368000	49.868009000	93.479975000
8	58.732849000	49.722407000	94.699821000
6	58.224837000	51.205382000	92.880463000
1	58.487876000	51.969658000	93.626596000
6	56.718703000	51.179497000	92.587420000
1	56.123337000	51.448340000	93.465999000
1	56.436888000	50.156903000	92.299933000
6	56.537599000	52.112985000	91.398520000
1	56.502749000	53.159750000	91.731418000
1	55.613118000	51.923943000	90.838815000
6	57.789170000	51.859960000	90.571818000
1	57.654534000	51.005581000	89.892296000
1	58.079937000	52.721299000	89.961212000
7	58.813248000	51.561394000	91.584609000
6	60.147192000	51.852779000	91.524717000
8	60.856488000	51.742510000	92.527902000
6	60.727476000	52.239116000	90.176210000
1	60.065474000	52.908658000	89.611434000
1	61.649147000	52.798150000	90.391499000
6	61.070119000	51.014921000	89.304732000
1	60.121960000	50.547319000	88.995353000
6	61.839043000	49.990962000	90.128120000
1	62.159218000	49.140416000	89.513490000
1	62.737415000	50.433835000	90.579402000
1	61.230301000	49.588029000	90.945966000
6	61.814512000	51.438693000	88.034552000
1	62.765673000	51.934178000	88.278169000
1	62.043788000	50.580311000	87.391714000
1	61.214376000	52.143863000	87.449366000
6	58.796475000	55.619253000	90.256874000
1	58.987887000	56.669568000	90.512939000
1	58.028208000	55.249183000	90.946352000
1	59.716839000	55.061601000	90.470974000
6	58.353054000	55.467890000	88.796832000
1	57.387624000	55.978770000	88.660803000
1	58.158017000	54.408807000	88.574808000
6	59.342311000	56.005903000	87.740433000
1	59.507534000	57.077450000	87.952925000
6	60.704788000	55.295203000	87.792925000
1	60.576914000	54.222520000	87.600462000
1	61.382185000	55.686767000	87.024019000
1	61.200420000	55.407300000	88.765336000
6	58.740817000	55.882548000	86.330769000
1	59.415526000	56.291202000	85.569530000
1	57.778932000	56.405953000	86.252846000
1	58.573433000	54.828258000	86.070873000
6	59.243008000	54.504277000	82.121147000
1	59.975808000	54.741878000	81.334714000
1	58.488333000	53.866156000	81.642440000
6	59.918290000	53.722699000	83.201111000
7	60.972290000	54.232092000	83.921542000

6	61.310989000	53.283921000	84.772463000
1	62.114829000	53.337165000	85.501945000
7	60.531787000	52.183571000	84.635474000
1	60.576741000	51.311151000	85.163696000
6	59.628785000	52.445524000	83.637664000
1	58.875393000	51.719562000	83.348194000
6	58.602650000	55.796773000	82.608506000
1	58.136517000	56.351825000	81.786300000
1	57.831196000	55.599017000	83.362383000
1	59.351592000	56.448139000	83.073409000
1	56.532001000	47.351191000	85.627015000

Transient Dihydride structure in [NiFe] hydrogenase:

28	57.806196000	47.734412000	85.128087000
26	57.751475000	49.701468000	86.775759000
1	57.166040000	48.060626000	86.533481000
6	56.037627000	49.964385000	87.458307000
7	54.972540000	50.073229000	87.954824000
6	58.208223000	48.995908000	88.451793000
7	58.367258000	48.537244000	89.527606000
6	58.281085000	51.325302000	87.100845000
8	58.663243000	52.407724000	87.303919000
16	58.486806000	47.041070000	83.078792000
6	58.964500000	48.525405000	82.115760000
1	59.688609000	49.099486000	82.710128000
1	58.083904000	49.167419000	81.980120000
6	59.537213000	48.120340000	80.773552000
1	59.849150000	49.003169000	80.202050000
1	60.410212000	47.465820000	80.884496000
1	58.793822000	47.582330000	80.172282000
16	58.438681000	45.702946000	85.847910000
6	57.843666000	45.514291000	87.569700000
1	57.976819000	46.459489000	88.109739000
1	56.769919000	45.295265000	87.555696000
6	58.608105000	44.405924000	88.262945000
1	58.250880000	44.281638000	89.293570000
1	58.495186000	43.444625000	87.746553000
1	59.680951000	44.631577000	88.308123000
16	59.745960000	49.043674000	85.721866000
6	60.777291000	47.973808000	86.788094000
1	61.194755000	48.595603000	87.589109000
1	60.120327000	47.232244000	87.257230000
6	61.844344000	47.305363000	85.947388000
1	62.502640000	48.038867000	85.466066000
1	61.375954000	46.700851000	85.161157000
1	62.468030000	46.642936000	86.561123000
16	57.085178000	49.820866000	84.528356000
6	55.260159000	49.685692000	84.344703000
1	54.818716000	50.578916000	84.802460000
1	54.914280000	48.818480000	84.916064000
6	54.832290000	49.599327000	82.896431000
1	55.202531000	50.469487000	82.331426000
1	53.734810000	49.644990000	82.862917000
7	55.256934000	48.364960000	82.251509000
1	55.960298000	47.796031000	82.722213000
6	54.707535000	47.987433000	81.071146000
8	53.890503000	48.695121000	80.479087000
6	55.018292000	46.594963000	80.536041000
1	54.797878000	46.600920000	79.464425000
1	54.264420000	45.934578000	81.000822000
7	56.354662000	46.073768000	80.731147000
1	56.891898000	46.342347000	81.562381000
6	56.874003000	45.110001000	79.921753000
8	56.276511000	44.668892000	78.939243000
6	58.257595000	44.612391000	80.308041000
1	58.956320000	44.838813000	79.495288000
1	58.222748000	43.522867000	80.406207000
1	58.638461000	45.048814000	81.236187000

