

SUPPORTING INFORMATION

Oxygen Reduction Reaction on [NiFe] Hydrogenases

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B3LYP Calculations

The single point energy calculation by B3LYP hybrid functional has been done (see **Fig. S1**). Except the O₂ binding step and the first H⁺/e⁻ injection showing a different trend with the BP86 result, the rest steps follow a similar plus-minus trend. Moreover, the **Ni-A** state is -47.2 kcal/mol lower with the **Ni-OOH-Fe** state, which also agrees with our hypothesis on the difficult reactivation for the **Ni-A** state.

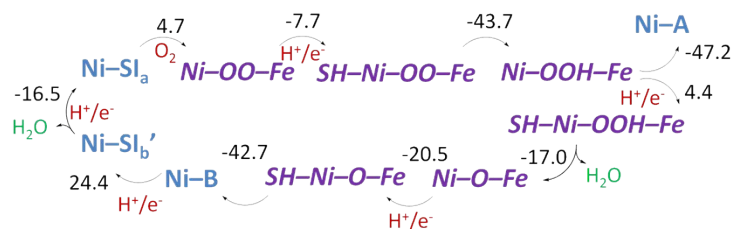


Fig S1. Total energy diagram for the ORR path along the [NiFe] hydrogenases by B3LYP single point energy calculation. (Note: The pH correction was not included for the H⁺/e⁻ injection steps)

Cartesian Coordinates

Frozen atoms are indicated by -1. The frozen atoms are the same for all systems.

Ni-SI_a state:

Free Energy: -4981.496567 a.u.

Charge, Multiplicity: -2, 1

Ni	0	58.21572300	47.04912900	84.89689800
Fe	0	57.45770500	48.97015300	86.77683900
C	0	57.93214700	48.60692700	88.57960300
C	0	57.25778200	50.63671100	87.07796300
C	0	55.63518400	48.55953700	87.13215800
N	0	58.28239400	48.40575500	89.68843300
O	0	57.14306100	51.79379700	87.26864100
N	0	54.49784900	48.30394300	87.31363500
C	-1	60.58610300	47.64972500	81.30907900
C	0	59.86953300	47.66728100	82.65352100
S	0	58.51334600	46.41918200	82.73696100
C	-1	55.00862200	49.12590500	82.52908000
C	0	55.37186900	48.62292900	83.94714100
S	0	57.13187700	48.96935100	84.44512500
C	-1	58.66838400	44.02194700	88.31142600
C	0	58.12693800	45.16200200	87.43221400
S	0	58.77802800	45.08806300	85.70603600
C	-1	62.19421100	47.81862300	86.78557000
C	0	60.71935000	47.82378000	87.27690100
S	0	59.49670100	48.43892100	86.03171500
H	0	62.38796300	48.66739600	86.09419400
H	-1	62.81971900	47.95843300	87.66639700
H	0	62.45419600	46.87826300	86.25961600
H	0	61.30398900	48.49610200	81.20482400
H	0	61.14476200	46.69972100	81.15704800
H	-1	59.84029200	47.71240600	80.51650800
H	-1	59.74340600	44.12117800	88.45971500
H	0	58.18193200	44.03455100	89.31299000
H	0	58.47855800	43.02822400	87.84805000
H	0	55.40205400	48.44199100	81.74836300
H	-1	53.91945800	49.25522500	82.39862900
H	0	55.46804300	50.12351000	82.34951000
H	0	60.58227800	48.48612400	88.15544300
H	0	60.39163400	46.81372400	87.58890900
H	0	58.36668100	46.15320100	87.87501800
H	0	57.01925900	45.12276300	87.38936100
H	0	60.58639600	47.47951900	83.47987600
H	0	59.43242800	48.66977000	82.84440600
H	0	55.20857200	47.53223300	84.05415800
H	0	54.75630400	49.10929300	84.73002600

Ni-OO-Fe state:

Free Energy: -5131.906436 a.u.

Charge, Multiplicity: -2, 1

Ni	0	58.34075200	47.50610000	85.23805700
Fe	0	58.04719800	50.29573400	86.20321500
C	0	58.83464400	50.95244300	87.80400000
C	0	58.35097500	51.80359000	85.45525400
C	0	56.29607300	50.84695000	86.68215800
N	0	59.39155200	51.39360600	88.74373400
O	0	58.55844200	52.83817700	84.94246300
N	0	55.18640300	51.17414600	86.90650700
C	-1	60.58606500	47.64967800	81.30913700
C	0	59.99288800	47.90567600	82.67375000
S	0	58.81731500	46.61555100	83.19998300
C	-1	55.00863900	49.12581200	82.52913500
C	0	55.45856400	49.08950600	84.01222700
S	0	57.29729400	49.30324100	84.19189600
C	-1	58.66846600	44.02216900	88.31108500
C	0	58.04885700	45.17912400	87.52507900
S	0	58.87903900	45.47104700	85.92884600
C	-1	62.19418000	47.81852400	86.78556100
C	0	60.90051400	48.64198600	87.05162800
S	0	59.94731100	49.10228000	85.58239400
H	0	62.74486000	48.20068700	85.89976800
H	-1	62.81970100	47.95850500	87.66639900
H	0	61.96212700	46.74566000	86.62491300
H	0	61.38049800	48.39671100	81.07341300
H	0	61.05179300	46.64046600	81.24924700
H	-1	59.84029400	47.71242400	80.51650700
H	-1	59.74338500	44.12104600	88.45995500
H	0	58.19577100	43.92654200	89.31702500
H	0	58.51806200	43.04916200	87.78834900
H	0	55.32961400	48.20729000	81.99370600
H	-1	53.91946600	49.25528300	82.39862500
H	0	55.49247800	49.98394400	82.01292000
H	0	61.11521900	49.60458000	87.56317900
H	0	60.16400200	48.13010000	87.72891900
H	0	58.09386600	46.15223300	88.08373200
H	0	56.97079200	44.97607600	87.33911400
H	0	60.79873500	47.95934300	83.43169600
H	0	59.47686700	48.88916900	82.70027600
H	0	55.17737700	48.13496700	84.50186700
H	0	55.00528500	49.90844100	84.60877100
O	0	57.67044100	48.30152900	86.89146400
O	0	58.15663000	47.99420400	88.10624700

