

## Electronic Supplementary Information

### Dehydrogenation of Ethanol to Acetaldehyde with Nitrous Oxide over the Metal-Organic Framework NU-1000: A Density Functional Theory Study

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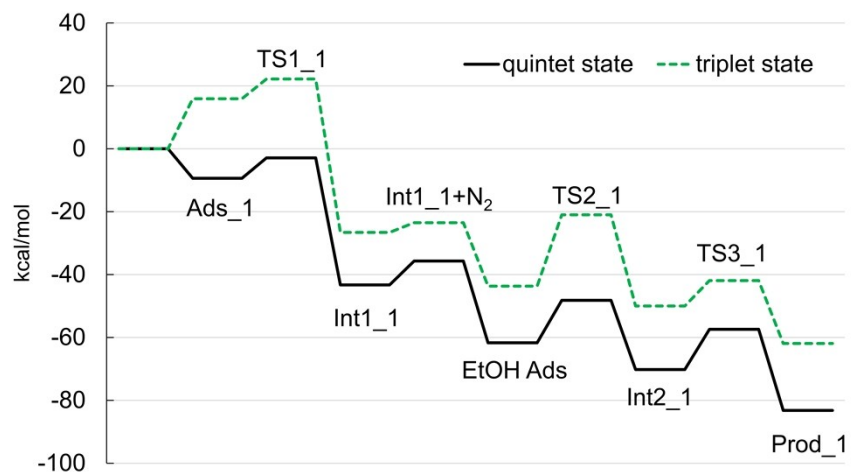
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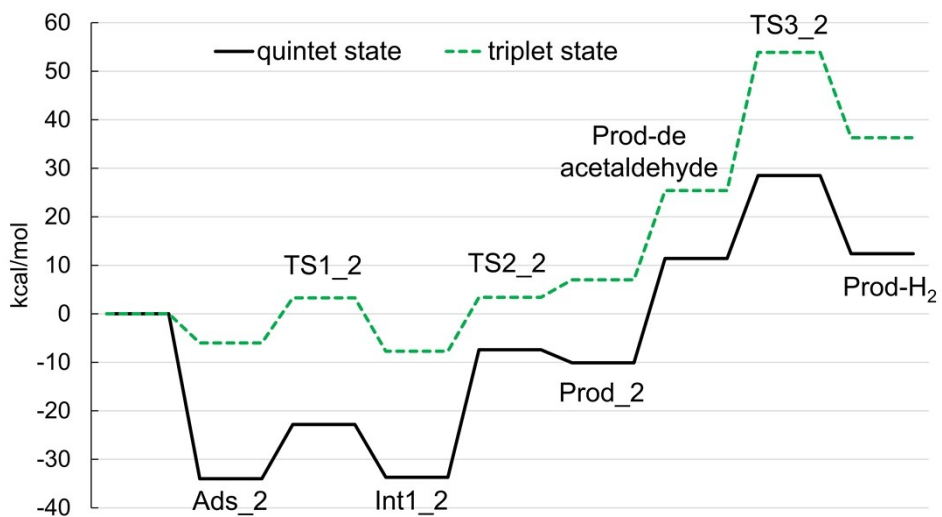
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## Section 1: Spin states



**Fig. S1** Relative energy without thermal corrections for the ethanol dehydration to acetaldehyde with  $N_2O$  over Fe-Zr-NU-1000.

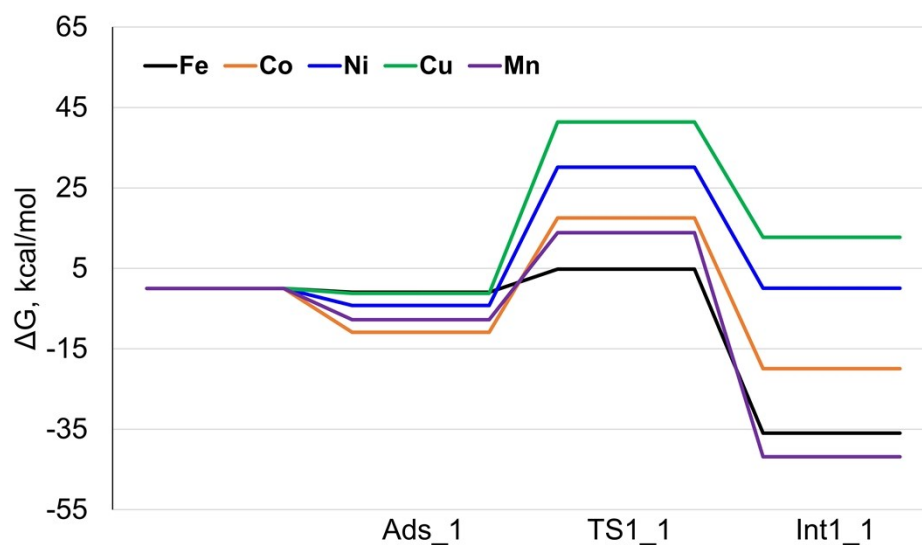


**Fig. S2** Relative energy without thermal corrections for the ethanol dehydration to acetaldehyde without  $N_2O$  over Fe-Zr-NU-1000.

## Section 2: N<sub>2</sub>O Decomposition M-Zr-NU1000

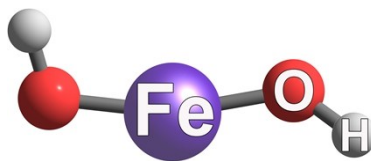
**Table S1** Relative electronic energy without thermal corrections for N<sub>2</sub>O decomposition on M-Zr-NU1000 (M = Co, Ni, Cu and Mn).

Reaction coordinates	Relative electronic energy (kcal/mol)							
	Co-Zr-NU-1000		Ni-Zr-NU-1000		Cu-Zr-NU-1000		Mn-Zr-NU-1000	
	Quartet	Doublet	Triplet	Singlet	Quartet	Doublet	Sextet	Quartet
M-Zr-NU-1000	0.0	18.4	0.0	79.3	87.6	0.0	0.0	30.9
N <sub>2</sub> O Ads (Ads_1)	-16.1	10.5	-12.8	32.5	78.0	-9.3	-16.7	23.8
TS (TS1_1)	10.9	32.1	24.8	69.2	45.6	35.5	12.6	7.2
Int (Int1_1)	-25.5	-10.0	-5.9	20.7	22.1	7.4	-16.8	-46.9



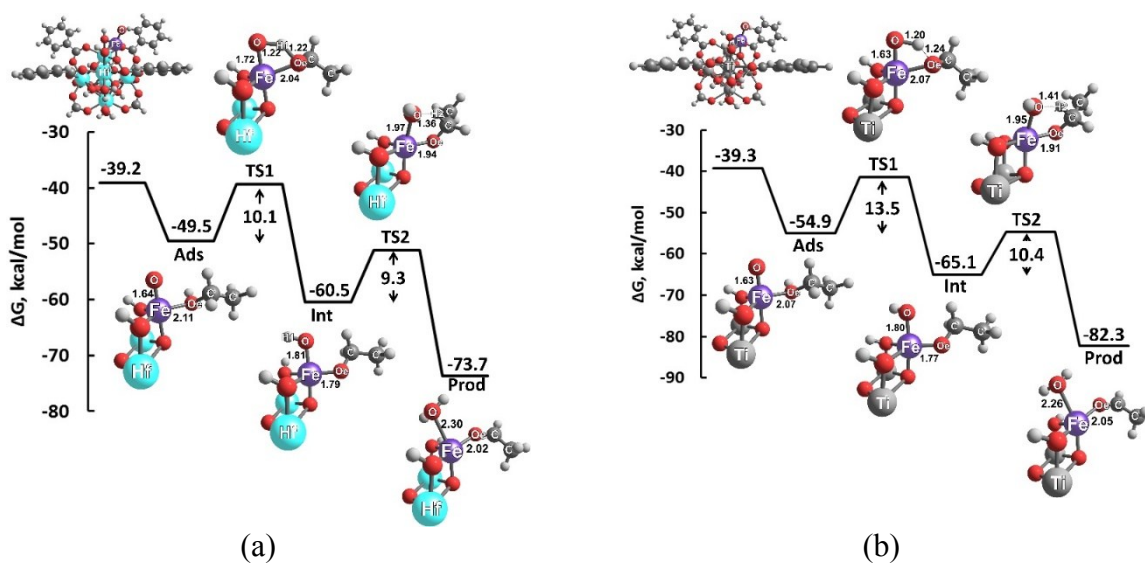
**Fig. S3** Gibbs free energy profile for N<sub>2</sub>O decomposition on M-Zr-NU1000 (M=Fe, Mn, Co, Ni and Cu). The superscript numbers in the energy profiles refer to the spin states of each complex.

### Section 3: Effect of supported NU-1000 framework



**Fig. S4** Cluster model of Fe-NU-1000 without the whole NU-1000 framework.

### Section 4: Ethanol dehydration on Fe-Hf-NU1000 and Fe-Ti-NU1000



**Fig. S5** Gibbs free energy profile for ethanol dehydration on Fe-Hf-NU1000 (a) and Fe-Ti-NU1000 (b).

### Section 5: Turnover frequencies (TOF) and energy span

The turnover frequencies (TOF) for the catalytic pathways using the energy span model of Kozuch and Shaik via equation (1):

$$TOF = \frac{k_B T}{h} \frac{e^{-\Delta G_r/RT} - 1}{\sum_{i=1, j=0}^N e^{(T_i - I_j - \delta G_{ij}/RT)}} \quad (1)$$

$k_B$  is Boltzmann's constant,  $h$  is Planck's constant,  $T$  is the absolute temperature,  $R$  is the universal gas constant,  $N$  is the number of steps in the catalytic cycle,  $\Delta G_r$  is the reaction Gibbs free energy,  $T_i$  is the energies of transition states,  $I_j$  is the energies of intermediates, and  $\delta G_{ij}$  is defined as

$$\delta G_{ij} = \begin{cases} \Delta G_r, & i > j \\ 0, & i \leq j \end{cases}$$

To calculate the equation 1, for the adsorption and desorption steps that there are no connecting transition state, we set the free energy of the transition states as the free energy of the adsorption (Ads) and the product complex (Prod), respectively which is the same strategies used in reference 26.

### Section 6: Geometry relaxation

The consequences of geometry relaxation was tested by calculating the reaction pathway with fixing only the para-C atoms of benzoate linkers of MOF for non-functionalized and for all functionalized systems, to compare with fixing entire linkers. In the non-functionalized system, both fixing variants give virtually the same relative free energies. For the functionalized system, the relative energies were lower when fixing only para-C atoms (see Table S2), due to hydrogen bond interactions between the reacting molecule and the functionalized groups. The activation energies differ within 1-2 kcal/mol between both sets of restraints. However, in both cases functionalization of the organic linker does not improve the catalytic activity of the MOF.

**Table S2** Relative free energy for the ethanol dehydration with N<sub>2</sub>O over non-functionalized and functionalized Fe-Zr-NU-1000 with fixing only para-C atoms.

Reaction Coordinates	Relative free energies (kcal/mol)				
	-H	-NH <sub>2</sub>	-OH	-NO <sub>2</sub>	-Br
Ads_4	-11.0	-16.0	-15.5	-9.2	-12.3
TS1_4	-1.4	-3.1	-3.3	3.8	-1.8
	(Ea=9.6)	(Ea=12.9)	(Ea=12.2)	(Ea=13.0)	(Ea=10.5)
Int1_4	-22.3	-26.2	-27.0	-21.7	-26.0
TS2_4	-12.2	-15.2	-16.4	-11.8	-15.3

	(Ea=10.1)	(Ea=11.0)	(Ea=10.6)	(Ea=9.9)	(Ea=10.7)
Prod 4	-36.4	-37.4	-42.0	-54.7	-40.3

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**Section 7: Coordinates of all optimized structures with total electronic and free energies**

**Reacting molecules**

N<sub>2</sub>O

Free Energy: -184.66497

Electronic Energy: -184.657689

N	-0.026220000	-0.629467000	0.000002000
O	0.752289000	-2.828363000	0.000046000
N	0.355243000	-1.707364000	0.000024000

N<sub>2</sub>

Free Energy: -109.527657

Electronic Energy: -109.5147253

N	-0.040704000	-0.588870000	0.000001000
N	0.329880000	-1.635434000	0.000022000

H<sub>2</sub>

Free Energy: -1.171624

Electronic Energy: -1.1700775

H	0.655919000	-2.556201000	0.000041000
H	0.407644000	-1.855047000	0.000027000

Ethanol

Free Energy: -154.963603

Electronic Energy: -155.0187494

C	-1.999636000	0.933761000	0.000000000
H	-1.637939000	1.466560000	0.883583000
H	-1.637936000	1.466559000	-0.883582000
H	-3.092447000	0.966877000	-0.000002000
C	-1.500108000	-0.488585000	0.000001000
H	-1.886045000	-1.023863000	-0.884627000
H	-1.886046000	-1.023862000	0.884630000
O	-0.084628000	-0.448375000	0.000002000
H	0.230554000	-1.356191000	0.000012000

Acetaldehyde

Free Energy: -153.782979

Electronic Energy: -153.8135709

C	-1.404571000	1.769809000	1.965373000
O	-0.381332000	1.939194000	1.344082000
H	-1.818564000	2.581161000	2.614650000
C	-2.216932000	0.512800000	1.953991000
H	-3.240967000	0.730454000	1.631983000
H	-1.771665000	-0.234425000	1.296194000
H	-2.297907000	0.112220000	2.970394000

**Reaction with N<sub>2</sub>O**

Fe-NU-1000

Free Energy: -4057.65154

Electronic Energy: -4057.8100964

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000

H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.970851000	-2.847065000	0.218981000
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H	0.011493000	4.083183000	-0.368329000
H	0.645251000	4.476385000	1.651872000
H	0.938614000	4.209255000	-1.650838000
H	1.874585000	0.160560000	2.977068000
H	-1.962513000	2.892160000	-0.091001000
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H	-0.003779000	-4.016888000	0.605089000
O	-1.117948000	0.121962000	1.536498000
O	-0.018492000	-3.887267000	1.616146000
O	1.038385000	1.518960000	0.024993000
O	1.313644000	0.155165000	2.194230000
O	-0.078491000	-1.090012000	4.079569000



O	-0.159966000	1.517939000	4.018534000
O	0.282805000	-2.033303000	-3.864666000
O	1.034666000	-1.463593000	0.207276000
O	-1.423001000	-2.054785000	0.218504000
O	-0.004989000	-3.968432000	-0.989823000
O	-0.087096000	4.000178000	1.246152000
O	0.051384000	3.945354000	-1.372669000
O	-1.423848000	2.094390000	-0.051982000
O	0.132569000	1.480827000	-4.011988000
O	1.339879000	-0.099493000	-2.043309000
O	-1.110906000	-0.082659000	-1.441678000
Zr	2.462104000	0.004423000	0.113390000
Zr	-0.086438000	-1.617152000	2.034852000
Zr	-0.043931000	1.956849000	1.758626000
Zr	-0.017781000	1.658044000	-1.775576000
Zr	-2.554956000	-0.003411000	0.043498000
Zr	-0.000017000	-1.930276000	-1.569901000
Fe	0.987952000	-0.248843000	-3.899145000

Fe-NU-1000 (Ads\_1)

Free Energy: -4242.318019

Electronic Energy: -4242.4827982

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161898000	-2.734602000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021308000	-2.724790000
C	-4.324800000	2.872000000	-3.007999000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223384000	-2.332228000	-2.105805000
C	-3.315195000	-2.089489000	2.441205000

C	-3.322908000	2.330099000	2.211501000
C	3.188500000	2.436997000	2.193702000
C	3.241992000	2.241996000	-2.085984000
C	3.280309000	-2.402405000	-1.851728000
C	-3.245504000	2.084763000	-2.346726000
C	3.174602000	-2.211102000	2.426603000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666621000	2.881883000
H	3.964843000	3.004754000	2.662579000
H	-4.111859000	2.914439000	2.636931000
H	3.948377000	-2.768397000	2.911976000
O	-3.663757000	1.472077000	1.337383000
O	-3.610003000	1.255376000	-1.456716000
O	-3.653955000	-1.258607000	1.542899000
O	-2.127256000	-2.310203000	2.835720000
O	1.970329000	-2.521817000	2.683609000
O	2.090008000	-2.742663000	-2.140682000
O	3.548194000	-1.286105000	1.640818000
O	3.614209000	-1.448400000	-1.083704000
O	3.557200000	1.485679000	1.438496000
O	3.591775000	1.320300000	-1.285291000
O	2.046390000	2.547602000	-2.386358000
O	1.986456000	2.771286000	2.435675000
O	-2.020211000	-2.554157000	-2.444516000
O	-3.603926000	-1.474693000	-1.248422000
O	-2.134339000	2.562387000	2.592268000
O	-2.045128000	2.316598000	-2.694348000
H	-1.973684000	-2.837890000	0.208662000
H	-1.036670000	1.804901000	4.309946000
H	-0.136596000	0.502659000	4.148161000

H	-0.739751000	1.463203000	-4.383655000
H	0.006680000	4.086969000	-0.354660000
H	0.643930000	4.479582000	1.660501000
H	0.929672000	4.226472000	-1.638786000
H	1.874954000	0.159382000	2.976548000
H	-1.971468000	2.895733000	-0.087070000
H	-0.816116000	-1.491223000	4.550649000
H	0.806857000	-2.635779000	-4.122504000
H	0.840238000	-4.187823000	1.920678000
H	0.785847000	-4.399158000	-1.331698000
H	-0.005701000	-4.004167000	0.585051000
O	-1.118421000	0.124735000	1.537133000
O	-0.018880000	-3.887007000	1.598228000
O	1.035275000	1.537088000	0.034799000
O	1.311336000	0.156479000	2.195645000
O	-0.078144000	-1.090703000	4.079285000
O	-0.161228000	1.514826000	4.023886000
O	0.274694000	-1.883584000	-3.839502000
O	1.033226000	-1.470453000	0.215096000
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O	-0.092051000	4.007139000	1.256927000
O	0.046166000	3.952422000	-1.360457000
O	-1.429383000	2.100368000	-0.048014000
O	0.141766000	1.472868000	-3.992147000
O	1.356930000	-0.089050000	-1.978699000
O	-1.110799000	-0.073166000	-1.442158000
Zr	2.444893000	0.005405000	0.118304000
Zr	-0.088472000	-1.618906000	2.031736000
Zr	-0.047074000	1.960544000	1.764802000
Zr	-0.026274000	1.665516000	-1.768311000
Zr	-2.555020000	-0.003646000	0.044322000
Zr	0.003620000	-1.910596000	-1.590129000
Fe	1.210766000	-0.146403000	-3.863893000
N	4.408525000	-0.583234000	-4.343272000
O	3.330743000	-0.988650000	-4.673709000
N	5.430476000	-0.198156000	-4.028159000

Fe-NU-1000 (TS1\_1)