8	52.252036000	48.186563000	84.468771000
8	52.714958000	46.134881000	83.660544000
6	52.147613000	47.262487000	83.610263000
6	51.273427000	47.542422000	82.391291000
1	51.878590000	48.038225000	81.621633000
1	50.448175000	48.215318000	82.644698000
1	50.883188000	46.614340000	81.962542000
1	53.185967000	47.836353000	85.838721000
7	53.705999000	47.590221000	86.716437000
1	54.120654000	48.337103000	87.272356000
6	53.880912000	46.310914000	87.018401000
7	53.414119000	45.376617000	86.181876000
1	53.170728000	45.660163000	85.199529000
1	53.682355000	44.418126000	86.339726000
7	54.478323000	45.934560000	88.166188000
1	54.576445000	44.942791000	88.318997000
6	55.094093000	46.833983000	89.129748000
1	55.769254000	46.225809000	89.743241000
1	55.739232000	47.554476000	88.600682000
6	54.092143000	47.569996000	90.001678000
1	53.493620000	46.843593000	90.571639000
1	53.379203000	48.099261000	89.353486000
6	54.742230000	48.573960000	90.944690000
1	55.249307000	48.055032000	91.770776000
1	55.535072000	49.119095000	90.402801000
6	53.732765000	49.572827000	91.486998000
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1	52.889256000	49.062191000	91.974613000
7	53.210694000	50.379658000	90.403966000
1	53.771000000	50.443983000	89.547700000
6	51.993116000	50.955234000	90.437139000
8	51.225645000	50.898319000	91.398690000
6	51.545855000	51.580116000	89.116533000
1	50.743047000	52.288620000	89.377711000
6	51.044966000	50.512210000	88.137894000
1	51.691906000	49.624737000	88.213005000
1	50.021645000	50.193912000	88.361056000
6	51.217531000	51.156272000	86.770173000
1	51.242462000	50.427214000	85.952086000
1	50.394933000	51.857758000	86.574074000
6	52.534674000	51.905527000	86.912204000
1	53.383324000	51.250712000	86.668320000
1	52.594077000	52.796118000	86.273875000
7	52.579294000	52.270042000	88.333798000
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8	53.206010000	53.526977000	90.100527000
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1	53.591606000	54.559620000	87.224940000
6	55.408228000	53.392999000	87.314974000
1	56.037027000	52.878380000	88.050908000
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8	57.445821000	46.462604000	91.408085000
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1	58.937386000	45.451430000	92.365949000

1	59.496850000	46.613219000	91.154330000
6	58.957933000	47.467823000	93.059403000
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8	58.692273000	49.701701000	94.696469000
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1	58.495519000	51.955962000	93.621337000
6	56.699334000	51.195421000	92.604163000
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1	56.393076000	50.173440000	92.342541000
6	56.521068000	52.105692000	91.396593000
1	56.506684000	53.160151000	91.705772000
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7	58.792114000	51.540017000	91.578141000
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6	61.066037000	51.009370000	89.300963000
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6	59.200703000	54.486162000	82.116754000
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6	59.870025000	53.691968000	83.191094000
7	60.933107000	54.186951000	83.907848000

6	61.266130000	53.232071000	84.753401000
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7	60.474628000	52.140558000	84.616091000
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1	59.374671000	56.425956000	83.066016000
1	56.532420000	47.068234000	84.970297000

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