SH-Ni-OO-Fe state:

Free Energy: -5132.487007 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.13065400	47.63280700	85.16979500
Fe	0	58.05634300	50.39333900	86.14822000
C	0	58.80289900	50.92335200	87.81648000
C	0	58.57563700	51.87157400	85.46537200
C	0	56.35195400	51.12672900	86.55495900
N	0	59.33714000	51.27429500	88.80671200

O	0	58.93253500	52.88913300	84.99962800
N	0	55.27774300	51.57708000	86.73868900
C	-1	60.58606500	47.64967800	81.30913700
C	0	59.98158600	47.90208500	82.67355300
S	0	58.74134200	46.65808300	83.17325200
C	-1	55.00863900	49.12581200	82.52913500
C	0	55.46175000	49.43106300	83.97099500
S	0	57.30180600	49.47802700	84.11828500
C	-1	58.66846600	44.02216900	88.31108500
C	0	58.02084100	45.21770700	87.62042000
S	0	58.58774100	45.52548700	85.89686800
C	-1	62.19418000	47.81852400	86.78556100
C	0	60.85630600	48.55674400	87.08089400
S	0	60.00695400	49.14658800	85.58340900
H	0	62.71413700	48.27768700	85.91778200
H	-1	62.81970100	47.95850500	87.66639900
H	0	62.05958500	46.73712900	86.56996900
H	0	61.38067200	48.39899600	81.08254700
H	0	61.05219800	46.64019700	81.24646600
H	-1	59.84029400	47.71242400	80.51650700
H	-1	59.74338500	44.12104600	88.45995500
H	0	58.21929200	43.87544600	89.32013300
H	0	58.51014500	43.07875100	87.74087900
H	0	55.28991500	48.09330300	82.23148400
H	-1	53.91946600	49.25528300	82.39862500
H	0	55.51014700	49.81499900	81.81524900
H	0	61.03048300	49.45123200	87.71455000
H	0	60.13355200	47.93529400	87.66130100
H	0	58.11320400	46.19988400	88.14523200
H	0	56.92962800	45.05255600	87.49337200
H	0	60.76746900	47.93596700	83.45235700
H	0	59.48826300	48.89699400	82.69945200
H	0	55.07440000	48.68928100	84.69797700
H	0	55.10647000	50.42213600	84.32255700
O	0	57.41886200	48.46285700	86.74802100
O	0	57.76559300	48.06215400	87.99065100
H	0	59.89327300	45.72932100	86.21172800

TS1 state (transition state between SH-Ni-OO-Fe and Ni-OOH-Fe):

Free Energy: -5132.484282 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.21781700	47.53130700	85.14952100
Fe	0	57.99627100	50.28010700	86.22168800
C	0	58.74579800	50.83114100	87.88253700
C	0	58.39844000	51.80826400	85.56141800
C	0	56.25441000	50.87866000	86.68082900
N	0	59.27670000	51.19909100	88.86818600
O	0	58.67669200	52.85820800	85.11538300
N	0	55.15281100	51.24388100	86.89037300
C	-1	60.58606500	47.64967800	81.30913700
C	0	59.95374200	47.84229900	82.67336000
S	0	58.63493700	46.63690400	83.07570900

C	-1	55.00863900	49.12581200	82.52913500
C	0	55.44189400	49.21287000	84.00879800
S	0	57.27986000	49.34931800	84.19093900
C	-1	58.66846600	44.02216900	88.31108500
C	0	58.03171500	45.07469800	87.39508300
S	0	59.14874600	45.69842500	86.07041800
C	-1	62.19418000	47.81852400	86.78556100
C	0	60.90388300	48.64253900	87.05896500
S	0	60.03360100	49.20186100	85.56564500
H	0	62.73980200	48.22143000	85.90569700
H	-1	62.81970100	47.95850500	87.66639900
H	0	62.00300700	46.74070600	86.60449000
H	0	61.36225600	48.42611200	81.11649800
H	0	61.07535600	46.65322900	81.21984000
H	-1	59.84029400	47.71242400	80.51650700
H	-1	59.74338500	44.12104600	88.45995500
H	0	58.19026900	44.03995900	89.31596700
H	0	58.52957500	42.99465300	87.90419600
H	0	55.32127300	48.16057800	82.07754900
H	-1	53.91946600	49.25528300	82.39862500
H	0	55.50249500	49.93048900	81.94179600
H	0	61.13439300	49.55350200	87.64886100
H	0	60.16806300	48.09388500	87.70115900
H	0	57.74097200	46.01784700	87.92493800
H	0	57.14307900	44.67461000	86.86632700
H	0	60.72407900	47.79132400	83.46715400
H	0	59.51183300	48.85873800	82.74635300
H	0	55.10228600	48.33487400	84.59386800
H	0	55.02965900	50.11001300	84.51647700
O	0	57.53972400	48.32369900	86.79324800
O	0	57.89603400	47.90164400	88.03066900
H	0	59.89633000	46.37333200	86.99150100

Ni-OOH-Fe state:

Free Energy: -5132.536856 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.04550400	47.49752100	85.13740000
Fe	0	57.86487400	50.17127800	86.28758400
C	0	58.34985900	50.29729800	88.11110600
C	0	58.59510700	51.67802500	85.90429400
C	0	56.20351500	51.05256100	86.58707300
N	0	58.64856800	50.26339100	89.25210600
O	0	59.08872900	52.71069200	85.65168600
N	0	55.19768300	51.60867100	86.72372600
C	-1	60.58609400	47.64975500	81.30908600
C	0	59.97583800	47.88649800	82.68215600
S	0	58.72225400	46.63455000	83.14622500
C	-1	55.00860100	49.12591400	82.52906500
C	0	55.48010500	49.42473000	83.96388000
S	0	57.31855000	49.47892300	84.11345100
C	-1	58.66838500	44.02193600	88.31142400
C	0	58.07390400	45.28767400	87.67412800