Free Energy: -4242.308821

Electronic Energy: -4242.4723745

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000

C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000

O	-3.61000000	1.25540000	-1.45670000
O	-3.65400000	-1.25860000	1.54290000
O	-2.12730000	-2.31020000	2.83570000
O	1.97030000	-2.52180000	2.68360000
O	2.09000000	-2.74270000	-2.14060000
O	3.54820000	-1.28610000	1.64080000
O	3.61420000	-1.44840000	-1.08370000
O	3.55720000	1.48570000	1.43850000
O	3.59180000	1.32030000	-1.28530000
O	2.04640000	2.54780000	-2.38640000
O	1.98650000	2.77130000	2.43570000
O	-2.02020000	-2.55450000	-2.44470000
O	-3.60400000	-1.47470000	-1.24840000
O	-2.13430000	2.56240000	2.59230000
O	-2.04510000	2.31670000	-2.69430000
H	-1.97464100	-2.84192500	0.21374300
H	-1.03343500	1.81358500	4.31413100
H	-0.13709700	0.50924500	4.15380600
H	-0.64529900	1.19161500	-4.40924800
H	0.00269300	4.08250000	-0.35731600
H	0.64059500	4.48242800	1.65698800
H	0.92456200	4.22508400	-1.64170700
H	1.87054900	0.16354800	2.98614600
H	-1.97295000	2.89588200	-0.08523700
H	-0.81332500	-1.48949200	4.56271000
H	0.45135800	-2.47678300	-4.27961200
H	0.84079300	-4.18955000	1.92575200
H	0.78909800	-4.39833200	-1.33281900
H	-0.00946100	-4.01094700	0.59568800
O	-1.12017400	0.12360300	1.54133400
O	-0.01954000	-3.88947500	1.60546400
O	1.03253400	1.53228400	0.03550100
O	1.31154100	0.15733200	2.20186200
O	-0.07851000	-1.08814200	4.08713700
O	-0.15999000	1.52001100	4.02557200
O	0.21990700	-1.67269000	-3.80506600
O	1.03261900	-1.47338800	0.22926600
O	-1.42546700	-2.05062500	0.21902200
O	-0.00810900	-3.95899000	-1.01771300
O	-0.09250100	4.00591000	1.25298000
O	0.04270700	3.94594800	-1.36323500
O	-1.43131000	2.10013200	-0.04689600
O	0.19739300	1.33608200	-3.96288700
O	1.36566400	-0.09841000	-1.93553400
O	-1.10445100	-0.07298100	-1.42845700
Zr	2.45342600	0.00359100	0.12872800
Zr	-0.09032700	-1.61768300	2.04194000
Zr	-0.04710900	1.96059800	1.76440700
Zr	-0.03098100	1.66082300	-1.76942900

Zr	-2.557594000	-0.001409000	0.047855000
Zr	0.005420000	-1.914608000	-1.564820000
Fe	1.467674000	-0.152840000	-3.803084000
N	4.386411000	-0.116162000	-4.195439000
O	3.221977000	-0.534966000	-4.557369000
N	5.520166000	-0.331917000	-4.142179000

Fe-NU-1000 (Int1\_1)

Free Energy: -4242.373808

Electronic Energy: -4242.5368585

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.292997000	-3.161921000	-2.734577000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341399000	3.021328000	-2.724767000
C	-4.324798000	2.872022000	-3.007977000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223415000	-2.332400000	-2.105766000
C	-3.315199000	-2.089484000	2.441202000
C	-3.322897000	2.330080000	2.211499000
C	3.188517000	2.437024000	2.193677000
C	3.241979000	2.242011000	-2.085859000
C	3.280341000	-2.402498000	-1.851748000
C	-3.245519000	2.084910000	-2.346686000
C	3.174575000	-2.211057000	2.426634000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000

H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101095000	-2.666615000	2.881890000
H	3.964843000	3.004768000	2.662561000
H	-4.111860000	2.914433000	2.636937000
H	3.948376000	-2.768371000	2.912006000
O	-3.663686000	1.472100000	1.337408000
O	-3.609978000	1.255468000	-1.456645000
O	-3.654020000	-1.258567000	1.542918000
O	-2.127309000	-2.310237000	2.835660000
O	1.970301000	-2.521778000	2.683569000
O	2.089996000	-2.742359000	-2.140644000
O	3.548250000	-1.286123000	1.640746000
O	3.614208000	-1.448470000	-1.083639000
O	3.557133000	1.485630000	1.438593000
O	3.591787000	1.320303000	-1.285310000
O	2.046421000	2.547577000	-2.386517000
O	1.986506000	2.771319000	2.435644000
O	-2.020213000	-2.554320000	-2.444846000
O	-3.604000000	-1.474740000	-1.248349000
O	-2.134298000	2.562423000	2.592289000
O	-2.045084000	2.316417000	-2.694327000
H	-1.957477000	-2.857516000	0.227435000
H	-1.032135000	1.819469000	4.292425000
H	-0.137246000	0.514043000	4.142000000
H	-0.347318000	1.560208000	-4.718826000
H	0.003621000	4.062331000	-0.397231000
H	0.644209000	4.474136000	1.631720000
H	0.935227000	4.174526000	-1.672247000
H	1.868695000	0.166263000	2.984459000
H	-1.959230000	2.885695000	-0.095057000
H	-0.815486000	-1.489692000	4.551063000
H	-0.367213000	-2.100355000	-4.482354000
H	0.840657000	-4.193164000	1.944696000
H	0.750588000	-4.433031000	-1.353205000
H	0.005727000	-4.019033000	0.599133000
O	-1.120362000	0.119320000	1.541762000
O	-0.011178000	-3.884735000	1.610652000

O	1.035839000	1.493966000	0.006989000
O	1.317083000	0.156067000	2.194990000
O	-0.078195000	-1.090040000	4.077758000
O	-0.157383000	1.523051000	4.009909000
O	0.200434000	-1.801186000	-3.766675000
O	1.040918000	-1.446546000	0.202689000
O	-1.419763000	-2.058243000	0.222915000
O	-0.010276000	-3.967391000	-0.990455000
O	-0.083814000	3.991011000	1.226568000
O	0.043686000	3.919631000	-1.399087000
O	-1.424507000	2.085398000	-0.053087000
O	0.205358000	1.347924000	-3.961793000
O	1.308856000	-0.114802000	-2.126840000
O	-1.119018000	-0.091952000	-1.421246000
Zr	2.474873000	0.004023000	0.121221000
Zr	-0.085145000	-1.616024000	2.035301000
Zr	-0.041972000	1.951943000	1.745916000
Zr	-0.037140000	1.622369000	-1.796823000
Zr	-2.562158000	-0.001361000	0.050352000
Zr	0.002650000	-1.926864000	-1.559939000
Fe	1.248550000	-0.254865000	-4.045754000
N	3.537448000	-0.175433000	-4.023928000
O	1.354490000	-0.355690000	-5.675627000
N	4.638729000	-0.143961000	-4.152010000

Fe-NU-1000 (Int1\_1+N<sub>2</sub>)

Free Energy: -4132.850814

Electronic Energy: -4133.0099428

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187703000	-2.459997000
C	-4.293001000	-3.161895000	-2.734605000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021292000	-2.724809000
C	-4.324801000	2.871991000	-3.008009000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000



C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223393000	-2.332292000	-2.105780000
C	-3.315196000	-2.089501000	2.441198000
C	-3.322899000	2.330098000	2.211499000
C	3.188509000	2.437018000	2.193684000
C	3.241994000	2.241993000	-2.086000000
C	3.280295000	-2.402406000	-1.851695000
C	-3.245498000	2.084781000	-2.346695000
C	3.174588000	-2.211087000	2.426611000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101095000	-2.666615000	2.881890000
H	3.964843000	3.004750000	2.662584000
H	-4.111860000	2.914436000	2.636934000
H	3.948377000	-2.768394000	2.911979000
O	-3.663703000	1.472098000	1.337385000
O	-3.610027000	1.255383000	-1.456728000
O	-3.653991000	-1.258610000	1.542882000
O	-2.127297000	-2.310157000	2.835679000
O	1.970308000	-2.521772000	2.683586000
O	2.089973000	-2.742935000	-2.140712000
O	3.548173000	-1.286056000	1.640825000
O	3.614184000	-1.448414000	-1.083660000
O	3.557305000	1.485691000	1.438468000
O	3.591853000	1.320324000	-1.285291000
O	2.046408000	2.547971000	-2.386299000
O	1.986479000	2.771327000	2.435704000
O	-2.020234000	-2.554647000	-2.444698000
O	-3.604006000	-1.474709000	-1.248417000

O	-2.134307000	2.562376000	2.592285000
O	-2.045115000	2.316842000	-2.694220000
H	-1.965348000	-2.852879000	0.222724000
H	-1.029523000	1.821778000	4.298306000
H	-0.136613000	0.514993000	4.145343000
H	-0.492261000	1.428037000	-4.613400000
H	0.007319000	4.077274000	-0.380496000
H	0.642471000	4.478481000	1.641384000
H	0.932768000	4.199456000	-1.664228000
H	1.868110000	0.165044000	2.984585000
H	-1.965555000	2.890971000	-0.089646000
H	-0.813253000	-1.489137000	4.554888000
H	0.243219000	-2.394685000	-4.487653000
H	0.840629000	-4.193232000	1.944196000
H	0.773843000	-4.424351000	-1.336078000
H	-0.002609000	-4.023186000	0.606973000
O	-1.119644000	0.120280000	1.538668000
O	-0.013987000	-3.887178000	1.614504000
O	1.034070000	1.501078000	0.012544000
O	1.316173000	0.155888000	2.195222000
O	-0.078337000	-1.088090000	4.079041000
O	-0.156518000	1.523792000	4.012145000
O	0.177436000	-1.723409000	-3.802007000
O	1.038241000	-1.453588000	0.205129000
O	-1.419347000	-2.059154000	0.220334000
O	-0.008717000	-3.972598000	-1.002022000
O	-0.083883000	3.995362000	1.233101000
O	0.045182000	3.937105000	-1.384661000
O	-1.426230000	2.093346000	-0.053960000
O	0.211644000	1.353150000	-3.961937000
O	1.346151000	-0.105254000	-2.070829000
O	-1.096468000	-0.085047000	-1.424955000
Zr	2.478712000	0.007013000	0.122876000
Zr	-0.086112000	-1.615016000	2.037856000
Zr	-0.042073000	1.954562000	1.749661000
Zr	-0.035793000	1.654494000	-1.790744000
Zr	-2.557661000	-0.001928000	0.045797000
Zr	0.006110000	-1.934685000	-1.554898000
Fe	1.317275000	-0.238756000	-3.920984000
O	2.043298000	-0.415033000	-5.363973000

Fe-NU-1000 (C<sub>2</sub>H<sub>5</sub>OH Ads)

Free Energy: -4287.830594

Electronic Energy: -4288.0701278

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000

C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000

H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.955611000	-2.858574000	0.228896000
H	-1.037154000	1.815810000	4.282139000
H	-0.137629000	0.513364000	4.138260000
H	-0.402591000	1.552332000	-4.694340000
H	0.003353000	4.057525000	-0.403710000
H	0.646242000	4.471303000	1.630067000
H	0.937546000	4.164860000	-1.674704000
H	1.869379000	0.166005000	2.983227000
H	-1.957426000	2.882655000	-0.096782000
H	-0.817903000	-1.489613000	4.546522000
H	-0.520465000	-2.100295000	-4.388557000
H	0.842990000	-4.189718000	1.941793000
H	0.752635000	-4.428890000	-1.351807000
H	0.008961000	-4.015574000	0.593668000
O	-1.120489000	0.118639000	1.542737000
O	-0.009941000	-3.884427000	1.607873000
O	1.037937000	1.491662000	0.004458000
O	1.317736000	0.155555000	2.193933000
O	-0.077527000	-1.091736000	4.076596000
O	-0.158742000	1.522472000	4.007561000
O	0.181360000	-1.880857000	-3.768064000
O	1.043184000	-1.446595000	0.202004000
O	-1.420391000	-2.057781000	0.223365000
O	-0.008479000	-3.966233000	-0.986317000
O	-0.083760000	3.990361000	1.226034000
O	0.043509000	3.916177000	-1.404565000
O	-1.423929000	2.081748000	-0.053357000
O	0.197577000	1.371929000	-3.965242000
O	1.276469000	-0.115515000	-2.152814000
O	-1.133535000	-0.096342000	-1.425086000
Zr	2.472195000	0.000863000	0.116693000

Zr	-0.084369000	-1.616433000	2.032245000
Zr	-0.040392000	1.950324000	1.741320000
Zr	-0.037675000	1.610574000	-1.803892000
Zr	-2.562249000	-0.001674000	0.051341000
Zr	0.001890000	-1.922565000	-1.566292000
Fe	1.178850000	-0.275045000	-4.099957000
O	1.110414000	-0.336069000	-5.736759000
C	4.033058000	0.205550000	-4.848234000
C	5.477764000	0.055256000	-4.460024000
H	3.848681000	0.107538000	-5.923087000
H	3.633000000	1.176838000	-4.538486000
H	5.573147000	0.111544000	-3.371826000
H	5.888644000	-0.902890000	-4.795128000
H	6.072701000	0.859896000	-4.902342000
O	3.228761000	-0.773999000	-4.136726000
H	3.295456000	-1.621016000	-4.601247000

Fe-NU-1000 (TS2\_1)

Free Energy: -4287.814494

Electronic Energy: -4288.0486191

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000

C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.954128000	-2.853152000	0.223615000
H	-1.031651000	1.820567000	4.280389000
H	-0.139438000	0.512736000	4.133031000
H	-0.587658000	1.566609000	-4.587779000
H	0.014884000	4.077540000	-0.389784000
H	0.646573000	4.474007000	1.640109000

H	0.93860000	4.19076000	-1.67513600
H	1.86165400	0.16366400	2.99080300
H	-1.95762300	2.89172700	-0.08734600
H	-0.81605500	-1.49329600	4.53563300
H	-0.48219200	-2.04185700	-4.44268200
H	0.84024800	-4.19564100	1.93824700
H	0.73827400	-4.43969700	-1.36595800
H	0.00836800	-4.01840200	0.58887900
O	-1.11923600	0.12083200	1.53877500
O	-0.00720500	-3.88005100	1.60022100
O	1.04350300	1.47790700	-0.00128300
O	1.32133500	0.15473500	2.19347100
O	-0.07771400	-1.09202000	4.06522000
O	-0.15630600	1.52171700	4.00161400
O	0.17467800	-1.81442600	-3.77708300
O	1.04582000	-1.42500600	0.17733100
O	-1.41442500	-2.05515900	0.21472400
O	-0.01495800	-3.96751800	-0.99559500
O	-0.07644500	3.98999800	1.22718400
O	0.04905600	3.93722800	-1.39258800
O	-1.42084500	2.09221800	-0.05599800
O	0.12207800	1.44263600	-3.95013400
O	1.31728500	-0.10528000	-2.23448500
O	-1.09347700	-0.08510300	-1.42288800
Zr	2.49609800	0.00991600	0.12975100
Zr	-0.08146600	-1.61345100	2.02242700
Zr	-0.03735100	1.94912300	1.73821000
Zr	-0.03385500	1.65392800	-1.80488800
Zr	-2.55399300	-0.00058700	0.04449900
Zr	0.00669100	-1.93312600	-1.57966000
Fe	1.15183900	-0.20367400	-4.08979000
O	1.02570800	-0.29232900	-5.80503600
C	4.02541600	-0.66282100	-4.82675000
C	5.20902000	-0.18812600	-4.02710600
H	3.64693400	-1.62266900	-4.44041100
H	4.30765300	-0.84441900	-5.87359800
H	5.57483600	0.76497400	-4.41983000
H	4.93508400	-0.04546600	-2.97665400
H	6.02018000	-0.92079800	-4.07908800
O	2.98759400	0.32009600	-4.81171400
H	2.17604700	0.09715100	-5.70304500

Fe-NU-1000 (Int2\_1)

Free Energy: -4287.847224

Electronic Energy: -4288.0836917

C	5.72718100	-2.88920500	-2.16011100
C	-5.63890000	-2.88510000	-2.45140000
C	4.38942500	-3.18809500	-2.46027400
C	-4.29300000	-3.16189800	-2.73460200

C	4.105980000	-4.252480000	-3.328510000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138196000	-5.020741000	-3.859348000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751198000	-3.537703000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755613000	-3.657663000	-2.695026000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223399000	-2.332322000	-2.105784000
C	-3.315200000	-2.089492000	2.441207000
C	-3.322901000	2.330086000	2.211511000
C	3.188501000	2.436997000	2.193705000
C	3.242001000	2.242013000	-2.085986000
C	3.280436000	-2.402359000	-1.851501000
C	-3.245500000	2.084810000	-2.346693000
C	3.174599000	-2.211094000	2.426607000
H	5.936268000	-2.056314000	-1.495647000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070804000	-4.466850000	-3.573363000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416505000	-2.445093000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000



H	3.964843000	3.004750000	2.662584000
H	-4.111859000	2.914439000	2.636931000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472105000	1.337396000
O	-3.610000000	1.255403000	-1.456697000
O	-3.654000000	-1.258608000	1.542895000
O	-2.127299000	-2.310202000	2.835699000
O	1.970300000	-2.521801000	2.683598000
O	2.090004000	-2.742667000	-2.140644000
O	3.548203000	-1.286101000	1.640789000
O	3.614198000	-1.448425000	-1.083670000
O	3.557196000	1.485699000	1.438500000
O	3.591794000	1.320297000	-1.285314000
O	2.046403000	2.547789000	-2.386408000
O	1.986502000	2.771309000	2.435689000
O	-2.020202000	-2.554482000	-2.444706000
O	-3.604000000	-1.474698000	-1.248399000
O	-2.134300000	2.562414000	2.592291000
O	-2.045105000	2.316682000	-2.694308000
H	-1.968561000	-2.848650000	0.224099000
H	-1.032086000	1.828837000	4.276126000
H	-0.139279000	0.522279000	4.136657000
H	-0.590358000	1.251273000	-4.474458000
H	0.007152000	4.073527000	-0.389341000
H	0.646742000	4.476155000	1.635513000
H	0.932409000	4.194647000	-1.672537000
H	1.864162000	0.168869000	2.986668000
H	-1.962307000	2.892251000	-0.085290000
H	-0.813356000	-1.487893000	4.545509000
H	0.256490000	-2.411132000	-4.341794000
H	0.847580000	-4.188990000	1.921564000
H	0.777032000	-4.410337000	-1.347155000
H	-0.005198000	-4.016392000	0.589045000
O	-1.121614000	0.120157000	1.539628000
O	-0.008817000	-3.882330000	1.597551000
O	1.037475000	1.485125000	-0.000712000
O	1.319143000	0.156757000	2.192711000
O	-0.075243000	-1.089007000	4.072812000
O	-0.155310000	1.529817000	4.002000000
O	0.139677000	-1.652858000	-3.761152000
O	1.041751000	-1.440552000	0.195741000
O	-1.422451000	-2.055283000	0.220157000
O	-0.013476000	-3.968430000	-1.018971000
O	-0.078675000	3.993497000	1.225319000
O	0.043526000	3.935303000	-1.393390000
O	-1.424600000	2.093361000	-0.057379000
O	0.209639000	1.338515000	-3.945213000
O	1.347748000	-0.111937000	-2.104756000
O	-1.096391000	-0.077803000	-1.423259000

Zr	2.491992000	0.011136000	0.122491000
Zr	-0.084930000	-1.611419000	2.030373000
Zr	-0.038474000	1.950623000	1.733339000
Zr	-0.029687000	1.656379000	-1.817919000
Zr	-2.556027000	0.001588000	0.043599000
Zr	-0.000449000	-1.921896000	-1.559809000
Fe	1.493176000	-0.246003000	-3.931942000
O	1.485396000	-0.543214000	-5.722901000
C	4.077270000	-0.144510000	-5.080411000
C	5.511259000	-0.021161000	-4.606662000
H	3.876406000	-1.165840000	-5.434883000
H	3.862953000	0.530427000	-5.921284000
H	5.763294000	1.016533000	-4.376569000
H	5.635301000	-0.616031000	-3.697524000
H	6.197679000	-0.392605000	-5.372938000
O	3.235121000	0.169415000	-3.994128000
H	0.586987000	-0.790640000	-5.980452000