S	0	58.63233400	45.49181200	85.93087000
C	-1	62.19422300	47.81862300	86.78559600
C	0	60.77565200	48.33160900	87.16217400
S	0	59.81295400	48.95916500	85.73404500
H	0	62.62820400	48.42490300	85.96160200
H	-1	62.81973500	47.95842700	87.66638700
H	0	62.17688300	46.75689200	86.46794500
H	0	61.37483900	48.40704200	81.09141200
H	0	61.05879100	46.64425400	81.24121900
H	-1	59.84029400	47.71237800	80.51650300
H	-1	59.74340500	44.12118500	88.45972000
H	0	58.20764500	43.82873100	89.30832900
H	0	58.49354100	43.12309300	87.67912000
H	0	55.28600300	48.09427500	82.22478800
H	-1	53.91945900	49.25522400	82.39862400
H	0	55.50339400	49.81538500	81.81007000
H	0	60.83163000	49.17553500	87.88048300
H	0	60.18402400	47.53418200	87.65401000
H	0	58.36119500	46.18572100	88.25521000
H	0	56.96572100	45.25809500	87.70466100
H	0	60.76607500	47.88219600	83.45894100
H	0	59.50362400	48.89069800	82.72659300
H	0	55.11401400	48.68646200	84.70584700
H	0	55.13148500	50.41580900	84.31943100
O	0	56.93179500	48.34503500	86.51606100
O	0	56.78259500	47.86924800	87.90002300
H	0	57.29604800	48.56234000	88.37953900

SH-Ni-OOH-Fe state:

Free Energy: -5133.108464 a.u.

Charge, Multiplicity: -2, 1

Ni	0	57.98288500	47.62468800	85.10212100
Fe	0	57.97230300	50.36674900	86.13693800
C	0	58.54454500	50.66510800	87.91724500
C	0	58.65121500	51.85035800	85.60807700
C	0	56.29656400	51.21657400	86.45720100
N	0	58.89751900	50.73146500	89.04332300
O	0	59.11077800	52.87119100	85.25410300
N	0	55.26153000	51.75969600	86.61292900
C	-1	60.58607100	47.64971000	81.30910700
C	0	59.97870800	47.90578500	82.68127500
S	0	58.69481300	46.69075800	83.17516200
C	-1	55.00863800	49.12553700	82.52920700
C	0	55.49134500	49.55902000	83.92223000
S	0	57.32942300	49.51295000	84.06460000
C	-1	58.66845000	44.02208700	88.31105500
C	0	58.05528100	45.28886600	87.70597100
S	0	58.51450900	45.62188600	85.93767500
C	-1	62.19414500	47.81841100	86.78559600
C	0	60.79808200	48.43274200	87.10448300
S	0	60.06414200	49.24814800	85.64550400
H	0	62.67070300	48.36588900	85.94415000

H	-1	62.81972300	47.95862500	87.66636400
H	0	62.14502200	46.74364200	86.50888400
H	0	61.38209200	48.39797200	81.08808100
H	0	61.05061400	46.63929900	81.24670900
H	-1	59.84029700	47.71242200	80.51650500
H	-1	59.74337500	44.12113200	88.45997300
H	0	58.21846400	43.81740900	89.30899000
H	0	58.49506200	43.12821400	87.67233700
H	0	55.26790000	48.06294600	82.33368900
H	-1	53.91949700	49.25551800	82.39859900
H	0	55.51002700	49.72730200	81.73979300
H	0	60.87750500	49.18292600	87.91867000
H	0	60.09924900	47.65225000	87.48440100
H	0	58.27988700	46.20613400	88.28158800
H	0	56.94831900	45.23001200	87.66804400
H	0	60.75673100	47.92145400	83.46934900
H	0	59.50711800	48.91044800	82.70852200
H	0	55.08108300	48.92918200	84.73636800
H	0	55.19788500	50.60150700	84.16320600
O	0	57.11064800	48.53425900	86.56116600
O	0	57.35126300	48.06606700	87.95540700
H	0	57.80846900	48.86217000	88.32205500
H	0	59.83321200	45.84932400	86.20049800

Ni-O-Fe state:

Free Energy: -5056.712593 a.u.

Charge, Multiplicity: -2, 1

Ni	0	58.14458800	47.37258400	85.17594800
Fe	0	57.60801000	49.65609400	86.69439200
C	0	58.10070300	49.65748900	88.52350300
C	0	58.11291000	51.33509100	86.59735500
C	0	55.82682500	50.20498000	86.98349900
N	0	58.49487200	49.64243700	89.63414000
O	0	58.49465700	52.44124400	86.54530200
N	0	54.71107000	50.56669300	87.10483000
C	-1	60.58603300	47.64972500	81.30913200
C	0	59.96382100	47.85980400	82.67892200
S	0	58.74802900	46.56989700	83.10176700
C	-1	55.00865500	49.12592200	82.52905200
C	0	55.39107000	48.94692300	84.01417800
S	0	57.18279200	49.27301500	84.30626700
C	-1	58.66839600	44.02195300	88.31137300
C	0	58.08137500	45.22278400	87.55882200
S	0	58.68240400	45.31458700	85.83576200
C	-1	62.19422300	47.81869000	86.78554500
C	0	60.72685100	48.12641100	87.18257100
S	0	59.76284100	48.83830400	85.79246800
H	0	62.55395700	48.53672100	86.01661200
H	-1	62.81971000	47.95837500	87.66641200
H	0	62.30629100	46.79485700	86.37588800
H	0	61.36863500	48.41657500	81.09673500
H	0	61.06668500	46.64887800	81.23405600