Fe-NU-1000 (TS3\_1)

Free Energy: -4287.833074

Electronic Energy: -4288.0632164

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000

C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.963536000	-2.855001000	0.235293000
H	-1.038078000	1.817343000	4.294779000
H	-0.136904000	0.516066000	4.148303000
H	-0.581653000	1.309137000	-4.502754000
H	0.005234000	4.068710000	-0.386861000

H	0.645328000	4.477172000	1.637204000
H	0.939718000	4.176604000	-1.662696000
H	1.871362000	0.170074000	2.987662000
H	-1.963388000	2.886642000	-0.092394000
H	-0.816268000	-1.487349000	4.557514000
H	-0.694474000	-1.761719000	-4.153449000
H	0.843432000	-4.183759000	1.964364000
H	0.728208000	-4.462193000	-1.343324000
H	0.001970000	-4.028576000	0.623177000
O	-1.119781000	0.121727000	1.545729000
O	-0.015070000	-3.889859000	1.633473000
O	1.035572000	1.509954000	0.019575000
O	1.315625000	0.159200000	2.201255000
O	-0.077365000	-1.087631000	4.086835000
O	-0.160255000	1.525340000	4.017422000
O	0.172032000	-1.784833000	-3.732624000
O	1.044344000	-1.461657000	0.225942000
O	-1.422058000	-2.058476000	0.226965000
O	-0.017103000	-3.982175000	-0.967970000
O	-0.087103000	3.997617000	1.235710000
O	0.045802000	3.928150000	-1.389659000
O	-1.425169000	2.088635000	-0.053573000
O	0.208081000	1.300228000	-3.952820000
O	1.368065000	-0.117335000	-2.015738000
O	-1.100909000	-0.088907000	-1.423334000
Zr	2.472970000	0.007613000	0.116210000
Zr	-0.082241000	-1.615454000	2.042712000
Zr	-0.040682000	1.955945000	1.751985000
Zr	-0.022887000	1.637478000	-1.790053000
Zr	-2.549583000	0.000045000	0.050931000
Zr	0.012961000	-1.943628000	-1.542291000
Fe	1.455465000	-0.239277000	-3.892751000
O	1.730506000	-0.755129000	-5.780534000
C	3.974556000	0.152413000	-5.231478000
C	5.141114000	-0.799325000	-5.197954000
H	3.024145000	-0.395403000	-5.897449000
H	4.141182000	1.093045000	-5.786823000
H	5.900445000	-0.433940000	-4.495887000
H	4.836376000	-1.791934000	-4.852123000
H	5.601066000	-0.893819000	-6.185110000
O	3.303632000	0.319121000	-4.096781000
H	1.543156000	-1.676323000	-6.006022000

Fe-NU-1000 (Prod\_1)

Free Energy: -4287.870046

Electronic Energy: -4288.1044535

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000

C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000

H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.970771000	-2.846667000	0.217442000
H	-1.043446000	1.807048000	4.292066000
H	-0.135854000	0.510738000	4.144693000
H	-0.586469000	1.483463000	-4.509205000
H	0.002241000	4.062075000	-0.389833000
H	0.645521000	4.475631000	1.640963000
H	0.937778000	4.180086000	-1.658951000
H	1.881178000	0.163060000	2.968391000
H	-1.965213000	2.878910000	-0.103935000
H	-0.820741000	-1.487115000	4.554120000
H	0.894637000	-2.739594000	-3.946727000
H	0.843379000	-4.180109000	1.931148000
H	0.790120000	-4.403383000	-1.311283000
H	-0.003466000	-4.003770000	0.593857000
O	-1.118838000	0.120575000	1.539442000
O	-0.019185000	-3.888385000	1.609398000
O	1.036304000	1.530040000	0.025898000
O	1.310001000	0.156426000	2.193230000
O	-0.078873000	-1.091309000	4.084986000
O	-0.162725000	1.520923000	4.017987000
O	0.236950000	-2.042579000	-3.824025000
O	1.035740000	-1.479958000	0.221540000
O	-1.427264000	-2.051735000	0.222318000
O	-0.001102000	-3.956599000	-0.993980000
O	-0.093800000	4.002853000	1.244152000
O	0.045547000	3.924448000	-1.390837000
O	-1.425923000	2.082423000	-0.053810000
O	0.199351000	1.402126000	-3.958953000

O	1.325544000	-0.106748000	-2.017280000
O	-1.137511000	-0.094371000	-1.446654000
Zr	2.428511000	0.006460000	0.108605000
Zr	-0.089542000	-1.618821000	2.038034000
Zr	-0.046322000	1.960371000	1.752420000
Zr	-0.021760000	1.617112000	-1.799135000
Zr	-2.558429000	-0.002439000	0.046787000
Zr	-0.002387000	-1.904058000	-1.572900000
Fe	1.228273000	-0.289966000	-4.033727000
O	0.304503000	-0.644464000	-6.134343000
C	4.148792000	-1.135766000	-4.709725000
C	4.905006000	-0.086078000	-3.999237000
H	4.694794000	-1.935915000	-5.236973000
H	0.941803000	-1.030759000	-6.743180000
H	4.676781000	0.896541000	-4.432500000
H	4.578279000	-0.040454000	-2.949944000
H	5.982735000	-0.249650000	-4.042370000
O	2.907314000	-1.163636000	-4.751307000
H	-0.144818000	-1.404112000	-5.721373000

### Reaction without N<sub>2</sub>O

Fe-NU-1000 (Ads\_2)

Free Energy: -4212.647726

Electronic Energy: -4212.8829931

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000

C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.964756000	-2.859643000	0.230329000
H	-1.045583000	1.811491000	4.305331000
H	-0.136075000	0.517403000	4.160129000
H	-0.566501000	1.466729000	-4.498674000
H	-0.006017000	4.052076000	-0.388373000
H	0.639591000	4.480165000	1.640724000
H	0.932089000	4.172429000	-1.653155000
H	1.883383000	0.168635000	2.981694000
H	-1.967386000	2.871946000	-0.106998000
H	-0.819790000	-1.485542000	4.580302000
H	-0.715458000	-1.808565000	-4.142225000
H	0.845481000	-4.178561000	1.966384000
H	0.737422000	-4.451585000	-1.335179000



H	0.000337000	-4.023706000	0.630287000
O	-1.117928000	0.118229000	1.549420000
O	-0.020592000	-3.898236000	1.642985000
O	1.037630000	1.547592000	0.044607000
O	1.307636000	0.158145000	2.209970000
O	-0.080547000	-1.090161000	4.106762000
O	-0.164941000	1.526217000	4.030478000
O	0.173949000	-1.832516000	-3.771519000
O	1.038084000	-1.501730000	0.263883000
O	-1.426406000	-2.061112000	0.233038000
O	-0.010622000	-3.973867000	-0.962880000
O	-0.102335000	4.005936000	1.250596000
O	0.040233000	3.912754000	-1.388788000
O	-1.427168000	2.076497000	-0.051317000
O	0.215262000	1.343326000	-3.953495000
O	1.343904000	-0.111310000	-1.901268000
O	-1.132981000	-0.105478000	-1.431213000
Zr	2.414389000	0.002179000	0.127444000
Zr	-0.092469000	-1.622423000	2.062083000
Zr	-0.047936000	1.964213000	1.762041000
Zr	-0.018770000	1.598231000	-1.789767000
Zr	-2.552922000	-0.001480000	0.053316000
Zr	0.017221000	-1.928116000	-1.528956000
Fe	1.368805000	-0.309440000	-3.906558000
C	4.408826000	0.128243000	-4.839019000
C	3.662692000	0.423197000	-6.111914000
H	4.998444000	0.992401000	-4.510513000
H	5.079007000	-0.732980000	-4.947983000
H	3.039411000	-0.431806000	-6.400576000
H	3.018471000	1.301591000	-5.991363000
H	4.351970000	0.620624000	-6.935885000
O	3.426798000	-0.178140000	-3.834417000
H	3.753879000	-0.075148000	-2.920408000

Fe-NU-1000 (TS1\_2)

Free Energy: -4212.63175

Electronic Energy: -4212.8651669

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000

C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.953948000	-2.854450000	0.220090000
H	-1.037829000	1.817085000	4.285997000
H	-0.137657000	0.515132000	4.142104000

H	-0.747299000	1.739746000	-4.406354000
H	0.001913000	4.061107000	-0.395826000
H	0.640740000	4.478672000	1.627477000
H	0.927789000	4.190583000	-1.674795000
H	1.869844000	0.166136000	2.987812000
H	-1.958325000	2.871128000	-0.108624000
H	-0.817738000	-1.488334000	4.553961000
H	-0.842092000	-2.210869000	-4.079690000
H	0.843376000	-4.193329000	1.955945000
H	0.726932000	-4.468023000	-1.357959000
H	0.004883000	-4.031806000	0.613820000
O	-1.114541000	0.117853000	1.539097000
O	-0.012647000	-3.893693000	1.624014000
O	1.043375000	1.508759000	0.017432000
O	1.315879000	0.155361000	2.200074000
O	-0.078500000	-1.090545000	4.082166000
O	-0.159711000	1.523894000	4.010428000
O	0.068661000	-2.012847000	-3.826951000
O	1.047519000	-1.467536000	0.222246000
O	-1.411405000	-2.058436000	0.214925000
O	-0.014211000	-3.984342000	-0.978047000
O	-0.088211000	3.994967000	1.224712000
O	0.041554000	3.921246000	-1.398924000
O	-1.416268000	2.075802000	-0.065533000
O	0.102716000	1.499625000	-4.020805000
O	1.373549000	-0.118243000	-2.061097000
O	-1.081374000	-0.100859000	-1.444919000
Zr	2.466018000	-0.000029000	0.130746000
Zr	-0.082968000	-1.622050000	2.040042000
Zr	-0.038734000	1.955421000	1.744941000
Zr	-0.004937000	1.629228000	-1.811205000
Zr	-2.537195000	-0.003630000	0.042583000
Zr	0.041761000	-1.953591000	-1.562889000
Fe	0.853960000	-0.312835000	-4.227548000
C	4.016385000	0.072758000	-4.435441000
C	3.770243000	1.106713000	-5.511591000
H	4.628389000	0.488833000	-3.622588000
H	4.581503000	-0.776145000	-4.848344000
H	3.243912000	0.659925000	-6.363390000
H	3.155018000	1.926344000	-5.125214000
H	4.708843000	1.534599000	-5.880081000
O	2.807360000	-0.409967000	-3.893599000
H	2.361081000	-0.189271000	-2.794195000

Fe-NU-1000 (Int\_2)

Free Energy: -4212.646402

Electronic Energy: -4212.8825188

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187699000	-2.460001000
C	-4.293000000	-3.161896000	-2.734604000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000

C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324799000	2.872005000	-3.007995000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223399000	-2.332291000	-2.105809000
C	-3.315205000	-2.089516000	2.441193000
C	-3.322902000	2.330108000	2.211496000
C	3.188514000	2.437000000	2.193705000
C	3.241990000	2.241978000	-2.086007000
C	3.280290000	-2.402372000	-1.851704000
C	-3.245499000	2.084799000	-2.346708000
C	3.174608000	-2.211099000	2.426603000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666620000	2.881885000
H	3.964843000	3.004752000	2.662581000
H	-4.111858000	2.914443000	2.636927000
H	3.948377000	-2.768399000	2.911974000
O	-3.663725000	1.472082000	1.337382000
O	-3.609978000	1.255408000	-1.456696000
O	-3.654040000	-1.258598000	1.542879000
O	-2.127263000	-2.310288000	2.835717000
O	1.970321000	-2.521831000	2.683578000
O	2.090037000	-2.742397000	-2.140549000
O	3.548206000	-1.286047000	1.640791000
O	3.614102000	-1.448414000	-1.083670000
O	3.557245000	1.485627000	1.438478000

O	3.591680000	1.320340000	-1.285269000
O	2.046441000	2.547498000	-2.386393000
O	1.986510000	2.771324000	2.435673000
O	-2.020200000	-2.554226000	-2.444679000
O	-3.603984000	-1.474720000	-1.248404000
O	-2.134276000	2.562462000	2.592297000
O	-2.045076000	2.316463000	-2.694294000
H	-1.966958000	-2.847738000	0.220829000
H	-1.034267000	1.816604000	4.287560000
H	-0.138372000	0.511789000	4.138200000
H	-0.780787000	1.495023000	-4.379982000
H	-0.002396000	4.072286000	-0.380212000
H	0.637625000	4.484656000	1.632799000
H	0.919399000	4.218825000	-1.664039000
H	1.858420000	0.166382000	3.000852000
H	-1.970474000	2.883380000	-0.091769000
H	-0.811280000	-1.490702000	4.549193000
H	-0.793700000	-2.030829000	-4.131856000
H	0.838023000	-4.200896000	1.949043000
H	0.711458000	-4.484864000	-1.364279000
H	-0.002184000	-4.034141000	0.608661000
O	-1.118637000	0.121353000	1.546203000
O	-0.016067000	-3.895183000	1.618124000
O	1.038336000	1.507065000	0.017316000
O	1.317196000	0.156334000	2.204147000
O	-0.074100000	-1.091166000	4.075645000
O	-0.157779000	1.521696000	4.008760000
O	0.064033000	-1.800060000	-3.761127000
O	1.042262000	-1.461609000	0.219989000
O	-1.415174000	-2.058132000	0.208908000
O	-0.025445000	-3.993200000	-0.986241000
O	-0.087416000	3.999691000	1.224601000
O	0.036841000	3.938642000	-1.387654000
O	-1.422107000	2.091688000	-0.064903000
O	0.075989000	1.339034000	-3.968417000
O	1.418647000	-0.121961000	-2.012057000
O	-1.033377000	-0.081091000	-1.409936000
Zr	2.466233000	-0.002476000	0.164228000
Zr	-0.085499000	-1.623732000	2.031192000
Zr	-0.041070000	1.956163000	1.743467000
Zr	-0.019749000	1.662650000	-1.816320000
Zr	-2.530759000	-0.003531000	0.043454000
Zr	0.029173000	-1.972729000	-1.591506000
Fe	1.202938000	-0.267199000	-4.369306000
C	4.126209000	0.022069000	-4.727883000
C	3.812098000	1.180623000	-5.653135000
H	4.627636000	0.395549000	-3.816151000
H	4.848819000	-0.658353000	-5.208422000
H	3.414855000	0.816613000	-6.607671000
H	3.055069000	1.835182000	-5.200060000
H	4.696274000	1.793844000	-5.860710000
O	2.987175000	-0.706908000	-4.371765000
H	2.277110000	-0.191977000	-2.472459000

Fe-NU-1000 (TS2\_2)

Free Energy: -4212.609396

Electronic Energy: -4212.8405911

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000

H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.959709000	-2.851547000	0.220623000
H	-1.034940000	1.814945000	4.296370000
H	-0.137614000	0.511392000	4.144968000
H	-0.779539000	1.605790000	-4.351741000
H	-0.000386000	4.070594000	-0.379404000
H	0.637888000	4.483882000	1.635562000
H	0.934491000	4.199869000	-1.654175000
H	1.863047000	0.165206000	2.997374000
H	-1.966726000	2.883422000	-0.093188000
H	-0.813423000	-1.491214000	4.554119000
H	-0.807950000	-2.126750000	-4.093026000
H	0.842817000	-4.195162000	1.946497000
H	0.727399000	-4.464003000	-1.362940000
H	-0.000034000	-4.028904000	0.609013000
O	-1.119026000	0.121075000	1.547493000
O	-0.013942000	-3.894006000	1.617926000
O	1.037193000	1.514027000	0.026683000
O	1.316213000	0.156399000	2.204562000
O	-0.075709000	-1.091512000	4.081570000
O	-0.158729000	1.521215000	4.015805000
O	0.069525000	-1.852826000	-3.796614000
O	1.041988000	-1.463949000	0.224003000
O	-1.413711000	-2.057943000	0.212379000
O	-0.019404000	-3.981461000	-0.992625000
O	-0.090074000	4.000080000	1.231109000
O	0.044624000	3.934476000	-1.385367000
O	-1.422416000	2.089206000	-0.060414000
O	0.067529000	1.340017000	-3.972334000
O	1.385786000	-0.109277000	-1.962021000
O	-1.057584000	-0.085939000	-1.411938000
Zr	2.472480000	0.002666000	0.146856000
Zr	-0.084173000	-1.620920000	2.036854000
Zr	-0.041232000	1.957204000	1.751061000
Zr	-0.013224000	1.651803000	-1.799074000
Zr	-2.536676000	-0.002599000	0.047814000

Zr	0.037310000	-1.953244000	-1.573758000
Fe	0.849085000	-0.317141000	-4.702624000
C	2.757373000	-0.112092000	-5.614885000
C	3.107391000	1.250201000	-6.147975000
H	3.103857000	-0.959223000	-6.225230000
H	1.189752000	-0.249881000	-6.309030000
H	2.540914000	2.027551000	-5.627819000
H	4.171063000	1.438294000	-5.958494000
H	2.920346000	1.326365000	-7.221868000
O	2.798304000	-0.288373000	-4.307679000
H	2.100436000	-0.103831000	-2.621748000

Fe-NU-1000 (Prod\_2)

Free Energy: -4212.61731

Electronic Energy: -4212.8448996

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187693000	-2.460009000
C	-4.293002000	-3.161888000	-2.734613000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341401000	3.021283000	-2.724819000
C	-4.324802000	2.871983000	-3.008017000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223387000	-2.332355000	-2.105720000
C	-3.315199000	-2.089508000	2.441202000
C	-3.322906000	2.330109000	2.211508000
C	3.188504000	2.436995000	2.193714000
C	3.242002000	2.241971000	-2.086037000
C	3.280308000	-2.402410000	-1.851706000
C	-3.245494000	2.084873000	-2.346633000
C	3.174610000	-2.211103000	2.426611000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000



H	-5.89900000	1.83020000	-1.98630000
H	3.03890000	4.19850000	-3.96280000
H	-2.97830000	4.10040000	-4.14500000
H	4.87690000	5.53410000	-4.95980000
H	-4.77430000	5.49830000	-5.13120000
H	7.73460000	3.29050000	-2.64450000
H	-7.71490000	3.20560000	-2.97220000
H	-7.13990000	-5.40920000	-4.21020000
H	7.28610000	-5.35680000	-3.94480000
H	-7.17290000	5.07750000	-4.54480000
H	7.25200000	5.10910000	-4.29360000
H	-4.10109300	-2.66662500	2.88188000
H	3.96484300	3.00475200	2.66258100
H	-4.11185800	2.91444500	2.63692500
H	3.94837700	-2.76839700	2.91197600
O	-3.66372400	1.47208500	1.33740600
O	-3.61002900	1.25540700	-1.45669500
O	-3.65396500	-1.25860500	1.54290700
O	-2.12728600	-2.31017600	2.83573400
O	1.97027700	-2.52177400	2.68363100
O	2.09006400	-2.74279400	-2.14054700
O	3.54814500	-1.28612100	1.64077600
O	3.61416000	-1.44840400	-1.08373100
O	3.55714400	1.48568400	1.43845500
O	3.59175700	1.32024800	-1.28533300
O	2.04628000	2.54787500	-2.38638500
O	1.98646200	2.77120900	2.43567700
O	-2.02000300	-2.55469500	-2.44466400
O	-3.60398500	-1.47471300	-1.24837900
O	-2.13433900	2.56235600	2.59228800
O	-2.04499500	2.31715900	-2.69440700
H	-1.96588400	-2.85040200	0.22089200
H	-1.03738700	1.81538900	4.28906500
H	-0.13803300	0.51379700	4.14213200
H	-0.75776500	1.61014200	-4.33293500
H	-0.00469200	4.06531100	-0.38451100
H	0.63752600	4.48446100	1.63491300
H	0.92408600	4.20217900	-1.66103000
H	1.86081100	0.16550300	2.99805100
H	-1.97199700	2.88436000	-0.09018100
H	-0.81202700	-1.48995400	4.55625200
H	-0.73787000	-2.09149200	-4.11844400
H	0.84263200	-4.19382500	1.93513700
H	0.73178100	-4.45422400	-1.36406300
H	-0.00275800	-4.02156700	0.59955400
O	-1.12148200	0.12129400	1.55086100
O	-0.01615000	-3.89458700	1.61043600
O	1.03715500	1.51733300	0.02564900
O	1.31466100	0.15648700	2.20485200
O	-0.07415000	-1.09200400	4.08258300
O	-0.15897700	1.52335600	4.01347900
O	0.09480700	-1.74437100	-3.77585600
O	1.03800800	-1.47090100	0.22956700
O	-1.41953200	-2.05716700	0.21376600
O	-0.02039500	-3.97532700	-1.00071800
O	-0.09157600	4.00265600	1.23035100