H	-1	59.84032400	47.71239500	80.51647700
H	-1	59.74340000	44.12117800	88.45975600
H	0	58.20217100	43.92061000	89.31910200
H	0	58.49075700	43.06954900	87.76395500
H	0	55.36253100	48.27381800	81.91181500
H	-1	53.91945300	49.25520400	82.39865400
H	0	55.48503400	50.04445400	82.12097200
H	0	60.67005600	48.87935500	87.99566300
H	0	60.19848100	47.22721400	87.54708900
H	0	58.31847200	46.19466700	88.04874700
H	0	56.97093600	45.18880200	87.54972200
H	0	60.74997100	47.86442000	83.46285400
H	0	59.46623200	48.85320500	82.73690200
H	0	55.17000400	47.92328200	84.37741100
H	0	54.83896200	49.65025900	84.67055100
O	0	57.36700000	47.82101100	86.76284200

SH-Ni-O-Fe state:

Free Energy: -5057.306621 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.71992200	47.08933700	84.85305800
Fe	0	57.53776300	49.31060100	86.64863200
C	0	57.96630300	48.93751900	88.46879700
C	0	57.84587000	51.06526400	86.70259400
C	0	55.74192100	49.77791000	87.13771800
N	0	58.26991400	48.62777300	89.56468300
O	0	57.99404000	52.22362100	86.69980900
N	0	54.63905400	50.10807100	87.38573800
C	-1	60.58602700	47.64973600	81.30913800
C	0	59.91863200	47.73291400	82.68138400
S	0	58.70864600	46.37697000	82.94615000
C	-1	55.00864100	49.12589200	82.52907200
C	0	55.39864200	49.26595800	84.00717000
S	0	57.21531100	49.18713500	84.26394000
C	-1	58.66839100	44.02201500	88.31139800
C	0	58.05148600	45.17260500	87.51064800
S	0	58.41512000	45.14213100	85.70346300
C	-1	62.19427900	47.81863300	86.78551600
C	0	60.69132900	47.96532000	87.13663200
S	0	59.87014900	49.21496700	86.08737000
H	0	62.50041600	48.58340500	86.03952900
H	-1	62.81965800	47.95842400	87.66644100
H	0	62.42865200	46.82470300	86.34525400
H	0	61.31972000	48.47723600	81.16339800
H	0	61.12998000	46.68740200	81.17738600
H	-1	59.84033100	47.71239400	80.51647000
H	-1	59.74340900	44.12112300	88.45972700
H	0	58.21545400	43.99850900	89.32779700
H	0	58.47733100	43.03444300	87.83651900
H	0	55.30677700	48.13130300	82.13429800
H	-1	53.91945700	49.25522600	82.39863900
H	0	55.51980000	49.89290200	81.90745400

H	0	60.53598800	48.24240900	88.19949000
H	0	60.16579100	46.99402400	87.00685600
H	0	58.31484200	46.17968100	87.89396700
H	0	56.94407300	45.15034500	87.53335200
H	0	60.66527700	47.71870300	83.50226200
H	0	59.37421600	48.69439900	82.79400400
H	0	54.93957600	48.48425700	84.64345400
H	0	55.06658200	50.23765900	84.42802700
O	0	57.01360300	47.55480500	86.42418700
H	0	59.72841100	45.48263800	85.80130500

TS2 state (transition state between SH-Ni-O-Fe and Ni-B state):

Free Energy: -5057.290795 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.81106200	47.30386300	84.81116300
Fe	0	57.86880500	49.77844100	86.41271100
C	0	58.33387700	49.81415300	88.26739900
C	0	58.05114900	51.51672900	86.11896200
C	0	56.06642200	50.17823300	86.96302700
N	0	58.63594100	49.81410600	89.40504300
O	0	58.12744300	52.65463100	85.86718900
N	0	54.95708800	50.45848100	87.23828700
C	-1	60.58605700	47.64978900	81.30910500
C	0	59.89514700	47.75930500	82.66360100
S	0	58.55173800	46.51726800	82.85751800
C	-1	55.00868500	49.12506400	82.52902600
C	0	55.46128300	49.40262700	83.96948100
S	0	57.29447600	49.32975500	84.12526300
C	-1	58.66841900	44.02204400	88.31117600
C	0	58.02400500	45.18996200	87.56478500
S	0	58.80701800	45.44930800	85.90723800
C	-1	62.19417000	47.81867400	86.78552800
C	0	60.81894800	48.45488600	87.12845800
S	0	60.13740300	49.57178200	85.85167200
H	0	62.68383800	48.33530100	85.93229900
H	-1	62.81967200	47.95843500	87.66643000
H	0	62.10679500	46.74212500	86.53228800
H	0	61.33736600	48.45984600	81.16265400
H	0	61.10780800	46.67343900	81.19263600
H	-1	59.84027800	47.71237700	80.51651900
H	-1	59.74338800	44.12115800	88.45985400
H	0	58.20232900	43.90238800	89.31615300
H	0	58.51319600	43.06353200	87.76586400
H	0	55.28888800	48.09459200	82.22274900
H	-1	53.91952400	49.25590200	82.39876300
H	0	55.51366300	49.81704000	81.82020700
H	0	60.87617400	49.04134400	88.06748900
H	0	60.05560900	47.67471900	87.33547300
H	0	58.10972200	46.14928100	88.11235200
H	0	56.94009700	45.01145200	87.41313400
H	0	60.61616500	47.64774000	83.49777500
H	0	59.44798300	48.76865500	82.78585300

H	0	55.02862400	48.69105700	84.69912600
H	0	55.16358700	50.41445800	84.31382100
O	0	57.51947500	47.92377600	86.50693500
H	0	58.79742600	46.90371000	86.20216600

Ni-B state:

Free Energy: -5057.364173 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.03546400	47.33746700	85.07615300
Fe	0	57.68336700	49.80897000	86.51964800
C	0	58.13053500	49.68423400	88.35786700
C	0	58.27601500	51.41440900	86.38208800
C	0	55.94221200	50.48388900	86.88604200
N	0	58.44278100	49.51551900	89.48283400
O	0	58.67636200	52.51584100	86.30306900
N	0	54.86148300	50.91956200	87.06454900
C	-1	60.58608600	47.64972500	81.30910500
C	0	59.96388500	47.86450700	82.67961400
S	0	58.74567800	46.56701600	83.09547100
C	-1	55.00864700	49.12586400	82.52911000
C	0	55.42331900	49.21875200	84.01004500
S	0	57.24524100	49.36425600	84.23863200
C	-1	58.66838000	44.02198400	88.31137300
C	0	58.09524100	45.25661700	87.60000300
S	0	58.70857000	45.36641900	85.86748300
C	-1	62.19419800	47.81859600	86.78557100
C	0	60.74187200	48.18567900	87.18992900
S	0	59.72926600	48.86318900	85.82028300
H	0	62.57012900	48.50576800	85.99675500
H	-1	62.81971500	47.95845500	87.66639600
H	0	62.26768600	46.78041200	86.40367300
H	0	61.36861500	48.41604500	81.09869200
H	0	61.06758500	46.64899300	81.23466500
H	-1	59.84030500	47.71239400	80.51649500
H	-1	59.74340600	44.12118000	88.45971600
H	0	58.20018400	43.88241900	89.31327900
H	0	58.48824000	43.09845300	87.71866400
H	0	55.31873100	48.15723400	82.08302500
H	-1	53.91945900	49.25524300	82.39863700
H	0	55.50376900	49.92853100	81.93962100
H	0	60.72712500	48.96602300	87.97836900
H	0	60.21528500	47.30719000	87.61151100
H	0	58.39341000	46.17021700	88.16357400
H	0	56.98450700	45.22792700	87.59993700
H	0	60.74444700	47.86903800	83.46691000
H	0	59.46133900	48.85356600	82.73562600
H	0	55.08503100	48.34708700	84.60589300
H	0	54.99233600	50.11335200	84.50440600
O	0	56.94677600	47.88173800	86.57813300
H	0	57.26499500	47.52707600	87.42505400

SH-Ni-OH-Fe state:

Free Energy: -5057.930519 a.u.

Charge, Multiplicity: -2, 1

Ni	0	57.77539200	47.23011400	84.92663500
Fe	0	57.57487100	49.63605900	86.56230500
C	0	57.94326200	49.22496100	88.37490700
C	0	58.24515300	51.21291600	86.62869700
C	0	55.84498400	50.34335600	86.92711400
N	0	58.17609900	48.79118400	89.44930300
O	0	58.69144400	52.29873000	86.69896900
N	0	54.77703600	50.80797800	87.11632600
C	-1	60.58606400	47.64971000	81.30911700
C	0	59.92606300	47.78627900	82.67923800
S	0	58.63217000	46.51932000	82.98337700
C	-1	55.00865300	49.12578800	82.52915000
C	0	55.40700000	49.34977000	83.99362900
S	0	57.22124600	49.31332200	84.25713400
C	-1	58.66839200	44.02198000	88.31126600
C	0	58.07905500	45.22167600	87.55782000
S	0	58.49351300	45.31398400	85.74850500
C	-1	62.19421200	47.81853400	86.78556800
C	0	60.71884500	48.06254000	87.19920500
S	0	59.77465400	48.88434700	85.87676800
H	0	62.50882600	48.57195600	86.03186800
H	-1	62.81970200	47.95851400	87.66639600
H	0	62.36322200	46.81121700	86.34895000
H	0	61.34192900	48.45227900	81.14437800
H	0	61.10278600	46.66949700	81.19859900
H	-1	59.84031200	47.71240400	80.51648900
H	-1	59.74339300	44.12120500	88.45979200
H	0	58.20763000	43.94687500	89.32109300
H	0	58.47774000	43.06746000	87.77499900
H	0	55.30050100	48.11004800	82.18681400
H	-1	53.91946800	49.25530400	82.39862500
H	0	55.51843900	49.85544500	81.86276200
H	0	60.66119200	48.68902600	88.11333400
H	0	60.23972300	47.09656400	87.48919100
H	0	58.36913000	46.18450700	88.03053200
H	0	56.97055800	45.18616500	87.55326800
H	0	60.66922700	47.73692900	83.50094200
H	0	59.44060600	48.77985500	82.77882000
H	0	54.96627700	48.59782400	84.67810200
H	0	55.06840400	50.33690800	84.37076400
O	0	56.72731300	47.75692900	86.44171000
H	0	57.00237700	47.37977400	87.29353600
H	0	59.79703700	45.66138700	85.93514100

Ni-SI₆ state:

Free Energy: -5057.924013 a.u.

Charge, Multiplicity: -2, 1

Ni	0	57.92197000	47.19401100	85.04489000
Fe	0	57.49172300	49.13084700	86.65539600

C	0	57.91188100	48.56174800	88.41828700
C	0	57.65275300	50.78479700	87.10293400
C	0	55.63418400	49.14033700	87.08761100
N	0	58.19741100	48.19678300	89.50373100
O	0	57.76157300	51.91509900	87.40758600
N	0	54.47936800	49.15686000	87.32652700
C	-1	60.58605600	47.64975500	81.30914300
C	0	59.94999000	47.81926000	82.68326800
S	0	58.76865400	46.47071800	83.06718600
C	-1	55.00865300	49.12574100	82.52913400
C	0	55.33011300	49.14244500	84.02998700
S	0	57.13159400	49.19132100	84.39347300
C	-1	58.66841300	44.02207800	88.31114700
C	0	58.07661700	45.25563300	87.62583600
S	0	58.20342800	45.23153100	85.81275100
C	-1	62.19421800	47.81863700	86.78553900
C	0	60.73383700	48.06737400	87.22702700
S	0	59.69065100	48.77982600	85.90150800
H	0	62.51416600	48.56887800	86.02909700
H	-1	62.81969700	47.95842300	87.66641400
H	0	62.33619500	46.80713000	86.35306100
H	0	61.34982200	48.44052300	81.11943900
H	0	61.09362100	46.66374300	81.21428400
H	-1	59.84030200	47.71235100	80.51649400
H	-1	59.74338700	44.12112100	88.45989200
H	0	58.21540700	43.90290100	89.32012100
H	0	58.47329100	43.09066100	87.73635900
H	0	55.33185700	48.17531600	82.05495900
H	-1	53.91946900	49.25533500	82.39864000
H	0	55.51967500	49.95761200	81.99683500
H	0	60.69742600	48.77344900	88.08165000
H	0	60.27663700	47.12770300	87.59053500
H	0	58.48894300	46.20738500	88.01457200
H	0	56.97781100	45.33468700	87.76783500
H	0	60.71248700	47.85546900	83.48735300
H	0	59.39942800	48.78088200	82.75084200
H	0	54.90167700	48.26917700	84.55738600
H	0	54.89727000	50.03564900	84.52619400
O	0	59.91128200	44.97474500	85.68616200
H	0	60.05555300	45.47109400	84.83441900
H	0	57.11826500	47.47157200	86.37042100