O	0.037192000	3.931320000	-1.390165000
O	-1.426412000	2.091039000	-0.060189000
O	0.085864000	1.346496000	-3.944986000
O	1.379617000	-0.116306000	-1.933307000
O	-1.067863000	-0.084392000	-1.402269000
Zr	2.452979000	0.001769000	0.156122000
Zr	-0.089436000	-1.622011000	2.036512000
Zr	-0.043530000	1.958242000	1.745182000
Zr	-0.027101000	1.645974000	-1.816473000
Zr	-2.541614000	-0.001326000	0.049861000
Zr	0.022137000	-1.941698000	-1.583339000
Fe	0.855059000	-0.289492000	-4.902686000
C	3.949054000	0.188975000	-4.560961000
C	4.291361000	0.811901000	-5.856292000
H	0.862725000	-0.195276000	-6.539314000
H	4.740527000	0.085891000	-3.797897000
H	3.429929000	0.823927000	-6.527100000
H	4.643365000	1.837256000	-5.680802000
H	5.128004000	0.282180000	-6.325345000
O	2.814316000	-0.215686000	-4.266837000
H	2.070282000	-0.165397000	-2.610596000

Fe-NU-1000 (Prod-deCH<sub>3</sub>CHO)

Free Energy: -4058.821544

Electronic Energy: -4058.9971256

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388901000	-3.187672000	-2.460036000
C	-4.293003000	-3.161878000	-2.734624000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341401000	3.021272000	-2.724833000
C	-4.324802000	2.871980000	-3.008020000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223386000	-2.332157000	-2.105837000
C	-3.315213000	-2.089525000	2.441212000
C	-3.322917000	2.330126000	2.211514000
C	3.188502000	2.437017000	2.193685000
C	3.241981000	2.241896000	-2.086036000
C	3.280272000	-2.402298000	-1.851735000
C	-3.245496000	2.084661000	-2.346745000

C	3.174600000	-2.211115000	2.426590000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101092000	-2.666632000	2.881873000
H	3.964843000	3.004756000	2.662576000
H	-4.111856000	2.914455000	2.636914000
H	3.948377000	-2.768402000	2.911970000
O	-3.663674000	1.472110000	1.337384000
O	-3.610011000	1.255303000	-1.456767000
O	-3.653962000	-1.258617000	1.542889000
O	-2.127302000	-2.310070000	2.835706000
O	1.970297000	-2.521744000	2.683639000
O	2.089956000	-2.743247000	-2.140488000
O	3.548165000	-1.286123000	1.640812000
O	3.614268000	-1.448332000	-1.083778000
O	3.557179000	1.485729000	1.438507000
O	3.591867000	1.320230000	-1.285380000
O	2.046359000	2.548335000	-2.386304000
O	1.986485000	2.771246000	2.435747000
O	-2.020185000	-2.554912000	-2.444513000
O	-3.604007000	-1.474621000	-1.248470000
O	-2.134311000	2.562251000	2.592320000
O	-2.045069000	2.317150000	-2.694194000
H	-1.964309000	-2.849769000	0.222773000
H	-1.031861000	1.819568000	4.286732000
H	-0.139352000	0.512611000	4.136614000
H	-0.794802000	1.597028000	-4.360615000
H	0.001456000	4.078717000	-0.379169000
H	0.636540000	4.485475000	1.636867000
H	0.916897000	4.228091000	-1.668854000
H	1.858116000	0.164138000	3.001049000
H	-1.969980000	2.883287000	-0.089832000
H	-0.811791000	-1.493085000	4.546063000
H	-0.783515000	-2.101260000	-4.121772000
H	0.836986000	-4.202499000	1.954146000
H	0.698236000	-4.491291000	-1.373073000
H	-0.000023000	-4.036478000	0.611103000
O	-1.116930000	0.120514000	1.543161000

O	-0.014032000	-3.892881000	1.619096000
O	1.041888000	1.499670000	0.014795000
O	1.318544000	0.155041000	2.203124000
O	-0.075613000	-1.092436000	4.071810000
O	-0.156948000	1.521767000	4.005827000
O	0.081392000	-1.865671000	-3.768890000
O	1.045693000	-1.452687000	0.206021000
O	-1.413128000	-2.059688000	0.208962000
O	-0.027454000	-3.991656000	-0.984107000
O	-0.084996000	3.998001000	1.225452000
O	0.037386000	3.944338000	-1.386081000
O	-1.420984000	2.091856000	-0.064878000
O	0.052761000	1.384706000	-3.954911000
O	1.404192000	-0.110798000	-2.080835000
O	-1.028837000	-0.084852000	-1.413032000
Zr	2.471940000	0.003369000	0.164651000
Zr	-0.084865000	-1.621808000	2.029333000
Zr	-0.039923000	1.955909000	1.741699000
Zr	-0.022551000	1.672515000	-1.819093000
Zr	-2.530996000	-0.002984000	0.041097000
Zr	0.027256000	-1.973674000	-1.588864000
Fe	1.027224000	-0.282772000	-4.492822000
H	2.338884000	-0.292859000	-5.444531000
H	2.273665000	-0.085547000	-2.508182000

Fe-NU-1000 (TS3\_2)

Free Energy: -4058.797888

Electronic Energy: -4058.969866

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000

C	3.24200000	2.24200000	-2.08600000
C	3.28030000	-2.40240000	-1.85170000
C	-3.24550000	2.08480000	-2.34670000
C	3.17460000	-2.21110000	2.42660000
H	5.93700000	-2.05670000	-1.49580000
H	-5.87170000	-2.04820000	-1.80050000
H	3.07080000	-4.46690000	-3.57330000
H	-2.94310000	-4.45000000	-3.79820000
H	4.90090000	-5.84720000	-4.52440000
H	-4.73720000	-5.87310000	-4.74900000
H	7.78600000	-3.41650000	-2.44510000
H	-7.68620000	-3.45250000	-2.74720000
H	5.87480000	1.98160000	-1.64250000
H	-5.89900000	1.83020000	-1.98630000
H	3.03890000	4.19850000	-3.96280000
H	-2.97830000	4.10040000	-4.14500000
H	4.87690000	5.53410000	-4.95980000
H	-4.77430000	5.49830000	-5.13120000
H	7.73460000	3.29050000	-2.64450000
H	-7.71490000	3.20560000	-2.97220000
H	-7.13990000	-5.40920000	-4.21020000
H	7.28610000	-5.35680000	-3.94480000
H	-7.17290000	5.07750000	-4.54480000
H	7.25200000	5.10910000	-4.29360000
H	-4.10109400	-2.66661800	2.88188700
H	3.96484300	3.00475000	2.66258300
H	-4.11185900	2.91444000	2.63693000
H	3.94837700	-2.76839700	2.91197600
O	-3.66370000	1.47210000	1.33740000
O	-3.61000000	1.25540000	-1.45670000
O	-3.65400000	-1.25860000	1.54290000
O	-2.12730000	-2.31020000	2.83570000
O	1.97030000	-2.52180000	2.68360000
O	2.09000000	-2.74270000	-2.14060000
O	3.54820000	-1.28610000	1.64080000
O	3.61420000	-1.44840000	-1.08370000
O	3.55720000	1.48570000	1.43850000
O	3.59180000	1.32030000	-1.28530000
O	2.04640000	2.54780000	-2.38640000
O	1.98650000	2.77130000	2.43570000
O	-2.02020000	-2.55450000	-2.44470000
O	-3.60400000	-1.47470000	-1.24840000
O	-2.13430000	2.56240000	2.59230000
O	-2.04510000	2.31670000	-2.69430000
H	-1.95706100	-2.85611900	0.22594800
H	-1.03629100	1.81821600	4.29490200
H	-0.13731200	0.51565700	4.14780700
H	-0.75224500	1.65922000	-4.40855100
H	0.00572400	4.07025600	-0.38303000
H	0.63964400	4.48104500	1.63780800
H	0.93427900	4.19503400	-1.66295600
H	1.87081600	0.16627100	2.98963900
H	-1.96152600	2.87772800	-0.10141700
H	-0.81660700	-1.48882600	4.55860500
H	-0.81163500	-2.14245400	-4.09744400
H	0.84301800	-4.19085200	1.96536500

H	0.721826000	-4.471065000	-1.355960000
H	0.003320000	-4.035161000	0.624777000
O	-1.115330000	0.119062000	1.540754000
O	-0.013790000	-3.893609000	1.632956000
O	1.041563000	1.514750000	0.024574000
O	1.315741000	0.156262000	2.202630000
O	-0.078690000	-1.089666000	4.085868000
O	-0.159602000	1.524334000	4.015785000
O	0.097728000	-1.976927000	-3.817837000
O	1.046438000	-1.467429000	0.224907000
O	-1.413815000	-2.060586000	0.219169000
O	-0.016686000	-3.985770000	-0.973017000
O	-0.089386000	3.997996000	1.234310000
O	0.046370000	3.930530000	-1.386706000
O	-1.419252000	2.082368000	-0.061083000
O	0.099394000	1.458049000	-4.005607000
O	1.373109000	-0.107427000	-2.023907000
O	-1.081872000	-0.097428000	-1.438743000
Zr	2.470437000	0.005943000	0.128755000
Zr	-0.082854000	-1.619502000	2.044152000
Zr	-0.039426000	1.957256000	1.751345000
Zr	-0.009783000	1.644269000	-1.798229000
Zr	-2.539191000	-0.002146000	0.044236000
Zr	0.034370000	-1.955495000	-1.548489000
Fe	0.961665000	-0.301538000	-4.146768000
H	2.716006000	-0.164557000	-3.849901000
H	2.288832000	-0.129747000	-2.905770000

Fe-NU-1000 (Prod-H<sub>2</sub>)

Free Energy: -4058.823065

Electronic Energy: -4058.9955589

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388899000	-3.187746000	-2.459942000
C	-4.292996000	-3.161929000	-2.734568000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341399000	3.021340000	-2.724754000
C	-4.324797000	2.872031000	-3.007969000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223415000	-2.332576000	-2.105681000

C	-3.315183000	-2.089466000	2.441192000
C	-3.322881000	2.330058000	2.211495000
C	3.188495000	2.436983000	2.193714000
C	3.242024000	2.242188000	-2.085903000
C	3.280347000	-2.402590000	-1.851618000
C	-3.245502000	2.085056000	-2.346593000
C	3.174605000	-2.211094000	2.426611000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101097000	-2.666604000	2.881901000
H	3.964843000	3.004747000	2.662587000
H	-4.111861000	2.914425000	2.636946000
H	3.948377000	-2.768393000	2.911980000
O	-3.663720000	1.472067000	1.337432000
O	-3.610004000	1.255546000	-1.456584000
O	-3.654027000	-1.258567000	1.542926000
O	-2.127291000	-2.310324000	2.835676000
O	1.970306000	-2.521850000	2.683544000
O	2.089991000	-2.742020000	-2.140838000
O	3.548208000	-1.286046000	1.640824000
O	3.614159000	-1.448511000	-1.083570000
O	3.557217000	1.485647000	1.438525000
O	3.591773000	1.320406000	-1.285186000
O	2.046419000	2.547174000	-2.386617000
O	1.986512000	2.771353000	2.435639000
O	-2.020230000	-2.553983000	-2.445011000
O	-3.604001000	-1.474831000	-1.248275000
O	-2.134293000	2.562529000	2.592259000
O	-2.045110000	2.316156000	-2.694567000
H	-1.958927000	-2.857499000	0.231392000
H	-1.040611000	1.812791000	4.311162000
H	-0.137894000	0.512878000	4.159466000
H	-0.680663000	1.422170000	-4.414408000
H	0.006002000	4.068443000	-0.374039000
H	0.643695000	4.476704000	1.649340000
H	0.938137000	4.186521000	-1.649328000
H	1.878890000	0.167184000	2.986561000
H	-1.961076000	2.884339000	-0.095219000

H	-0.819730000	-1.488912000	4.569486000
H	-0.707829000	-1.944803000	-4.165240000
H	0.843648000	-4.182613000	1.966303000
H	0.739723000	-4.448103000	-1.340274000
H	0.003617000	-4.025155000	0.625630000
O	-1.117839000	0.120391000	1.546475000
O	-0.016570000	-3.891759000	1.636902000
O	1.039162000	1.529712000	0.039216000
O	1.312134000	0.158105000	2.208083000
O	-0.081215000	-1.089531000	4.097984000
O	-0.163624000	1.522605000	4.029855000
O	0.174670000	-1.874842000	-3.782460000
O	1.042038000	-1.474715000	0.242215000
O	-1.421502000	-2.058181000	0.229885000
O	-0.009683000	-3.973425000	-0.966119000
O	-0.093526000	4.000911000	1.252075000
O	0.048350000	3.926857000	-1.376016000
O	-1.425236000	2.085309000	-0.046720000
O	0.177841000	1.378128000	-3.978229000
O	1.337308000	-0.106294000	-1.968629000
O	-1.125446000	-0.094118000	-1.432451000
Zr	2.456112000	0.004895000	0.112818000
Zr	-0.085121000	-1.617875000	2.053786000
Zr	-0.043877000	1.958690000	1.766324000
Zr	-0.014222000	1.624549000	-1.765109000
Zr	-2.552989000	-0.000927000	0.052637000
Zr	0.020184000	-1.930652000	-1.529549000
Fe	1.228130000	-0.264933000	-3.930167000
H	2.725857000	-0.301467000	-4.928038000
H	2.995156000	-0.250350000	-4.158051000

### Reaction on Fe-Hf-NU-1000

Fe-Hf-NU-1000-O

Free Energy: -4138.843903

Electronic Energy: -4138.9967777

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000



C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.964626000	-2.853542000	0.223683000
H	-1.012932000	1.831350000	4.298973000
H	-0.129475000	0.515627000	4.135749000
H	-0.482249000	1.443494000	-4.603475000
H	0.000910000	4.067364000	-0.377019000

H	0.617075000	4.492774000	1.638663000
H	0.919053000	4.203001000	-1.668493000
H	1.868234000	0.162495000	2.982124000
H	-1.964339000	2.889533000	-0.087650000
H	-0.790330000	-1.483671000	4.568229000
H	0.174062000	-2.374240000	-4.477459000
H	0.825233000	-4.192941000	1.956138000
H	0.752446000	-4.438800000	-1.329814000
H	-0.008764000	-4.014423000	0.611165000
O	-1.122084000	0.121723000	1.539260000
O	-0.021455000	-3.872381000	1.620443000
O	1.036687000	1.499807000	0.013525000
O	1.318988000	0.153791000	2.191116000
O	-0.071250000	-1.080042000	4.072522000
O	-0.147903000	1.526628000	3.996849000
O	0.172374000	-1.719344000	-3.773827000
O	1.037700000	-1.455385000	0.207838000
O	-1.422639000	-2.057284000	0.220129000
O	-0.016372000	-3.968586000	-0.991599000
O	-0.090627000	3.987629000	1.226519000
O	0.038562000	3.923555000	-1.383976000
O	-1.427740000	2.090166000	-0.054877000
O	0.207886000	1.351973000	-3.940241000
O	1.351483000	-0.103140000	-2.061892000
O	-1.096534000	-0.087598000	-1.422870000
Hf	2.483701000	0.006959000	0.119580000
Hf	-0.083535000	-1.609050000	2.032202000
Hf	-0.042725000	1.946953000	1.744584000
Hf	-0.034712000	1.652881000	-1.782574000
Hf	-2.562309000	-0.002679000	0.044997000
Hf	0.002538000	-1.931689000	-1.545570000
Fe	1.317226000	-0.238173000	-3.912398000
O	2.011533000	-0.407848000	-5.371803000

Fe-Hf-NU-1000 (Ads\_3)

Free Energy: -4293.823934

Electronic Energy: -4294.05740768

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000

C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.955466000	-2.857846000	0.227344000
H	-1.020427000	1.824731000	4.282908000
H	-0.130106000	0.513641000	4.127938000

H	-0.414775000	1.541774000	-4.666936000
H	-0.003055000	4.048878000	-0.399842000
H	0.621331000	4.486186000	1.628460000
H	0.925032000	4.168301000	-1.677747000
H	1.869045000	0.163088000	2.979285000
H	-1.956839000	2.882062000	-0.095190000
H	-0.795806000	-1.483885000	4.558557000
H	-0.516763000	-2.095800000	-4.369890000
H	0.827854000	-4.189804000	1.950983000
H	0.727167000	-4.442733000	-1.347783000
H	0.001478000	-4.006691000	0.595948000
O	-1.123130000	0.120302000	1.542565000
O	-0.017589000	-3.870048000	1.612246000
O	1.040195000	1.491359000	0.005539000
O	1.320346000	0.153411000	2.188143000
O	-0.070407000	-1.083914000	4.069156000
O	-0.149782000	1.524988000	3.991808000
O	0.180798000	-1.873826000	-3.745965000
O	1.042312000	-1.450573000	0.204690000
O	-1.424065000	-2.054722000	0.223312000
O	-0.018233000	-3.960127000	-0.977696000
O	-0.090458000	3.983643000	1.220495000
O	0.037287000	3.903367000	-1.403040000
O	-1.425990000	2.079534000	-0.053543000
O	0.193512000	1.368699000	-3.943163000
O	1.286660000	-0.113437000	-2.136786000
O	-1.132045000	-0.097540000	-1.424584000
Hf	2.477231000	0.000695000	0.113224000
Hf	-0.082420000	-1.611110000	2.025725000
Hf	-0.041716000	1.943576000	1.735794000
Hf	-0.035200000	1.610201000	-1.795466000
Hf	-2.567282000	-0.002670000	0.050682000
Hf	0.000918000	-1.917341000	-1.557791000
Fe	1.190053000	-0.273521000	-4.081133000
O	1.115669000	-0.334564000	-5.718277000
C	4.040184000	0.203568000	-4.844511000
C	5.485701000	0.052519000	-4.459435000
H	3.852462000	0.103087000	-5.918531000
H	3.642235000	1.176090000	-4.535944000
H	5.583568000	0.110824000	-3.371521000
H	5.894792000	-0.906709000	-4.793561000
H	6.080401000	0.855678000	-4.904690000
O	3.236988000	-0.773555000	-4.128137000
H	3.299150000	-1.621131000	-4.592346000

Fe-Hf-NU-1000 (TS1\_3)

Free Energy: -4293.807869

Electronic Energy: -4294.03598764

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000

C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000

O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.953359000	-2.853152000	0.222507000
H	-1.013498000	1.829993000	4.280593000
H	-0.131921000	0.512473000	4.121413000
H	-0.579759000	1.568253000	-4.580835000
H	0.008309000	4.067742000	-0.388485000
H	0.621541000	4.488782000	1.636221000
H	0.925345000	4.193480000	-1.681078000
H	1.860788000	0.160997000	2.988277000
H	-1.956016000	2.890090000	-0.086973000
H	-0.794442000	-1.486658000	4.545692000
H	-0.487629000	-2.045311000	-4.419113000
H	0.826028000	-4.195290000	1.946927000
H	0.714014000	-4.454210000	-1.361405000
H	0.001541000	-4.009922000	0.590671000
O	-1.121287000	0.122310000	1.538078000
O	-0.013922000	-3.865729000	1.604188000
O	1.045887000	1.475469000	-0.001805000
O	1.325018000	0.152711000	2.188061000
O	-0.069820000	-1.084313000	4.056899000
O	-0.146664000	1.523822000	3.984536000
O	0.172084000	-1.817036000	-3.756977000
O	1.046266000	-1.428059000	0.179999000
O	-1.417721000	-2.052635000	0.214386000
O	-0.023007000	-3.962060000	-0.986560000
O	-0.082392000	3.982451000	1.219339000
O	0.042511000	3.923344000	-1.393695000
O	-1.421899000	2.088932000	-0.057454000
O	0.121365000	1.438206000	-3.935637000
O	1.320962000	-0.103848000	-2.225874000
O	-1.093797000	-0.087430000	-1.423486000
Hf	2.503972000	0.010335000	0.130915000
Hf	-0.079112000	-1.608275000	2.014580000
Hf	-0.038577000	1.941785000	1.731404000
Hf	-0.031647000	1.651742000	-1.799021000
Hf	-2.558674000	-0.001491000	0.042855000
Hf	0.004918000	-1.928500000	-1.571891000
Fe	1.154296000	-0.207593000	-4.079435000
O	1.018811000	-0.297658000	-5.794048000
C	4.026200000	-0.664415000	-4.828816000
C	5.209875000	-0.188437000	-4.030017000
H	3.651206000	-1.626470000	-4.444625000
H	4.307240000	-0.841887000	-5.876673000
H	5.574291000	0.765183000	-4.422790000
H	4.936967000	-0.046515000	-2.979211000
H	6.021820000	-0.920186000	-4.082942000
O	2.985495000	0.315583000	-4.810059000
H	2.170804000	0.090562000	-5.697526000

Fe-Hf-NU-1000 (Int\_3)

Free Energy: -4293.841505

Electronic Energy: -4294.07253596

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000

H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.967548000	-2.848487000	0.226611000
H	-1.016454000	1.833379000	4.282593000
H	-0.129490000	0.520344000	4.128145000
H	-0.574657000	1.208416000	-4.457402000
H	0.004190000	4.065300000	-0.388262000
H	0.621695000	4.491975000	1.633976000
H	0.924994000	4.193778000	-1.677269000
H	1.864966000	0.166485000	2.983075000
H	-1.961186000	2.892608000	-0.085380000
H	-0.792917000	-1.481162000	4.559190000
H	0.270791000	-2.403950000	-4.318862000
H	0.828579000	-4.188949000	1.941023000
H	0.760427000	-4.422602000	-1.332383000
H	-0.009146000	-4.006549000	0.597537000
O	-1.123120000	0.123693000	1.540805000
O	-0.019158000	-3.868513000	1.608204000
O	1.039897000	1.490689000	0.003010000
O	1.321131000	0.155663000	2.188458000
O	-0.069671000	-1.079476000	4.067942000
O	-0.147562000	1.530651000	3.989242000
O	0.147628000	-1.648998000	-3.735328000
O	1.041092000	-1.445668000	0.201581000
O	-1.425457000	-2.052547000	0.221691000
O	-0.018576000	-3.962724000	-1.003788000
O	-0.086175000	3.988105000	1.220730000
O	0.041071000	3.922863000	-1.394140000
O	-1.426172000	2.092132000	-0.057179000
O	0.219571000	1.318360000	-3.924224000
O	1.352377000	-0.111299000	-2.071410000
O	-1.099147000	-0.080950000	-1.420708000
Hf	2.493803000	0.012735000	0.118481000
Hf	-0.081604000	-1.605336000	2.026205000
Hf	-0.040316000	1.946430000	1.732687000
Hf	-0.028458000	1.653068000	-1.804709000
Hf	-2.560913000	0.001423000	0.045352000
Hf	-0.005666000	-1.917328000	-1.549580000



Fe	1.517642000	-0.249541000	-3.901942000
O	1.526469000	-0.574278000	-5.687322000
C	4.153951000	-0.440333000	-4.880157000
C	5.528501000	0.154826000	-4.660809000
H	4.181813000	-1.532982000	-4.731396000
H	3.798006000	-0.264018000	-5.905022000
H	5.533981000	1.224930000	-4.884664000
H	5.839506000	0.025598000	-3.619932000
H	6.257018000	-0.343134000	-5.308079000
O	3.264076000	0.146092000	-3.959828000
H	0.632375000	-0.823641000	-5.957014000

Fe-Hf-NU-1000 (TS2\_3)

Free Energy: -4293.82665

Electronic Energy: -4294.05058362

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000

H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.958452000	-2.854710000	0.225631000
H	-1.023316000	1.818512000	4.297890000
H	-0.130937000	0.508720000	4.138935000
H	-0.696499000	1.245269000	-4.349680000
H	-0.002594000	4.062455000	-0.368044000
H	0.618956000	4.489474000	1.646239000
H	0.923302000	4.195792000	-1.650744000
H	1.871657000	0.157669000	2.985250000
H	-1.966245000	2.884684000	-0.083223000
H	-0.796030000	-1.488616000	4.566107000
H	-0.595803000	-1.814720000	-4.270005000
H	0.830528000	-4.188449000	1.954871000
H	0.714052000	-4.456196000	-1.350131000
H	-0.004295000	-4.012759000	0.608113000
O	-1.121354000	0.121415000	1.546300000
O	-0.019417000	-3.874451000	1.621310000
O	1.043936000	1.513263000	0.030012000
O	1.318602000	0.151930000	2.197122000
O	-0.071854000	-1.086221000	4.076913000
O	-0.152691000	1.520872000	4.005004000
O	0.220358000	-1.765059000	-3.762178000
O	1.039176000	-1.460766000	0.216276000
O	-1.422336000	-2.054674000	0.220581000
O	-0.026111000	-3.966520000	-0.978023000
O	-0.096250000	3.990514000	1.239605000

O	0.039019000	3.921365000	-1.374679000
O	-1.429595000	2.085752000	-0.048600000
O	0.152702000	1.315570000	-3.901059000
O	1.369256000	-0.092933000	-2.007807000
O	-1.103088000	-0.092836000	-1.422959000
Hf	2.477519000	0.002311000	0.113286000
Hf	-0.080789000	-1.612362000	2.032374000
Hf	-0.040242000	1.946411000	1.751403000
Hf	-0.026530000	1.638943000	-1.768963000
Hf	-2.554898000	-0.003685000	0.050589000
Hf	0.016695000	-1.931776000	-1.553941000
Fe	1.477354000	-0.256400000	-3.884775000
O	1.826552000	0.251252000	-5.756779000
C	4.095655000	-0.481576000	-5.066893000
C	4.681145000	-1.650064000	-5.813559000
H	3.175060000	0.041015000	-5.776740000
H	4.777006000	0.374852000	-4.906318000
H	5.405028000	-2.176802000	-5.178803000
H	3.901527000	-2.368083000	-6.083674000
H	5.192799000	-1.321932000	-6.722175000
O	3.343140000	-0.771386000	-4.010881000
H	1.559654000	1.155982000	-5.971038000

Fe-Hf-NU-1000 (Prod\_3)

Free Energy: -4293.86248

Electronic Energy: -4294.0909427

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000

C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.970679000	-2.846590000	0.216574000
H	-1.027393000	1.815899000	4.292332000
H	-0.128944000	0.510889000	4.134110000
H	-0.581639000	1.486785000	-4.500816000
H	-0.004552000	4.051986000	-0.387701000
H	0.622896000	4.488375000	1.637911000
H	0.923612000	4.183100000	-1.664166000
H	1.881178000	0.160234000	2.963675000
H	-1.965246000	2.877950000	-0.102632000
H	-0.800141000	-1.481865000	4.564549000
H	0.881692000	-2.739117000	-3.937255000
H	0.828046000	-4.180414000	1.941686000
H	0.769316000	-4.416873000	-1.307964000
H	-0.008776000	-3.994496000	0.596060000

O	-1.121828000	0.122000000	1.538964000
O	-0.026662000	-3.873743000	1.613559000
O	1.036994000	1.528814000	0.025238000
O	1.312281000	0.154192000	2.187062000
O	-0.072525000	-1.083948000	4.076882000
O	-0.154363000	1.523246000	4.001812000
O	0.231554000	-2.037042000	-3.804170000
O	1.033742000	-1.481440000	0.221364000
O	-1.430852000	-2.049370000	0.221341000
O	-0.008527000	-3.951484000	-0.986365000
O	-0.100265000	3.995643000	1.237789000
O	0.038197000	3.910486000	-1.391004000
O	-1.428754000	2.079707000	-0.054379000
O	0.196298000	1.399109000	-3.941226000
O	1.332231000	-0.105253000	-2.008804000
O	-1.136263000	-0.095487000	-1.446846000
Hf	2.432864000	0.006420000	0.102519000
Hf	-0.087619000	-1.613076000	2.030982000
Hf	-0.048088000	1.953307000	1.746419000
Hf	-0.019578000	1.615332000	-1.793411000
Hf	-2.563440000	-0.003165000	0.045264000
Hf	-0.003994000	-1.901095000	-1.566504000
Fe	1.238144000	-0.289295000	-4.021257000
O	0.302701000	-0.637978000	-6.114670000
C	4.149174000	-1.137032000	-4.711220000
C	4.906812000	-0.089035000	-3.999606000
H	4.693206000	-1.934078000	-5.244698000
H	0.934471000	-1.029591000	-6.725849000
H	4.680581000	0.894136000	-4.432955000
H	4.580324000	-0.043015000	-2.950345000
H	5.984333000	-0.254041000	-4.042927000
O	2.906912000	-1.165405000	-4.747547000
H	-0.153288000	-1.393094000	-5.700895000

**Reaction on Fe-Ti-NU-1000**

Fe-Ti-NU-1000-O

Free Energy: -4200.160371

Electronic Energy: -4200.325477

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000

C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.918698000	-2.722549000	0.224199000
H	-0.993390000	1.922916000	3.892116000

H	-0.151105000	0.577926000	3.881593000
H	-0.680630000	1.569315000	-4.170394000
H	0.045520000	3.816968000	-0.458675000
H	0.682601000	4.093923000	1.704619000
H	0.886039000	3.794600000	-1.800147000
H	1.819597000	0.149612000	2.839903000
H	-1.888294000	2.767438000	-0.085095000
H	-0.833290000	-1.555496000	4.167743000
H	-0.695192000	-2.038165000	-3.931427000
H	0.816224000	-3.797593000	2.039489000
H	0.769544000	-4.050417000	-1.424635000
H	0.028893000	-3.759622000	0.658771000
O	-1.121768000	0.114869000	1.448040000
O	-0.044923000	-3.579388000	1.640289000
O	1.032990000	1.393675000	-0.004626000
O	1.288661000	0.144628000	2.032810000
O	-0.082722000	-1.110159000	3.748650000
O	-0.109629000	1.558999000	3.704166000
O	0.105375000	-1.780614000	-3.453656000
O	1.042259000	-1.350482000	0.181791000
O	-1.396859000	-1.909478000	0.210227000
O	-0.007541000	-3.653936000	-1.003652000
O	-0.058275000	3.665244000	1.251139000
O	-0.001525000	3.621981000	-1.432584000
O	-1.389009000	1.941072000	-0.042105000
O	0.072643000	1.313121000	-3.622971000
O	1.266611000	-0.109275000	-1.928923000
O	-1.131455000	-0.079542000	-1.322770000
Ti	2.430109000	-0.034737000	0.098895000
Ti	-0.124213000	-1.460931000	1.894333000
Ti	0.022046000	1.814092000	1.588850000
Ti	-0.082174000	1.475223000	-1.632100000
Ti	-2.519426000	0.004953000	0.053972000
Ti	-0.005353000	-1.807594000	-1.421336000
Fe	1.154370000	-0.252424000	-3.803320000
O	1.528016000	-0.330369000	-5.377424000

Fe-Ti-NU-1000 (Ads\_3)

Free Energy: -4355.148865

Electronic Energy: -4355.39421433

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000

C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000



H	-1.924023000	-2.714490000	0.222447000
H	-0.994284000	1.919523000	3.881783000
H	-0.150285000	0.576175000	3.872886000
H	-0.703368000	1.596666000	-4.163624000
H	0.046881000	3.804363000	-0.467958000
H	0.685388000	4.087956000	1.700791000
H	0.881297000	3.787140000	-1.809312000
H	1.822656000	0.147795000	2.832677000
H	-1.884002000	2.760782000	-0.092796000
H	-0.837233000	-1.553853000	4.160077000
H	-0.707232000	-2.085017000	-3.927113000
H	0.818368000	-3.789271000	2.014518000
H	0.787678000	-4.014432000	-1.413774000
H	0.027461000	-3.736130000	0.631891000
O	-1.121647000	0.116176000	1.447329000
O	-0.044706000	-3.571817000	1.619768000
O	1.037093000	1.391431000	-0.009824000
O	1.287840000	0.142603000	2.028415000
O	-0.083669000	-1.111207000	3.743802000
O	-0.108502000	1.557898000	3.698767000
O	0.100277000	-1.815767000	-3.468225000
O	1.039240000	-1.344203000	0.170204000
O	-1.403060000	-1.901138000	0.208043000
O	-0.006716000	-3.634651000	-1.010929000
O	-0.058677000	3.664193000	1.248003000
O	-0.004678000	3.613902000	-1.441301000
O	-1.386863000	1.933599000	-0.045169000
O	0.078775000	1.381289000	-3.638588000
O	1.194066000	-0.104423000	-1.975446000
O	-1.165130000	-0.084128000	-1.338020000
Ti	2.407018000	-0.041518000	0.094560000
Ti	-0.127687000	-1.459463000	1.887240000
Ti	0.023557000	1.812320000	1.579946000
Ti	-0.082275000	1.451765000	-1.652001000
Ti	-2.523196000	0.006989000	0.051531000
Ti	-0.025928000	-1.783616000	-1.455348000
Fe	1.068579000	-0.230417000	-3.940809000
O	0.864727000	-0.285564000	-5.558391000
C	3.899903000	0.247305000	-4.840449000
C	5.349853000	0.054115000	-4.493825000
H	3.676243000	0.121011000	-5.905225000
H	3.541179000	1.237406000	-4.540691000
H	5.481352000	0.123646000	-3.410251000
H	5.718487000	-0.921952000	-4.827169000
H	5.956198000	0.831153000	-4.968172000
O	3.089237000	-0.683591000	-4.070469000
H	3.183935000	-1.571988000	-4.445000000

Fe-Ti-NU-1000 (TS1\_3)

Free Energy: -4355.127378

Electronic Energy: -4355.36762066

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000

C	-3.98600000	-4.23630000	-3.58270000
C	5.13820000	-5.02070000	-3.85940000
C	-4.99820000	-5.03520000	-4.10760000
C	6.48280000	-4.75120000	-3.53770000
C	-6.35110000	-4.78220000	-3.80710000
C	6.75580000	-3.65750000	-2.69490000
C	-6.64970000	-3.67970000	-2.98340000
C	5.67340000	2.76200000	-2.36940000
C	-5.66880000	2.62890000	-2.68460000
C	4.34140000	3.02130000	-2.72480000
C	-4.32480000	2.87200000	-3.00800000
C	4.06990000	4.01780000	-3.67330000
C	-4.01940000	3.90710000	-3.90490000
C	5.10590000	4.76070000	-4.23120000
C	-5.03300000	4.69270000	-4.44890000
C	6.44470000	4.52640000	-3.86170000
C	-6.38420000	4.46260000	-4.12340000
C	6.70820000	3.50040000	-2.93460000
C	-6.68050000	3.40860000	-3.23760000
C	-3.22340000	-2.33230000	-2.10580000
C	-3.31520000	-2.08950000	2.44120000
C	-3.32290000	2.33010000	2.21150000
C	3.18850000	2.43700000	2.19370000
C	3.24200000	2.24200000	-2.08600000
C	3.28030000	-2.40240000	-1.85170000
C	-3.24550000	2.08480000	-2.34670000
C	3.17460000	-2.21110000	2.42660000
H	5.93700000	-2.05670000	-1.49580000
H	-5.87170000	-2.04820000	-1.80050000
H	3.07080000	-4.46690000	-3.57330000
H	-2.94310000	-4.45000000	-3.79820000
H	4.90090000	-5.84720000	-4.52440000
H	-4.73720000	-5.87310000	-4.74900000
H	7.78600000	-3.41650000	-2.44510000
H	-7.68620000	-3.45250000	-2.74720000
H	5.87480000	1.98160000	-1.64250000
H	-5.89900000	1.83020000	-1.98630000
H	3.03890000	4.19850000	-3.96280000
H	-2.97830000	4.10040000	-4.14500000
H	4.87690000	5.53410000	-4.95980000
H	-4.77430000	5.49830000	-5.13120000
H	7.73460000	3.29050000	-2.64450000
H	-7.71490000	3.20560000	-2.97220000
H	-7.13990000	-5.40920000	-4.21020000
H	7.28610000	-5.35680000	-3.94480000
H	-7.17290000	5.07750000	-4.54480000
H	7.25200000	5.10910000	-4.29360000
H	-4.10109400	-2.66661800	2.88188700
H	3.96484300	3.00475000	2.66258300
H	-4.11185900	2.91444000	2.63693000
H	3.94837700	-2.76839700	2.91197600
O	-3.66370000	1.47210000	1.33740000
O	-3.61000000	1.25540000	-1.45670000
O	-3.65400000	-1.25860000	1.54290000
O	-2.12730000	-2.31020000	2.83570000
O	1.97030000	-2.52180000	2.68360000

O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.915910000	-2.708849000	0.215356000
H	-0.991323000	1.926271000	3.866454000
H	-0.152540000	0.579948000	3.864554000
H	-0.760838000	1.602497000	-4.115709000
H	0.054016000	3.823326000	-0.469936000
H	0.680249000	4.094528000	1.700836000
H	0.892031000	3.801938000	-1.814252000
H	1.815865000	0.148764000	2.837652000
H	-1.879083000	2.768620000	-0.085477000
H	-0.838171000	-1.552232000	4.144913000
H	-0.719909000	-2.012806000	-3.930926000
H	0.816941000	-3.792626000	2.019017000
H	0.764372000	-4.046206000	-1.434093000
H	0.030373000	-3.745770000	0.634175000
O	-1.114232000	0.119968000	1.437583000
O	-0.041214000	-3.567650000	1.618129000
O	1.049366000	1.381470000	-0.023881000
O	1.295125000	0.142884000	2.023943000
O	-0.082752000	-1.108744000	3.731998000
O	-0.105961000	1.560348000	3.687061000
O	0.101805000	-1.794353000	-3.468652000
O	1.053808000	-1.325342000	0.145996000
O	-1.391298000	-1.897623000	0.199002000
O	-0.008335000	-3.642899000	-1.012514000
O	-0.051904000	3.662224000	1.237242000
O	0.004556000	3.631879000	-1.444189000
O	-1.378649000	1.942391000	-0.054561000
O	0.049614000	1.403664000	-3.626775000
O	1.254233000	-0.100430000	-2.034240000
O	-1.123439000	-0.074810000	-1.341260000
Ti	2.443838000	-0.026907000	0.106016000
Ti	-0.120173000	-1.455050000	1.877446000
Ti	0.031906000	1.809909000	1.568930000
Ti	-0.072523000	1.490817000	-1.662938000
Ti	-2.509438000	0.007432000	0.036192000
Ti	-0.002181000	-1.797807000	-1.455614000
Fe	1.083213000	-0.217559000	-3.903361000
O	0.866725000	-0.292305000	-5.604126000
C	3.923507000	-0.668529000	-4.776583000
C	5.135981000	-0.189108000	-4.025467000
H	3.578033000	-1.642604000	-4.397424000
H	4.151600000	-0.817605000	-5.841278000
H	5.474434000	0.771556000	-4.423727000
H	4.910636000	-0.061133000	-2.962009000
H	5.949265000	-0.914446000	-4.124895000