Ni-C state:

Free Energy: -4982.08882 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.08894300	47.31606200	85.08860600
Fe	0	57.53379400	49.24586800	86.66656200
C	0	57.61273300	50.93586500	87.03441700
C	0	55.67967700	49.18693300	87.10040800
C	0	57.98395100	48.77742300	88.45366100
O	0	57.65864300	52.08184300	87.28567700
N	0	54.52359600	49.17709300	87.32938500

N	0	58.29942900	48.49378900	89.55368000
C	-1	60.58588800	47.64983700	81.30900100
C	0	59.95451300	47.86911600	82.67516700
S	0	58.70309400	46.58885300	83.05285700
C	-1	55.00960200	49.12485900	82.52922400
C	0	55.36160300	48.99156700	84.02317900
S	0	57.15171000	49.25865100	84.39768900
C	-1	58.66800800	44.02205000	88.31153800
C	0	58.04320800	45.23582300	87.62108500
S	0	58.57980600	45.32885900	85.86412300
C	-1	62.19415800	47.81762000	86.78506100
C	0	60.72868000	48.10135600	87.19926400
S	0	59.69221100	48.87602500	85.89301400
H	-1	62.81954400	47.95873500	87.66647300
H	0	62.31949800	46.79699000	86.37054100
H	0	62.54057500	48.54359600	86.01665300
H	0	61.37504700	48.40941600	81.09630400
H	0	61.05835200	46.64463900	81.24145000
H	-1	59.84026500	47.71231500	80.51652600
H	-1	59.74338500	44.12109700	88.45992200
H	0	58.21624700	43.86765000	89.31954200
H	0	58.49609500	43.09116900	87.72521000
H	0	55.49909100	50.02299700	82.09171900
H	0	55.35737900	48.24546900	81.94821800
H	-1	53.91945600	49.25518500	82.39860800
H	0	57.33086000	47.57078500	86.47684400
H	0	58.31059100	46.17815400	88.14231000
H	0	56.93493100	45.17384900	87.65493900
H	0	60.21576700	47.17937000	87.53028500
H	0	60.68360200	48.80083000	88.05796200
H	0	60.72676800	47.84695300	83.47062200
H	0	59.47537400	48.86945000	82.73914800
H	0	54.82084100	49.73732600	84.64050200
H	0	55.07972300	48.00194700	84.43404900

Ni-SI_b' state:

Free Energy: - 5057.332928 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.98742400	47.05743100	84.89963600
Fe	0	57.47204500	49.05006000	86.76249300
C	0	57.92046300	48.53839500	88.53582000
C	0	57.44835000	50.71155500	87.15169000
C	0	55.62692200	48.75829000	87.13517000
N	0	58.25118100	48.22312600	89.62534100
O	0	57.44066900	51.86521400	87.40229300
N	0	54.48075400	48.55705900	87.33314600
C	-1	60.58602500	47.64972300	81.30916000
C	0	59.92847000	47.65031100	82.67667600
S	0	58.82554000	46.20625000	82.92367900
C	-1	55.00865700	49.12574500	82.52910900
C	0	55.31752500	48.98027900	84.03192500
S	0	57.11272600	49.11200500	84.44249300

C	-1	58.66842900	44.02210200	88.31111800
C	0	58.07473800	45.27785100	87.65872900
S	0	57.79272800	45.13616100	85.86736500
C	-1	62.19418900	47.81855000	86.78559300
C	0	60.71658300	47.83717000	87.24698800
S	0	59.52686400	48.43126900	85.96523200
H	0	62.40021800	48.66425400	86.09355600
H	-1	62.81972000	47.95849000	87.66638700
H	0	62.46476300	46.87885100	86.26181200
H	0	61.28319000	48.51412800	81.19004100
H	0	61.17230300	46.71885700	81.13903400
H	-1	59.84032300	47.71238000	80.51647700
H	-1	59.74338700	44.12112000	88.45989600
H	0	58.22465000	43.86844900	89.31948900
H	0	58.47914500	43.10724100	87.71224200
H	0	55.35359600	48.24183700	81.95306700
H	-1	53.91946600	49.25533100	82.39866300
H	0	55.51111300	50.02197000	82.10385200
H	0	60.57293800	48.50738800	88.11807700
H	0	60.40349900	46.83009800	87.58774100
H	0	58.66254600	46.18883700	87.86793400
H	0	57.05250600	45.51447900	88.02146000
H	0	60.68495400	47.66189700	83.48758200
H	0	59.32321100	48.56977700	82.81871900
H	0	54.93673700	48.02432100	84.44067800
H	0	54.82029900	49.77740700	84.62150500
O	0	59.21934400	44.30246100	85.39351200
H	0	59.48086900	44.85100700	84.58956100

Ni-A state:

Free Energy: -5132.610284 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.03150800	47.27455200	85.06102800
Fe	0	57.62263600	49.66252500	86.57283300
C	0	58.01766600	49.38760300	88.40715600
C	0	58.23432900	51.26565200	86.56080500
C	0	55.88012500	50.33374800	86.94688400
N	0	58.28313100	49.10225400	89.52067400
O	0	58.64628100	52.36532300	86.56959000
N	0	54.80061800	50.76683600	87.13768200
C	-1	60.58606900	47.64978900	81.30914100
C	0	59.95703400	47.82633200	82.68194500
S	0	58.73833600	46.52065200	83.06859900
C	-1	55.00864100	49.12570400	82.52916200
C	0	55.40953800	49.22358300	84.01300000
S	0	57.22653300	49.37077700	84.26148400
C	-1	58.66841300	44.02213100	88.31113000
C	0	58.12883900	45.24592200	87.56705100
S	0	58.76277200	45.29119800	85.82345900
C	-1	62.19422100	47.81852300	86.78555600
C	0	60.73556800	48.11633000	87.21300600
S	0	59.67437400	48.75117000	85.86192000

H	0	62.53769300	48.54077900	86.01325100
H	-1	62.81969000	47.95851800	87.66640400
H	0	62.28215600	46.79239200	86.37842500
H	0	61.35400500	48.43494700	81.11574500
H	0	61.08663800	46.66022400	81.21758200
H	-1	59.84029600	47.71232600	80.51649800
H	-1	59.74339100	44.12108300	88.45988800
H	0	58.18909500	43.92538200	89.31065000
H	0	58.48001600	43.08394100	87.74441700
H	0	55.31999200	48.15534200	82.08794500
H	-1	53.91947500	49.25536600	82.39862300
H	0	55.50616500	49.92682400	81.93968800
H	0	60.68728300	48.89117900	88.00562100
H	0	60.26949800	47.20529800	87.63614500
H	0	58.43187400	46.18507200	88.07923200
H	0	57.02277500	45.23999100	87.47250200
H	0	60.73112800	47.80526700	83.47524600
H	0	59.45071900	48.81132300	82.76335500
H	0	55.06164700	48.35373200	84.60630800
H	0	54.96875400	50.11833600	84.49797600
O	0	60.28231400	45.18813700	85.99726900
O	0	56.83937600	47.73693500	86.51637400
H	0	57.08973700	47.39464200	87.39011400

Ni-A TS state:

Free Energy: -5132.520086 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.89096000	47.19404600	85.02223500
Fe	0	58.03087100	50.25317900	86.08434500
C	0	58.68875300	50.73608800	87.80543700
C	0	59.11327400	51.37127500	85.31601200
C	0	56.69050600	51.61206500	86.04153500
N	0	59.13502700	50.94105100	88.87751800
O	0	59.83705400	52.14459700	84.81975300
N	0	55.86146900	52.44443000	85.95589800
C	-1	60.58606900	47.64978900	81.30914100
C	0	59.99164500	47.82036300	82.69412300
S	0	58.94819300	46.41026900	83.20909300
C	-1	55.00864100	49.12570400	82.52916200
C	0	55.47894500	49.30480300	83.98556100
S	0	57.31595400	49.25096300	84.09265300
C	-1	58.66841300	44.02213100	88.31113000
C	0	58.01866000	45.31997000	87.76904000
S	0	57.44789900	45.20489700	86.02254800
C	-1	62.19422100	47.81852300	86.78555600
C	0	60.74449000	48.17939600	87.20415900
S	0	59.64824100	48.57127100	85.78701700
H	0	62.55236600	48.51012200	85.99417700
H	-1	62.81969000	47.95851800	87.66640400
H	0	62.27877100	46.78081500	86.40313500
H	0	61.34239200	48.44472700	81.10689800
H	0	61.10460800	46.66983300	81.20289600
H	-1	59.84029600	47.71232600	80.51649800

H	-1	59.74339100	44.12108300	88.45988800
H	0	58.23516400	43.73994800	89.29688000
H	0	58.49862500	43.16575300	87.62386200
H	0	55.28689900	48.12022400	82.14642100
H	-1	53.91947500	49.25536600	82.39862300
H	0	55.50591800	49.87082200	81.87102000
H	0	60.72732200	49.08593900	87.84644500
H	0	60.29485900	47.36052700	87.80604100
H	0	58.70875900	46.18368400	87.82152500
H	0	57.12962800	45.60302600	88.36638800
H	0	60.79413900	47.94075000	83.44940200
H	0	59.38429500	48.74878400	82.74019800
H	0	55.09717400	48.52005300	84.67016400
H	0	55.18379300	50.28965200	84.40258100
O	0	56.69735500	47.31273300	86.39134100
O	0	56.69454000	49.09213000	86.97185000
H	0	57.09874000	48.81617100	87.81310700

Ni-B to Ni-Sib' TS1 state:

Free Energy: -5057.341136 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.84399900	47.10185900	84.99665900
Fe	0	57.60399800	49.37049900	86.62752000
C	0	57.95264100	48.89682000	88.42920600
C	0	58.14235000	50.95851600	86.83308700
C	0	55.81640400	49.86907500	87.05856600
N	0	58.21623600	48.57595700	89.53314400
O	0	58.52491800	52.06140800	86.97248200
N	0	54.72193400	50.23282800	87.30070700
C	-1	60.58590600	47.64930700	81.30919800
C	0	59.95048500	47.78427300	82.68212200
S	0	58.71555400	46.47729400	82.97047400
C	-1	55.00900600	49.12521500	82.52924200
C	0	55.37784900	49.22125600	84.02303900
S	0	57.18838700	49.23236500	84.34470600
C	-1	58.66862300	44.02226900	88.31105000
C	0	58.05491300	45.19016000	87.53755700
S	0	58.65055600	45.17800100	85.79734800
C	-1	62.19358400	47.81695300	86.78560800
C	0	60.69036000	47.79853400	87.16930900
S	0	59.59137100	48.50472000	85.86552400
H	0	62.40934900	48.66829400	86.10258900
H	-1	62.81963100	47.95997900	87.66621300
H	0	62.49385500	46.88759000	86.25863400
H	0	61.34600700	48.44653400	81.12870000
H	0	61.09720900	46.66688000	81.19766900
H	-1	59.84042200	47.71284200	80.51642000
H	-1	59.74339900	44.12098500	88.45990400
H	0	58.20861600	43.93710300	89.32292500
H	0	58.49317900	43.05904400	87.78140300
H	0	55.31393900	48.14506300	82.10715400
H	-1	53.91951200	49.25585000	82.39879100
H	0	55.51652700	49.91638100	81.93435200