O	2.867779000	0.295721000	-4.688657000
H	2.009718000	0.087225000	-5.565530000

Fe-Ti-NU-1000 (Int\_3)

Free Energy: -4355.165108

Electronic Energy: -4355.40682698

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000

H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.914873000	-2.723865000	0.231451000
H	-0.992640000	1.925420000	3.878895000
H	-0.149815000	0.581527000	3.874670000
H	-0.686859000	1.427464000	-4.128988000
H	0.039533000	3.801464000	-0.470720000
H	0.680199000	4.090652000	1.692108000
H	0.895015000	3.777982000	-1.802302000
H	1.821455000	0.157874000	2.839298000
H	-1.893306000	2.754832000	-0.085924000
H	-0.838521000	-1.549626000	4.159619000
H	-0.841851000	-1.666655000	-3.708748000
H	0.817252000	-3.798344000	2.052026000
H	0.753404000	-4.074928000	-1.416728000
H	0.030384000	-3.766592000	0.670587000
O	-1.116845000	0.114877000	1.448592000
O	-0.044512000	-3.583505000	1.652445000
O	1.038191000	1.385589000	-0.015662000
O	1.292197000	0.147621000	2.031306000
O	-0.080008000	-1.109625000	3.748813000
O	-0.107379000	1.561964000	3.696280000
O	0.081631000	-1.733139000	-3.418833000
O	1.050874000	-1.355034000	0.189463000
O	-1.392857000	-1.911115000	0.215876000
O	-0.007195000	-3.662784000	-0.983262000
O	-0.058704000	3.659652000	1.238051000
O	0.000325000	3.613327000	-1.446209000
O	-1.386603000	1.932694000	-0.053952000
O	0.104782000	1.241997000	-3.608246000
O	1.291092000	-0.123078000	-1.900238000
O	-1.125430000	-0.088484000	-1.326120000
Ti	2.436048000	-0.013842000	0.094053000
Ti	-0.115657000	-1.463247000	1.894595000
Ti	0.024885000	1.808093000	1.575794000
Ti	-0.080778000	1.471100000	-1.673891000

Ti	-2.505681000	0.007390000	0.051566000
Ti	0.008224000	-1.812769000	-1.401508000
Fe	1.395191000	-0.326307000	-3.752192000
O	1.301830000	-0.745256000	-5.504309000
C	3.984491000	-0.432633000	-4.835132000
C	5.349812000	0.192901000	-4.653119000
H	4.027463000	-1.515314000	-4.635784000
H	3.606645000	-0.309695000	-5.860367000
H	5.335927000	1.255071000	-4.910960000
H	5.676203000	0.101740000	-3.613330000
H	6.075467000	-0.316164000	-5.294454000
O	3.085784000	0.179861000	-3.938053000
H	0.659834000	-1.461457000	-5.607388000

Fe-Ti-NU-1000 (TS2\_3)

Free Energy: -4355.148563

Electronic Energy: -4355.38536989

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000

H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.926580000	-2.715117000	0.217379000
H	-0.999703000	1.908374000	3.899727000
H	-0.146775000	0.569556000	3.883832000
H	-0.821245000	1.349415000	-3.956817000
H	0.033522000	3.816279000	-0.434943000
H	0.686362000	4.092980000	1.713784000
H	0.882119000	3.810675000	-1.769391000
H	1.829801000	0.140713000	2.829295000
H	-1.909109000	2.754617000	-0.080306000
H	-0.837648000	-1.556155000	4.168173000
H	-0.732092000	-1.801839000	-3.870060000
H	0.822764000	-3.793667000	2.022714000
H	0.789483000	-4.035865000	-1.419393000
H	0.025775000	-3.750744000	0.647805000
O	-1.122767000	0.113222000	1.454497000
O	-0.045025000	-3.584776000	1.632387000
O	1.031380000	1.419131000	0.016521000
O	1.283477000	0.141977000	2.032811000
O	-0.082903000	-1.114824000	3.752747000
O	-0.112256000	1.553053000	3.713900000
O	0.148238000	-1.686948000	-3.486637000
O	1.032414000	-1.369258000	0.194020000
O	-1.397378000	-1.907089000	0.206409000

O	-0.002655000	-3.647676000	-1.018632000
O	-0.065267000	3.674405000	1.268467000
O	-0.005866000	3.629986000	-1.411870000
O	-1.395265000	1.937776000	-0.037521000
O	0.060835000	1.281466000	-3.565559000
O	1.319191000	-0.093389000	-1.834986000
O	-1.119570000	-0.084122000	-1.321481000
Ti	2.396991000	-0.038137000	0.086287000
Ti	-0.126154000	-1.466698000	1.895280000
Ti	0.018037000	1.819944000	1.599435000
Ti	-0.075753000	1.477406000	-1.622016000
Ti	-2.502739000	-0.002266000	0.057236000
Ti	0.015766000	-1.803024000	-1.449060000
Fe	1.433347000	-0.222564000	-3.742929000
O	1.884395000	0.668353000	-5.420293000
C	4.082463000	-0.324741000	-4.815344000
C	4.804534000	-1.241707000	-5.763276000
H	3.265270000	0.401925000	-5.439645000
H	4.705001000	0.442549000	-4.315585000
H	5.479650000	-1.897602000	-5.199628000
H	4.098221000	-1.879705000	-6.300465000
H	5.397923000	-0.675741000	-6.485294000
O	3.202379000	-0.900888000	-4.002730000
H	1.617768000	1.599742000	-5.433420000

Fe-Ti-NU-1000 (Prod\_3)

Free Energy: -4355.192431

Electronic Energy: -4355.42970317

C	5.726499000	-2.889201000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187703000	-2.459996000
C	-4.293001000	-3.161893000	-2.734608000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021294000	-2.724808000
C	-4.324801000	2.871994000	-3.008006000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223387000	-2.332289000	-2.105806000
C	-3.315197000	-2.089490000	2.441208000
C	-3.322923000	2.330098000	2.211511000
C	3.188491000	2.436975000	2.193655000



C	3.241995000	2.242006000	-2.085991000
C	3.280283000	-2.402408000	-1.851683000
C	-3.245500000	2.084807000	-2.346694000
C	3.174651000	-2.211229000	2.426735000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	3.070800000	-4.466900000	-3.573300000
H	-2.943100000	-4.450000000	-3.798200000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	3.038900000	4.198500000	-3.962800000
H	-2.978300000	4.100400000	-4.145000000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666621000	2.881884000
H	3.964843000	3.004756000	2.662576000
H	-4.111858000	2.914443000	2.636927000
H	3.948377000	-2.768441000	2.911924000
O	-3.663737000	1.472052000	1.337378000
O	-3.609930000	1.255374000	-1.456651000
O	-3.653912000	-1.258606000	1.542947000
O	-2.127301000	-2.310194000	2.835706000
O	1.970073000	-2.521668000	2.683433000
O	2.090000000	-2.742698000	-2.140602000
O	3.548256000	-1.286010000	1.640825000
O	3.614119000	-1.448407000	-1.083665000
O	3.557214000	1.485761000	1.438516000
O	3.591771000	1.320352000	-1.285261000
O	2.046400000	2.547804000	-2.386396000
O	1.986508000	2.771194000	2.435573000
O	-2.020200000	-2.554504000	-2.444696000
O	-3.603874000	-1.474675000	-1.248371000
O	-2.134301000	2.562396000	2.592305000
O	-2.045099000	2.316708000	-2.694292000
H	-1.969972000	-2.687442000	0.200614000
H	-1.004135000	1.908229000	3.914521000
H	-0.145584000	0.572692000	3.885057000
H	-0.726301000	1.564137000	-4.039803000
H	0.040207000	3.814037000	-0.447327000
H	0.701847000	4.079661000	1.708304000
H	0.880006000	3.815510000	-1.786159000
H	1.833888000	0.146893000	2.808975000
H	-1.907037000	2.757335000	-0.105082000
H	-0.837881000	-1.546763000	4.180791000
H	0.540708000	-2.650441000	-3.701110000
H	0.822118000	-3.764522000	1.992966000

H	0.843652000	-3.973073000	-1.319004000
H	-0.010168000	-3.720162000	0.636252000
O	-1.136496000	0.121862000	1.450742000
O	-0.060922000	-3.574948000	1.625981000
O	1.021510000	1.442456000	0.021106000
O	1.265976000	0.150211000	2.027868000
O	-0.090141000	-1.102579000	3.756932000
O	-0.117192000	1.558451000	3.719125000
O	0.132624000	-1.795798000	-3.513400000
O	1.000455000	-1.378092000	0.209418000
O	-1.426832000	-1.889159000	0.206670000
O	-0.010391000	-3.620231000	-1.031463000
O	-0.070184000	3.684480000	1.274953000
O	-0.004437000	3.631355000	-1.423047000
O	-1.395117000	1.940313000	-0.046729000
O	0.112470000	1.374824000	-3.598739000
O	1.271494000	-0.095127000	-1.826188000
O	-1.149713000	-0.080257000	-1.349069000
Ti	2.323244000	-0.021906000	0.085589000
Ti	-0.151539000	-1.458862000	1.897252000
Ti	-0.005971000	1.831124000	1.605456000
Ti	-0.062213000	1.468455000	-1.641015000
Ti	-2.520084000	-0.001943000	0.040770000
Ti	-0.028709000	-1.756823000	-1.463327000
Fe	1.279890000	-0.201709000	-3.865147000
O	0.464205000	-0.479427000	-5.955007000
C	4.192152000	-1.108349000	-4.590309000
C	4.989785000	-0.074967000	-3.907181000
H	4.707791000	-1.947377000	-5.089191000
H	1.041504000	-1.037203000	-6.487145000
H	4.812527000	0.902312000	-4.372886000
H	4.646999000	0.019913000	-2.864434000
H	6.058124000	-0.292557000	-3.931183000
O	2.954813000	-1.090809000	-4.641695000
H	-0.249672000	-1.063595000	-5.657260000

### Functionalization

Fe-NU-1000-Br-O

Free Energy: -14415.349938

Electronic Energy: -14415.503777

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885101000	-2.451399000
C	4.388901000	-3.187701000	-2.460000000
C	-4.293000000	-3.161899000	-2.734602000
C	4.106398000	-4.252600000	-3.328502000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138201000	-5.020698000	-3.859400000
C	-4.998200000	-5.035200000	-4.107601000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807101000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628902000	-2.684597000
C	4.341400000	3.021298000	-2.724803000
C	-4.324801000	2.872001000	-3.008000000

C	4.069899000	4.017800000	-3.673300000
C	-4.019398000	3.907100000	-3.904901000
C	5.105900000	4.760700000	-4.231200000
C	-5.033001000	4.692698000	-4.448901000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462598000	-4.123403000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223395000	-2.332286000	-2.105808000
C	-3.315199000	-2.089495000	2.441202000
C	-3.322904000	2.330108000	2.211494000
C	3.188500000	2.437001000	2.193694000
C	3.241996000	2.241993000	-2.086004000
C	3.280300000	-2.402406000	-1.851693000
C	-3.245500000	2.084796000	-2.346712000
C	3.174603000	-2.211104000	2.426596000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847201000	-4.524399000
H	-4.737200000	-5.873101000	-4.748999000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498302000	-5.131197000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004751000	2.662582000
H	-4.111859000	2.914441000	2.636929000
H	3.948377000	-2.768397000	2.911976000
O	-3.663737000	1.472099000	1.337384000
O	-3.609988000	1.255406000	-1.456701000
O	-3.654004000	-1.258599000	1.542896000
O	-2.127282000	-2.310232000	2.835706000
O	1.970307000	-2.521843000	2.683591000
O	2.090039000	-2.742561000	-2.140628000
O	3.548214000	-1.286096000	1.640805000
O	3.614183000	-1.448424000	-1.083686000
O	3.557201000	1.485682000	1.438499000
O	3.591764000	1.320306000	-1.285291000
O	2.046372000	2.547621000	-2.386366000
O	1.986495000	2.771332000	2.435669000
O	-2.020186000	-2.554256000	-2.444701000
O	-3.603963000	-1.474712000	-1.248397000
O	-2.134302000	2.562461000	2.592292000
O	-2.045114000	2.316507000	-2.694236000
H	-1.959422000	-2.858525000	0.224442000
H	-1.027354000	1.823044000	4.290461000
H	-0.133717000	0.517462000	4.137752000
H	-0.284869000	1.616914000	-4.730197000

H	0.015710000	4.081191000	-0.419814000
H	0.651045000	4.478603000	1.620236000
H	0.843927000	4.269715000	-1.771844000
H	1.869484000	0.166778000	2.977670000
H	-1.956518000	2.892808000	-0.099108000
H	-0.811756000	-1.486254000	4.551221000
H	0.386301000	-2.506055000	-4.416365000
H	0.845725000	-4.195741000	1.941727000
H	0.679071000	-4.484058000	-1.408581000
H	0.005356000	-4.031616000	0.602169000
O	-1.118064000	0.120506000	1.537571000
O	-0.007872000	-3.889856000	1.609565000
O	1.031822000	1.498627000	0.004215000
O	1.316307000	0.156606000	2.189206000
O	-0.076063000	-1.087193000	4.074930000
O	-0.153645000	1.526191000	4.005239000
O	0.198867000	-1.782695000	-3.807356000
O	1.039094000	-1.456666000	0.203089000
O	-1.419280000	-2.060775000	0.220895000
O	-0.027409000	-3.971358000	-0.999822000
O	-0.073960000	3.994219000	1.211142000
O	0.009170000	3.929670000	-1.420333000
O	-1.423742000	2.090870000	-0.059591000
O	0.201627000	1.298710000	-3.964917000
O	1.338223000	-0.109552000	-2.079203000
O	-1.097471000	-0.089863000	-1.425538000
Zr	2.470649000	0.006404000	0.121760000
Zr	-0.085080000	-1.617759000	2.034292000
Zr	-0.040684000	1.958570000	1.741451000
Zr	-0.036126000	1.648388000	-1.805942000
Zr	-2.551728000	-0.002431000	0.046215000
Zr	0.005332000	-1.943205000	-1.560547000
Fe	1.304865000	-0.273033000	-3.931038000
O	2.071603000	-0.445243000	-5.352979000
Br	-2.300426000	4.418256000	-4.559096000
Br	2.362672000	4.551689000	-4.345590000
Br	2.399257000	-4.854926000	-3.951759000
Br	-2.256694000	-4.810441000	-4.147746000

Fe-NU-1000-Br (Ads\_4)

Free Energy: -14570.331083

Electronic Energy: -14570.5634629

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000

C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.948982000	-2.861123000	0.226858000
H	-1.035447000	1.816679000	4.275902000

H	-0.135117000	0.515456000	4.132533000
H	-0.363283000	1.623514000	-4.716617000
H	0.013883000	4.065064000	-0.432225000
H	0.654966000	4.471803000	1.617135000
H	0.848270000	4.246048000	-1.774043000
H	1.869181000	0.166338000	2.979830000
H	-1.947867000	2.888368000	-0.101473000
H	-0.816274000	-1.488284000	4.543125000
H	-0.462687000	-2.193218000	-4.413165000
H	0.850988000	-4.191289000	1.927686000
H	0.655377000	-4.481692000	-1.422369000
H	0.011883000	-4.021190000	0.582685000
O	-1.118928000	0.119581000	1.543380000
O	-0.002794000	-3.885869000	1.596352000
O	1.038853000	1.490270000	0.000187000
O	1.318415000	0.155715000	2.189917000
O	-0.075506000	-1.091597000	4.072841000
O	-0.156223000	1.524413000	4.002709000
O	0.171407000	-1.870380000	-3.765583000
O	1.043708000	-1.446632000	0.198399000
O	-1.419298000	-2.056602000	0.222736000
O	-0.033953000	-3.962309000	-0.995145000
O	-0.073783000	3.990737000	1.211064000
O	0.008292000	3.913551000	-1.430282000
O	-1.421642000	2.082676000	-0.056157000
O	0.186683000	1.371792000	-3.968930000
O	1.271178000	-0.114483000	-2.165169000
O	-1.132955000	-0.095524000	-1.423482000
Zr	2.468926000	0.001034000	0.116303000
Zr	-0.082728000	-1.618057000	2.028816000
Zr	-0.038079000	1.954142000	1.735318000
Zr	-0.035037000	1.612688000	-1.812967000
Zr	-2.555358000	-0.000890000	0.052444000
Zr	0.001868000	-1.924310000	-1.572386000
Br	-2.300484000	4.416907000	-4.559120000
Br	2.366435000	4.513639000	-4.379804000
Br	2.401023000	-4.789758000	-4.006711000
Br	-2.256626000	-4.800775000	-4.160698000
Fe	1.155537000	-0.273205000	-4.115148000
O	1.094876000	-0.339206000	-5.751093000
C	3.984109000	0.205162000	-4.912785000
C	5.453848000	0.025231000	-4.647858000
H	3.717468000	0.141565000	-5.972744000
H	3.621436000	1.172531000	-4.547754000
H	5.657441000	0.085219000	-3.574885000
H	5.811505000	-0.944845000	-5.009596000
H	6.026026000	0.811190000	-5.149853000
O	3.217881000	-0.782977000	-4.172716000
H	3.237897000	-1.614249000	-4.670479000

Fe-NU-1000-Br (TS1\_4)

Free Energy: -14570.314732

Electronic Energy: -14570.5422833

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000

C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000

O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.947795000	-2.855917000	0.221194000
H	-1.029966000	1.821426000	4.273923000
H	-0.136596000	0.515289000	4.126848000
H	-0.484288000	1.670887000	-4.654401000
H	0.023981000	4.088028000	-0.425449000
H	0.655326000	4.475494000	1.623351000
H	0.842797000	4.273489000	-1.784021000
H	1.862988000	0.164026000	2.985061000
H	-1.949024000	2.897473000	-0.092773000
H	-0.814433000	-1.491133000	4.532341000
H	-0.411770000	-2.115721000	-4.473217000
H	0.849190000	-4.196055000	1.924161000
H	0.629240000	-4.498102000	-1.441708000
H	0.011864000	-4.024100000	0.578205000
O	-1.117513000	0.122179000	1.539038000
O	0.000240000	-3.881684000	1.588988000
O	1.042889000	1.478262000	-0.005974000
O	1.321614000	0.155180000	2.188457000
O	-0.075610000	-1.091363000	4.061446000
O	-0.153627000	1.524175000	3.996523000
O	0.168156000	-1.793609000	-3.776250000
O	1.045527000	-1.427012000	0.174212000
O	-1.413842000	-2.054013000	0.214145000
O	-0.041815000	-3.962986000	-1.003961000
O	-0.065999000	3.990722000	1.208434000
O	0.010247000	3.936070000	-1.424519000
O	-1.419235000	2.093318000	-0.059127000
O	0.124253000	1.429202000	-3.949778000
O	1.314498000	-0.103497000	-2.236483000
O	-1.093014000	-0.084958000	-1.420365000
Zr	2.489981000	0.010130000	0.128415000
Zr	-0.080394000	-1.615099000	2.019028000
Zr	-0.035338000	1.954179000	1.731871000
Zr	-0.033489000	1.655251000	-1.814370000
Zr	-2.547417000	0.000178000	0.045484000
Zr	0.006219000	-1.935448000	-1.586620000
Br	-2.301306000	4.411796000	-4.563615000
Br	2.363452000	4.523947000	-4.364643000
Br	2.401925000	-4.802649000	-3.992093000
Br	-2.256759000	-4.800045000	-4.161596000
Fe	1.157510000	-0.202415000	-4.095386000
O	1.068868000	-0.282428000	-5.811136000
C	4.034720000	-0.656181000	-4.807797000
C	5.229408000	-0.196220000	-4.015288000
H	3.646066000	-1.612667000	-4.421313000
H	4.309455000	-0.842388000	-5.855894000
H	5.600608000	0.754477000	-4.409364000



H	4.962314000	-0.052383000	-2.963081000
H	6.035314000	-0.934209000	-4.075034000
O	3.011678000	0.340440000	-4.782831000
H	2.210827000	0.123973000	-5.685534000

Fe-NU-1000-Br (Int\_4)

Free Energy: -14570.34715

Electronic Energy: -14570.579847

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000

H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.961844000	-2.853544000	0.228227000
H	-1.030933000	1.826017000	4.272710000
H	-0.134089000	0.522745000	4.130429000
H	-0.422187000	1.401539000	-4.633235000
H	0.017287000	4.077449000	-0.431192000
H	0.654798000	4.477192000	1.613626000
H	0.847772000	4.259654000	-1.781183000
H	1.865597000	0.170601000	2.980263000
H	-1.954451000	2.894079000	-0.096207000
H	-0.813710000	-1.483778000	4.543035000
H	0.514847000	-2.548857000	-4.207772000
H	0.848907000	-4.190513000	1.928778000
H	0.682897000	-4.471037000	-1.407192000
H	0.004781000	-4.022335000	0.590165000
O	-1.119585000	0.122345000	1.540312000
O	-0.005886000	-3.885236000	1.599491000
O	1.033981000	1.484980000	-0.007100000
O	1.318795000	0.158247000	2.187504000
O	-0.074723000	-1.086284000	4.070547000
O	-0.153259000	1.530724000	3.997598000
O	0.192349000	-1.748555000	-3.770938000
O	1.043111000	-1.445693000	0.196165000
O	-1.422450000	-2.055540000	0.223335000
O	-0.031457000	-3.963523000	-1.006931000
O	-0.069622000	3.993024000	1.203415000
O	0.008992000	3.927848000	-1.431140000
O	-1.422532000	2.091426000	-0.063066000
O	0.221407000	1.266494000	-3.932940000
O	1.342524000	-0.119525000	-2.099429000
O	-1.099271000	-0.085318000	-1.422167000
Zr	2.482467000	0.012161000	0.120225000
Zr	-0.082707000	-1.613872000	2.028708000
Zr	-0.037283000	1.956428000	1.729258000
Zr	-0.033037000	1.648571000	-1.828295000
Zr	-2.550053000	0.000315000	0.047277000
Zr	-0.002338000	-1.926795000	-1.564069000

Br	-2.302245000	4.411346000	-4.563668000
Br	2.364270000	4.514400000	-4.374887000
Br	2.401740000	-4.812999000	-3.998830000
Br	-2.256755000	-4.805257000	-4.153935000
Fe	1.499500000	-0.281329000	-3.931702000
O	1.494682000	-0.601310000	-5.712748000
C	4.131043000	-0.438901000	-4.926773000
C	5.506990000	0.154397000	-4.709363000
H	4.158411000	-1.533493000	-4.785960000
H	3.774566000	-0.260435000	-5.951010000
H	5.508970000	1.227401000	-4.921265000
H	5.825224000	0.015059000	-3.671597000
H	6.233986000	-0.332987000	-5.366354000
O	3.245000000	0.145393000	-4.002888000
H	0.636944000	-0.992291000	-5.932182000

Fe-NU-1000-Br (TS2\_4)

Free Energy: -14570.333624

Electronic Energy: -14570.5575419

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000

H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.957031000	-2.858228000	0.234953000
H	-1.035791000	1.819209000	4.286796000
H	-0.133775000	0.519434000	4.141335000
H	-0.492553000	1.431043000	-4.594156000
H	0.012725000	4.073893000	-0.422580000
H	0.653298000	4.478300000	1.618551000
H	0.848795000	4.251376000	-1.768238000
H	1.872991000	0.171317000	2.981319000
H	-1.954565000	2.890548000	-0.098967000
H	-0.815082000	-1.484413000	4.553694000
H	-0.671874000	-1.835003000	-4.188567000
H	0.851167000	-4.183892000	1.954917000
H	0.589146000	-4.539357000	-1.419657000
H	0.002292000	-4.037546000	0.617700000
O	-1.118138000	0.122831000	1.546392000
O	-0.009101000	-3.891875000	1.627174000
O	1.034589000	1.507329000	0.012101000
O	1.316207000	0.159664000	2.195673000
O	-0.075197000	-1.086752000	4.082831000
O	-0.157022000	1.528429000	4.011047000
O	0.170232000	-1.791690000	-3.723132000
O	1.044827000	-1.463216000	0.221671000
O	-1.422071000	-2.057246000	0.227720000
O	-0.051813000	-3.980247000	-0.968693000
O	-0.077400000	3.997279000	1.215742000

O	0.007381000	3.922678000	-1.422243000
O	-1.423234000	2.087949000	-0.058081000
O	0.209078000	1.280469000	-3.954658000
O	1.368656000	-0.118163000	-2.029751000
O	-1.098140000	-0.090774000	-1.419438000
Zr	2.467186000	0.007755000	0.114555000
Zr	-0.080695000	-1.617095000	2.039451000
Zr	-0.038358000	1.960128000	1.744006000
Zr	-0.022901000	1.635380000	-1.804017000
Zr	-2.542739000	0.000651000	0.052454000
Zr	0.010653000	-1.949860000	-1.547700000
Br	-2.301826000	4.413993000	-4.561277000
Br	2.364659000	4.506397000	-4.383040000
Br	2.401243000	-4.783526000	-4.009869000
Br	-2.256015000	-4.792741000	-4.165611000
Fe	1.448492000	-0.251625000	-3.908335000
O	1.730583000	-0.840506000	-5.768319000
C	3.947053000	0.156224000	-5.276579000
C	5.108278000	-0.801648000	-5.212995000
H	3.007540000	-0.429163000	-5.918320000
H	4.113987000	1.076085000	-5.865363000
H	5.862882000	-0.435645000	-4.506151000
H	4.784568000	-1.785811000	-4.859253000
H	5.578320000	-0.918326000	-6.192936000
O	3.280230000	0.361673000	-4.145324000
H	1.591173000	-1.785778000	-5.923015000

Fe-NU-1000-Br (Prod\_4)

Free Energy: -14570.371931

Electronic Energy: -14570.5983449

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000

C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.962783000	-2.851796000	0.219984000
H	-1.042115000	1.808397000	4.285948000
H	-0.133620000	0.513431000	4.139636000
H	-0.547003000	1.557274000	-4.544318000
H	0.010396000	4.067882000	-0.421315000
H	0.652580000	4.476826000	1.625154000
H	0.847468000	4.256617000	-1.760231000
H	1.882644000	0.164478000	2.965023000
H	-1.955763000	2.883028000	-0.108352000
H	-0.819877000	-1.485372000	4.551546000
H	0.830323000	-2.763908000	-3.981814000
H	0.849700000	-4.181213000	1.928265000
H	0.700515000	-4.460380000	-1.378284000
H	0.003637000	-4.010769000	0.589804000

O	-1.117232000	0.121243000	1.540762000
O	-0.012525000	-3.890123000	1.605272000
O	1.037300000	1.528397000	0.021773000
O	1.310774000	0.156945000	2.190407000
O	-0.077117000	-1.091078000	4.082554000
O	-0.160523000	1.523354000	4.013486000
O	0.219141000	-2.031556000	-3.810242000
O	1.037623000	-1.479464000	0.220108000
O	-1.425913000	-2.052339000	0.223473000
O	-0.021401000	-3.953833000	-0.992256000
O	-0.084954000	4.002526000	1.226916000
O	0.008450000	3.919356000	-1.419669000
O	-1.424037000	2.081501000	-0.056672000
O	0.193109000	1.380390000	-3.955309000
O	1.327721000	-0.106211000	-2.027224000
O	-1.134545000	-0.096828000	-1.443069000
Zr	2.426001000	0.006479000	0.107004000
Zr	-0.087278000	-1.620530000	2.036151000
Zr	-0.043576000	1.963967000	1.746541000
Zr	-0.019539000	1.615923000	-1.807767000
Zr	-2.550864000	-0.002289000	0.048931000
Zr	0.000447000	-1.909354000	-1.575379000
Br	-2.300917000	4.411160000	-4.563005000
Br	2.365196000	4.515182000	-4.373229000
Br	2.403109000	-4.847536000	-3.968650000
Br	-2.256651000	-4.803652000	-4.149880000
Fe	1.218775000	-0.306935000	-4.045937000
O	0.295497000	-0.662781000	-6.139487000
C	4.130278000	-1.133504000	-4.742167000
C	4.892334000	-0.071614000	-4.053575000
H	4.668108000	-1.934765000	-5.276425000
H	0.930170000	-1.087038000	-6.726026000
H	4.672544000	0.901566000	-4.513495000
H	4.563009000	0.002145000	-3.006887000
H	5.969627000	-0.241914000	-4.090608000
O	2.887017000	-1.165866000	-4.756776000
H	-0.201162000	-1.396249000	-5.735009000

Fe-NU-1000-NH<sub>2</sub>-O

Free Energy: -4354.174994

Electronic Energy: -4354.4459874

C	5.726500000	-2.889197000	-2.160203000
C	-5.638900000	-2.885099000	-2.451401000
C	4.388912000	-3.187715000	-2.459985000
C	-4.293000000	-3.161884000	-2.734616000
C	4.106379000	-4.252607000	-3.328502000
C	-3.986003000	-4.236297000	-3.582702000
C	5.138208000	-5.020693000	-3.859394000
C	-4.998199000	-5.035201000	-4.107600000
C	6.482800000	-4.751202000	-3.537698000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369401000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000

C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907101000	-3.904899000
C	5.105900000	4.760701000	-4.231199000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526401000	-3.861699000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223402000	-2.332249000	-2.105829000
C	-3.315200000	-2.089499000	2.441195000
C	-3.322896000	2.330083000	2.211506000
C	3.188497000	2.437002000	2.193698000
C	3.242009000	2.242024000	-2.086021000
C	3.280301000	-2.402489000	-1.851592000
C	-3.245495000	2.084780000	-2.346703000
C	3.174599000	-2.211105000	2.426596000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847197000	-4.524404000
H	-4.737200000	-5.873100000	-4.748999000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534099000	-4.959801000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101095000	-2.666613000	2.881892000
H	3.964843000	3.004750000	2.662583000
H	-4.111860000	2.914435000	2.636935000
H	3.948376000	-2.768392000	2.911982000
O	-3.663682000	1.472095000	1.337394000
O	-3.609955000	1.255397000	-1.456714000
O	-3.653975000	-1.258618000	1.542896000
O	-2.127298000	-2.310244000	2.835710000
O	1.970294000	-2.521876000	2.683623000
O	2.090019000	-2.742733000	-2.140519000
O	3.548222000	-1.286116000	1.640803000
O	3.614225000	-1.448477000	-1.083643000
O	3.557211000	1.485685000	1.438499000
O	3.591822000	1.320294000	-1.285292000
O	2.046253000	2.548015000	-2.386623000
O	1.986509000	2.771304000	2.435694000
O	-2.020185000	-2.554370000	-2.444694000
O	-3.603975000	-1.474693000	-1.248418000
O	-2.134287000	2.562377000	2.592298000
O	-2.045207000	2.316699000	-2.694277000
H	-1.964459000	-2.857364000	0.224894000
H	-1.027146000	1.824299000	4.293116000
H	-0.136965000	0.515439000	4.138634000



H	-0.477049000	1.516373000	-4.657655000
H	-0.005242000	4.080866000	-0.428552000
H	0.650306000	4.475854000	1.595615000
H	0.903998000	4.233581000	-1.719777000
H	1.864512000	0.165351000	2.984407000
H	-1.960233000	2.887316000	-0.097039000
H	-0.814211000	-1.488910000	4.547731000
H	-0.519324000	-2.048899000	-4.405928000
H	0.858297000	-4.197611000	1.903793000
H	0.752168000	-4.452818000	-1.384096000
H	-0.004533000	-4.033148000	0.581845000
O	-1.116246000	0.118679000	1.527404000
O	0.000315000	-3.889746000	1.584598000
O	1.038180000	1.485210000	0.003432000
O	1.317231000	0.155217000	2.191715000
O	-0.079777000	-1.087029000	4.071776000
O	-0.155691000	1.524175000	4.004340000
O	0.187779000	-1.849688000	-3.782246000
O	1.046419000	-1.449149000	0.197012000
O	-1.416152000	-2.065290000	0.217761000
O	-0.032771000	-3.996876000	-1.057656000
O	-0.074027000	3.986333000	1.191163000
O	0.026151000	3.941568000	-1.434181000
O	-1.421803000	2.089203000	-0.058975000
O	0.187567000	1.369223000	-3.976876000
O	1.341533000	-0.115409000	-2.130654000
O	-1.098470000	-0.091322000	-1.432982000
Zr	2.501353000	0.002469000	0.120438000
Zr	-0.083472000	-1.614473000	2.031954000
Zr	-0.039797000	1.952435000	1.743260000
Zr	-0.029167000	1.636038000	-1.783042000
Zr	-2.566130000	-0.002058000	0.039817000
Zr	0.011261000	-1.940469000	-1.547674000
N	2.785352000	4.360065000	-4.084857000
H	2.097411000	3.626648000	-4.008583000
H	2.768762000	4.841578000	-4.970888000
N	-2.736390000	4.202670000	-4.335436000
H	-2.628602000	5.132300000	-4.708084000
H	-1.986438000	3.889948000	-3.740017000
N	-2.693295000	-4.562234000	-3.964982000
H	-1.959928000	-4.240044000	-3.351552000
H	-2.588172000	-5.513792000	-4.279668000
N	2.826424000	-4.645479000	-3.695186000
H	2.801636000	-5.191377000	-4.542024000
H	2.109190000	-3.940508000	-3.632878000
Fe	1.220766000	-0.261327000	-3.980433000
O	1.835436000	-0.348751000	-5.482730000

Fe-NU-1000-NH<sub>2</sub> (Ads\_4)

Free Energy: -4509.156997

Electronic Energy: -4509.5079679

C	5.726500000	-2.889201000	-2.160198000
C	-5.638900000	-2.885101000	-2.451399000
C	4.388896000	-3.187695000	-2.460004000
C	-4.292999000	-3.161913000	-2.734586000
C	4.106408000	-4.252598000	-3.328498000

C	-3.985999000	-4.236302000	-3.582698000
C	5.138197000	-5.020703000	-3.859402000
C	-4.998200000	-5.035199000	-4.107601000
C	6.482800000	-4.751199000	-3.537701000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341401000	3.021302000	-2.724798000
C	-4.324800000	2.872003000	-3.007997000
C	4.069899000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105901000	4.760699000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223401000	-2.332346000	-2.105783000
C	-3.315199000	-2.089500000	2.441202000
C	-3.322901000	2.330109000	2.211494000
C	3.188501000	2.436997000	2.193702000
C	3.241997000	2.241997000	-2.085989000
C	3.280301000	-2.402361000	-1.851753000
C	-3.245502000	2.084815000	-2.346699000
C	3.174600000	-2.211098000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847201000	-4.524399000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666620000	2.881885000
H	3.964843000	3.004749000	2.662585000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768399000	2.911974000
O	-3.663727000	1.472101000	1.337394000
O	-3.610017000	1.255411000	-1.456693000
O	-3.654019000	-1.258591000	1.542892000
O	-2.127289000	-2.310196000	2.835699000
O	1.970300000	-2.521777000	2.683583000
O	2.089969000	-2.742601000	-2.140665000
O	3.548195000	-1.286088000	1.640795000
O	3.614180000	-1.448379000	-1.083713000
O	3.557196000	1.485695000	1.438500000

O	3.591779000	1.320311000	-1.285294000
O	2.046487000	2.547620000	-2.386289000
O	1.986488000	2.771316000	2.435684000
O	-2.020192000	-2.554461000	-2.444699000
O	-3.603996000	-1.474714000	-1.248387000
O	-2.134301000	2.562438000	2.592287000
O	-2.045053000	2.316614000	-2.694281000
H	-1.965073000	-2.849294000	0.221919000
H	-1.033886000	1.822128000	4.279767000
H	-0.137427000	0.517956000	4.133980000
H	-0.456605000	1.540061000	-4.662334000
H	-0.009395000	4.069579000	-0.440351000
H	0.650689000	4.475195000	1.594790000
H	0.916401000	4.208543000	-1.713262000
H	1.865292000	0.166340000	2.980753000
H	-1.957094000	2.884823000	-0.101132000
H	-0.817355000	-1.486734000	4.543104000
H	-0.530428000	-2.101084000	-4.399528000
H	0.852634000	-4.186042000	1.893673000
H	0.792755000	-4.410769000	-1.312925000
H	-0.018364000	-4.009779000	0.573967000
O	-1.119013000	0.121318000	1.531325000
O	-0.009624000	-3.882767000	1.582134000
O	1.040213000	1.486462000	0.000257000
O	1.317042000	0.156329000	2.188942000
O	-0.079468000	-1.086999000	4.070825000
O	-0.157261000	1.526641000	4.001714000
O	0.180154000	-1.896526000	-3.781405000
O	1.045513000	-1.447351000	0.193884000
O	-1.420265000	-2.055156000	0.218312000
O	-0.027313000	-3.979758000	-1.051372000
O	-0.077416000	3.988777000	1.193642000
O	0.029573000	3.931557000	-1.443031000
O	-1.422159000	2.084898000	-0.057496000
O	0.214571000	1.431069000	-3.979689000
O	1.265374000	-0.115313000	-2.169883000
O	-1.140333000	-0.093215000	-1.436215000
Zr	2.486950000	0.001687000	0.115793000
Zr	-0.086581000	-1.609739000	2.027567000
Zr	-0.040437000	1.953956000	1.736498000
Zr	-0.032856000	1.606914000	-1.797484000
Zr	-2.574626000	0.000026000	0.043696000
Zr	0.000662000	-1.904660000	-1.567709000
N	2.788612000	4.348316000	-4.091113000
H	2.082805000	3.637433000	-3.972449000
H	2.755448000	4.838664000	-4.970765000
N	-2.736390000	4.202131000	-4.334466000
H	-2.625405000	5.133314000	-4.701833000
H	-1.986309000	3.878293000	-3.744597000
N	-2.693206000	-4.561125000	-3.965201000
H	-1.960065000	-4.228187000	-3.356895000
H	-2.585800000	-5.513981000	-4.274552000
N	2.848951000	-4.522808000	-3.831807000
H	2.728840000	-5.407877000	-4.293354000
H	2.051168000	-4.112869000	-3.375270000
Fe	1.151036000	-0.263988000	-4.114889000