H	0	60.48544800	48.38988700	88.08393100
H	0	60.34377300	46.76223000	87.35930400
H	0	58.29037200	46.16624800	88.01206800
H	0	56.94706600	45.09559700	87.57230200
H	0	60.72099700	47.72746300	83.47820500
H	0	59.46138500	48.77570500	82.79484400
H	0	54.98076400	48.36987000	84.61395000
H	0	54.98502600	50.14627700	84.49150200
O	0	56.11230900	46.83828000	85.65297000
H	0	56.09679900	46.00218100	86.14700000

OH-Ni-Fe state:

Free Energy: -5057.345438 a.u.

Charge, Multiplicity: -2, 2

Ni	0	57.91204700	47.04020500	85.01671900
Fe	0	57.59753100	49.31462800	86.65052400
C	0	57.99835600	48.88600200	88.45224100
C	0	58.02565300	50.93909800	86.84582200
C	0	55.78400500	49.64651100	87.10849500
N	0	58.28920900	48.60239900	89.55970200
O	0	58.33536100	52.06738300	86.96994000
N	0	54.65870200	49.88831200	87.36320200
C	-1	60.58590600	47.64930700	81.30919800
C	0	59.94535200	47.74417200	82.68060900
S	0	58.68883300	46.44745200	82.89025600
C	-1	55.00900600	49.12521500	82.52924200
C	0	55.33881400	48.99961900	84.03325500
S	0	57.13592800	49.11713500	84.41150900
C	-1	58.66862300	44.02226900	88.31105000
C	0	58.09453100	45.18320200	87.49912100
S	0	58.78653100	45.14638000	85.79943600
C	-1	62.19358400	47.81695300	86.78560800
C	0	60.69154300	47.78005200	87.16924400
S	0	59.56224400	48.44743000	85.86254600
H	0	62.40182300	48.67426500	86.10748100
H	-1	62.81963100	47.95997900	87.66621300
H	0	62.50201300	46.89383900	86.25223200
H	0	61.33501400	48.46075600	81.14440700
H	0	61.11202700	46.67700400	81.17904000
H	-1	59.84042200	47.71284200	80.51642000
H	-1	59.74339900	44.12098500	88.45990400
H	0	58.19719500	43.96876500	89.31955800
H	0	58.48869700	43.04939500	87.80122200
H	0	55.34800900	48.22889900	81.97041300
H	-1	53.91951200	49.25585000	82.39879100
H	0	55.50611700	50.01250700	82.07863400
H	0	60.47694100	48.38779700	88.07027000
H	0	60.36354700	46.74222500	87.38118400
H	0	58.32049900	46.16008900	87.97853200
H	0	56.98821000	45.11965000	87.43763500
H	0	60.70983900	47.64944300	83.47926000
H	0	59.46686700	48.73662000	82.82533500

H	0	55.02217100	48.01695600	84.44303100
H	0	54.85000000	49.78920700	84.63873600
O	0	56.20809400	46.28095600	84.97192500
H	0	56.39485700	45.32625200	85.05771000

Ni-B to Ni-Sib' TS2 state:

Free Energy: -5057.302797 a.u.

Charge, Multiplicity: -2, 2

Ni	0	58.19319900	47.06496100	84.92426600
Fe	0	57.49161300	49.08373800	86.73877300
C	0	57.95359300	48.69297300	88.53800900
C	0	57.46441300	50.76540400	87.00167000
C	0	55.64222700	48.89987000	87.14036600
N	0	58.30233200	48.45201000	89.63908900
O	0	57.47223700	51.93094500	87.16893400
N	0	54.48587000	48.81594200	87.35516900
C	-1	60.58606200	47.64945800	81.30909300
C	0	59.88153600	47.65821800	82.65969600
S	0	58.50554200	46.43600700	82.73931200
C	-1	55.00902300	49.12536600	82.52922800
C	0	55.36627600	48.63131100	83.95169000
S	0	57.12996100	48.97506400	84.43562000
C	-1	58.66858200	44.02225200	88.31122700
C	0	58.13505100	45.17281400	87.44154700
S	0	58.84093500	45.15191300	85.74735000
C	-1	62.19364700	47.81693400	86.78558300
C	0	60.72068200	47.89834200	87.27191600
S	0	59.51246400	48.47662700	85.99868800
H	0	62.42360900	48.63377000	86.06781500
H	-1	62.81960700	47.95998300	87.66623000
H	0	62.41780000	46.84946800	86.29304100
H	0	61.30167400	48.49779500	81.20615000
H	0	61.14755200	46.70235400	81.14917400
H	-1	59.84036100	47.71275300	80.51647000
H	-1	59.74341600	44.12097500	88.45978400
H	0	58.18042400	44.03853300	89.31057300
H	0	58.46755200	43.03663400	87.83970500
H	0	55.39988700	48.43396400	81.75411800
H	-1	53.91949700	49.25572000	82.39878700
H	0	55.46991100	50.12082200	82.34250000
H	0	60.60729600	48.61858300	88.10727500
H	0	60.36456300	46.92385100	87.65891800
H	0	58.34524100	46.16262200	87.90022200
H	0	57.03848400	45.10922300	87.30455000
H	0	60.60249900	47.45329000	83.47846100
H	0	59.45798200	48.66344100	82.86611500
H	0	55.20646300	47.54131400	84.06990700
H	0	54.75717500	49.13002300	84.73222000
O	0	56.71669600	44.46211600	85.01188500
H	0	56.99719800	44.59554400	84.08712600