O	1.057977000	-0.315491000	-5.749763000
C	4.028963000	0.091878000	-4.870928000
C	5.471457000	-0.180621000	-4.547146000
H	3.797790000	0.036297000	-5.940114000
H	3.720886000	1.082415000	-4.517367000
H	5.630789000	-0.122005000	-3.467425000
H	5.778866000	-1.176485000	-4.884439000
H	6.112044000	0.561643000	-5.031847000
O	3.173519000	-0.838899000	-4.154234000
H	3.205325000	-1.697550000	-4.604405000

Fe-NU-1000-NH<sub>2</sub> (TS1\_4)

Free Energy: -4509.140643

Electronic Energy: -4509.4881216

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000

H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.959345000	-2.850458000	0.215988000
H	-1.029100000	1.823724000	4.275380000
H	-0.139274000	0.514371000	4.125880000
H	-0.606850000	1.584722000	-4.580419000
H	0.004974000	4.088799000	-0.436511000
H	0.654736000	4.474163000	1.598028000
H	0.901726000	4.240750000	-1.738457000
H	1.857737000	0.162988000	2.986808000
H	-1.955709000	2.891882000	-0.094129000
H	-0.815879000	-1.491468000	4.529113000
H	-0.526677000	-2.040008000	-4.421408000
H	0.856949000	-4.199917000	1.880757000
H	0.757323000	-4.436032000	-1.392989000
H	-0.001493000	-4.019215000	0.553909000
O	-1.116170000	0.120603000	1.524158000
O	0.004058000	-3.881174000	1.559655000
O	1.045403000	1.469204000	-0.009337000
O	1.320697000	0.154544000	2.187104000
O	-0.079119000	-1.089505000	4.056782000
O	-0.155287000	1.523228000	3.993452000
O	0.187315000	-1.863018000	-3.797316000
O	1.049701000	-1.425077000	0.167763000
O	-1.412463000	-2.057422000	0.208592000
O	-0.031152000	-3.982593000	-1.072509000
O	-0.066124000	3.985045000	1.187106000
O	0.027625000	3.948988000	-1.440718000
O	-1.418280000	2.092840000	-0.061636000
O	0.134106000	1.494080000	-3.970222000
O	1.300116000	-0.107963000	-2.262633000
O	-1.100499000	-0.084972000	-1.438550000

Zr	2.511581000	0.009326000	0.129889000
Zr	-0.082426000	-1.611512000	2.015375000
Zr	-0.037381000	1.950525000	1.731397000
Zr	-0.030367000	1.647427000	-1.800603000
Zr	-2.565620000	-0.000717000	0.035240000
Zr	0.008937000	-1.923843000	-1.579922000
N	2.784612000	4.339361000	-4.097811000
H	2.116087000	3.584415000	-4.039653000
H	2.773071000	4.818158000	-4.985672000
N	-2.737226000	4.200689000	-4.336999000
H	-2.627852000	5.126036000	-4.719206000
H	-1.983227000	3.886518000	-3.747588000
N	-2.693899000	-4.562646000	-3.964464000
H	-1.958505000	-4.235361000	-3.356346000
H	-2.587563000	-5.513574000	-4.280084000
N	2.828457000	-4.636653000	-3.702267000
H	2.793555000	-5.194572000	-4.540149000
H	2.099571000	-3.946499000	-3.613708000
Fe	1.107767000	-0.201291000	-4.109551000
O	0.965932000	-0.286663000	-5.823120000
C	3.977032000	-0.654377000	-4.839650000
C	5.153508000	-0.175532000	-4.033036000
H	3.594313000	-1.609494000	-4.443725000
H	4.266853000	-0.848243000	-5.882101000
H	5.529491000	0.771661000	-4.430351000
H	4.871771000	-0.022052000	-2.986391000
H	5.959578000	-0.914738000	-4.068997000
O	2.936488000	0.328613000	-4.847649000
H	2.119042000	0.096017000	-5.733016000

Fe-NU-1000-NH<sub>2</sub> (Int\_4)

Free Energy: -4509.175844

Electronic Energy: -4509.5266461

C	5.726500000	-2.889202000	-2.160197000
C	-5.638900000	-2.885106000	-2.451393000
C	4.388900000	-3.187724000	-2.459971000
C	-4.292995000	-3.161933000	-2.734566000
C	4.106399000	-4.252604000	-3.328495000
C	-3.985999000	-4.236310000	-3.582687000
C	5.138201000	-5.020698000	-3.859402000
C	-4.998200000	-5.035199000	-4.107601000
C	6.482800000	-4.751199000	-3.537702000
C	-6.351100000	-4.782198000	-3.807102000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.761999000	-2.369401000
C	-5.668799000	2.628905000	-2.684594000
C	4.341460000	3.021353000	-2.724759000
C	-4.324796000	2.872035000	-3.007967000
C	4.069797000	4.017808000	-3.673344000
C	-4.019399000	3.907109000	-3.904889000
C	5.105944000	4.760658000	-4.231175000
C	-5.033000000	4.692699000	-4.448901000
C	6.444700000	4.526398000	-3.861702000
C	-6.384200000	4.462598000	-4.123402000
C	6.708200000	3.500400000	-2.934600000

C	-6.680500000	3.408600000	-3.237600000
C	-3.223438000	-2.332414000	-2.105856000
C	-3.315197000	-2.089480000	2.441199000
C	-3.322890000	2.330080000	2.211501000
C	3.188494000	2.436985000	2.193707000
C	3.242012000	2.242113000	-2.085943000
C	3.280315000	-2.402487000	-1.851640000
C	-3.245524000	2.084897000	-2.346741000
C	3.174595000	-2.211088000	2.426599000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873098000	-4.749003000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876899000	5.534111000	-4.959788000
H	-4.774300000	5.498298000	-5.131202000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101096000	-2.666608000	2.881897000
H	3.964842000	3.004739000	2.662597000
H	-4.111861000	2.914429000	2.636942000
H	3.948376000	-2.768390000	2.911984000
O	-3.663726000	1.472089000	1.337396000
O	-3.609958000	1.255455000	-1.456658000
O	-3.654014000	-1.258601000	1.542897000
O	-2.127284000	-2.310291000	2.835696000
O	1.970317000	-2.521860000	2.683561000
O	2.090023000	-2.742347000	-2.140755000
O	3.548203000	-1.286089000	1.640808000
O	3.614163000	-1.448465000	-1.083629000
O	3.557212000	1.485679000	1.438517000
O	3.591777000	1.320374000	-1.285223000
O	2.046444000	2.547416000	-2.386560000
O	1.986508000	2.771378000	2.435641000
O	-2.020261000	-2.553914000	-2.444743000
O	-3.603949000	-1.474766000	-1.248348000
O	-2.134287000	2.562484000	2.592264000
O	-2.045138000	2.316158000	-2.694291000
H	-1.966554000	-2.859407000	0.237171000
H	-1.031818000	1.831626000	4.278184000
H	-0.136995000	0.526234000	4.137505000
H	-0.507851000	1.324578000	-4.573271000
H	-0.005388000	4.072701000	-0.446080000
H	0.652214000	4.475671000	1.585437000
H	0.906526000	4.212521000	-1.735517000
H	1.862898000	0.173689000	2.988099000
H	-1.960015000	2.883073000	-0.099702000
H	-0.815549000	-1.483070000	4.551972000
H	-0.741179000	-1.646237000	-4.077864000

H	0.856067000	-4.190091000	1.926787000
H	0.751523000	-4.465594000	-1.357386000
H	-0.005508000	-4.036220000	0.602604000
O	-1.117341000	0.118989000	1.531020000
O	-0.003964000	-3.889780000	1.605672000
O	1.037332000	1.477110000	-0.004521000
O	1.318083000	0.158935000	2.193902000
O	-0.078934000	-1.083361000	4.077556000
O	-0.156117000	1.533237000	4.000045000
O	0.149065000	-1.796702000	-3.731740000
O	1.053566000	-1.451757000	0.209833000
O	-1.419228000	-2.066877000	0.226980000
O	-0.028625000	-4.002919000	-1.030714000
O	-0.072379000	3.985549000	1.182352000
O	0.024438000	3.932187000	-1.449941000
O	-1.421167000	2.085217000	-0.064259000
O	0.227499000	1.314731000	-3.952021000
O	1.343998000	-0.132242000	-2.092600000
O	-1.104462000	-0.097234000	-1.432685000
Zr	2.504868000	0.010394000	0.119543000
Zr	-0.082779000	-1.610933000	2.038403000
Zr	-0.038150000	1.952430000	1.732831000
Zr	-0.029080000	1.627502000	-1.808728000
Zr	-2.563527000	0.000213000	0.040932000
Zr	0.012734000	-1.943188000	-1.524694000
N	2.784832000	4.339288000	-4.098544000
H	2.110400000	3.591415000	-4.025416000
H	2.769265000	4.815952000	-4.987225000
N	-2.738608000	4.200336000	-4.337553000
H	-2.625385000	5.127029000	-4.714837000
H	-1.982712000	3.872227000	-3.758410000
N	-2.696856000	-4.555520000	-3.974455000
H	-1.953398000	-4.203766000	-3.390483000
H	-2.581525000	-5.505976000	-4.287250000
N	2.828813000	-4.640362000	-3.700448000
H	2.791994000	-5.198199000	-4.538044000
H	2.094103000	-3.958909000	-3.599124000
Fe	1.461595000	-0.302393000	-3.925038000
O	1.458170000	-0.703291000	-5.694146000
C	4.096283000	-0.399207000	-4.907580000
C	5.456154000	0.219472000	-4.669727000
H	4.132342000	-1.484529000	-4.714231000
H	3.760349000	-0.270632000	-5.946225000
H	5.455869000	1.283625000	-4.920586000
H	5.739871000	0.122006000	-3.618068000
H	6.206911000	-0.286734000	-5.284090000
O	3.172432000	0.208046000	-4.033760000
H	0.843120000	-1.439005000	-5.818941000

Fe-NU-1000-NH<sub>2</sub> (TS2\_4)

Free Energy: -4509.161457

Electronic Energy: -4509.5052988

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000



C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000

O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.979118000	-2.843510000	0.231299000
H	-1.035787000	1.828972000	4.288193000
H	-0.135833000	0.527886000	4.144062000
H	-0.620748000	1.196436000	-4.456463000
H	-0.008884000	4.071587000	-0.444007000
H	0.649301000	4.483624000	1.587762000
H	0.910327000	4.214403000	-1.726359000
H	1.866799000	0.176282000	2.985051000
H	-1.959284000	2.884739000	-0.107507000
H	-0.814771000	-1.479134000	4.559711000
H	-0.735261000	-1.716390000	-4.126167000
H	0.847804000	-4.174973000	1.930154000
H	0.780703000	-4.446044000	-1.268509000
H	-0.032365000	-4.021060000	0.617501000
O	-1.119073000	0.125452000	1.535501000
O	-0.021609000	-3.887212000	1.622580000
O	1.036185000	1.505982000	0.012157000
O	1.313548000	0.162896000	2.196828000
O	-0.078554000	-1.079184000	4.085028000
O	-0.158635000	1.535850000	4.009631000
O	0.132714000	-1.769189000	-3.711337000
O	1.048027000	-1.468599000	0.227836000
O	-1.424783000	-2.056035000	0.225226000
O	-0.032905000	-3.998595000	-1.016815000
O	-0.080347000	3.996154000	1.190578000
O	0.027422000	3.930793000	-1.447358000
O	-1.420614000	2.087236000	-0.063790000
O	0.212564000	1.243782000	-3.974733000
O	1.388404000	-0.126394000	-2.007392000
O	-1.100147000	-0.087762000	-1.428886000
Zr	2.477078000	0.010308000	0.118880000
Zr	-0.087225000	-1.606698000	2.042974000
Zr	-0.042901000	1.962700000	1.742298000
Zr	-0.009466000	1.620492000	-1.800459000
Zr	-2.562169000	0.003338000	0.042917000
Zr	0.007166000	-1.927083000	-1.536152000
N	2.785952000	4.341769000	-4.096615000
H	2.112237000	3.592864000	-4.029517000
H	2.770869000	4.823328000	-4.982619000
N	-2.738937000	4.199710000	-4.337807000
H	-2.624232000	5.126548000	-4.714076000
H	-1.982848000	3.866694000	-3.761540000
N	-2.697956000	-4.552435000	-3.976649000
H	-1.951698000	-4.190865000	-3.402481000
H	-2.578792000	-5.499232000	-4.297859000
N	2.835589000	-4.517795000	-3.837508000
H	2.741975000	-5.426117000	-4.264978000
H	2.058042000	-4.229842000	-3.263422000

Fe	1.525199000	-0.292148000	-3.890945000
O	2.423269000	-1.588237000	-5.000198000
C	4.125907000	0.186386000	-5.029767000
C	5.395351000	0.002789000	-4.238069000
H	3.660349000	-0.931732000	-5.244750000
H	4.257427000	0.578622000	-6.054055000
H	5.959538000	0.941626000	-4.194834000
H	5.157622000	-0.293912000	-3.211851000
H	6.036995000	-0.759894000	-4.689745000
O	3.090690000	0.738111000	-4.389042000
H	2.349572000	-2.541693000	-4.801375000

Fe-NU-1000-NH<sub>2</sub> (Prod\_4)

Free Energy: -4509.19791

Electronic Energy: -4509.5428187

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000

H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.981217000	-2.833168000	0.206130000
H	-1.041026000	1.811637000	4.291238000
H	-0.135943000	0.513730000	4.140928000
H	-0.613322000	1.553784000	-4.483668000
H	-0.010920000	4.077364000	-0.420904000
H	0.649518000	4.479730000	1.611164000
H	0.916551000	4.228310000	-1.690999000
H	1.877364000	0.162265000	2.965577000
H	-1.964904000	2.881490000	-0.108066000
H	-0.820431000	-1.484418000	4.548772000
H	0.933584000	-2.678804000	-4.018510000
H	0.844422000	-4.176018000	1.894364000
H	0.847519000	-4.370006000	-1.233464000
H	-0.036777000	-3.997811000	0.582961000
O	-1.117266000	0.124446000	1.527781000
O	-0.026101000	-3.885808000	1.592904000
O	1.040232000	1.529964000	0.024627000
O	1.309274000	0.157544000	2.188016000
O	-0.080552000	-1.086893000	4.077918000
O	-0.161918000	1.523928000	4.013585000
O	0.232640000	-2.038218000	-3.835963000
O	1.038969000	-1.479935000	0.211460000
O	-1.425897000	-2.046561000	0.214657000
O	-0.006476000	-3.968920000	-1.045738000
O	-0.089148000	4.003101000	1.217463000
O	0.032005000	3.943317000	-1.423665000
O	-1.423769000	2.086320000	-0.056957000
O	0.205210000	1.504496000	-3.975369000
O	1.314777000	-0.101228000	-2.035950000

O	-1.143243000	-0.090625000	-1.460541000
Zr	2.440320000	0.008662000	0.106820000
Zr	-0.092594000	-1.611119000	2.031298000
Zr	-0.047030000	1.964959000	1.750003000
Zr	-0.016304000	1.615166000	-1.788690000
Zr	-2.569727000	-0.001343000	0.037875000
Zr	0.001901000	-1.886594000	-1.582406000
N	2.788919000	4.353163000	-4.083531000
H	2.075475000	3.650618000	-3.958022000
H	2.749287000	4.856265000	-4.955358000
N	-2.736337000	4.200209000	-4.335928000
H	-2.624103000	5.131847000	-4.701712000
H	-1.985608000	3.873536000	-3.747794000
N	-2.699963000	-4.543804000	-3.982928000
H	-1.950602000	-4.117087000	-3.457739000
H	-2.559897000	-5.496918000	-4.273702000
N	2.832939000	-4.585985000	-3.769938000
H	2.758300000	-5.519482000	-4.142758000
H	2.078144000	-4.304928000	-3.164872000
Fe	1.162866000	-0.244536000	-4.065767000
O	0.253263000	-0.612849000	-6.142228000
C	4.100395000	-1.141391000	-4.693171000
C	4.892786000	-0.124513000	-3.974174000
H	4.618194000	-1.978001000	-5.193567000
H	0.896822000	-0.990746000	-6.750232000
H	4.706774000	0.868194000	-4.403133000
H	4.558555000	-0.068159000	-2.927807000
H	5.962692000	-0.334323000	-4.006032000
O	2.864339000	-1.101175000	-4.779231000
H	-0.214367000	-1.377835000	-5.762581000

Fe-NU-1000-NO<sub>2</sub>-O

Free Energy: -4950.74742

Electronic Energy: -4950.947371

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000

C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554501000	-2.444701000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045099000	2.316700000	-2.694300000
H	-1.948844000	-2.860111000	0.219745000
H	-1.024182000	1.826082000	4.287089000
H	-0.131583000	0.520617000	4.131912000
H	-0.019687000	1.815613000	-4.760975000
H	0.004656000	4.100820000	-0.460481000
H	0.659987000	4.480719000	1.601016000
H	0.637341000	4.422466000	-1.903794000
H	1.872610000	0.167263000	2.970793000
H	-1.945016000	2.895409000	-0.111038000
H	-0.810716000	-1.483689000	4.548523000

H	0.399390000	-2.554641000	-4.425494000
H	0.845042000	-4.203511000	1.936801000
H	0.514985000	-4.577246000	-1.477467000
H	0.006229000	-4.039018000	0.596462000
O	-1.113524000	0.122009000	1.536641000
O	-0.005382000	-3.890195000	1.604015000
O	1.034599000	1.501366000	-0.001415000
O	1.316687000	0.157183000	2.184218000
O	-0.075153000	-1.086009000	4.070869000
O	-0.150827000	1.529221000	4.000735000
O	0.227237000	-1.826116000	-3.813348000
O	1.040328000	-1.458111000	0.198456000
O	-1.418071000	-2.055777000	0.219147000
O	-0.044059000	-3.958712000	-0.992892000
O	-0.068581000	3.994559000	1.200417000
O	-0.055581000	3.920313000	-1.448955000
O	-1.421956000	2.087287000	-0.062234000
O	0.193515000	1.299970000	-3.976462000
O	1.327908000	-0.113410000	-2.090959000
O	-1.099893000	-0.090063000	-1.432595000
Zr	2.463028000	0.005505000	0.124429000
Zr	-0.083441000	-1.621401000	2.032325000
Zr	-0.039016000	1.966604000	1.737651000
Zr	-0.029366000	1.646454000	-1.812000000
Zr	-2.542396000	-0.000874000	0.050614000
Zr	0.008542000	-1.947345000	-1.570335000
N	2.692650000	4.397811000	-4.037016000
N	-2.642319000	4.221178000	-4.328832000
N	-2.600553000	-4.613926000	-3.917411000
N	2.730688000	-4.628897000	-3.701060000
O	-2.136973000	-4.152655000	-4.952730000
O	-2.058503000	-5.412391000	-3.165702000
O	2.203626000	-5.509484000	-3.030806000
O	2.246804000	-4.075893000	-4.680121000
O	-2.188145000	3.566760000	-5.259189000
O	-2.095752000	5.156519000	-3.760485000
O	2.127021000	5.186902000	-3.281340000
O	2.244403000	3.951687000	-5.080722000
Fe	1.272901000	-0.272419000	-3.953589000
O	2.050198000	-0.375168000	-5.373793000

Fe-NU-1000-NO<sub>2</sub> (Ads\_4)

Free Energy: -5105.729051

Electronic Energy: -5106.0095965

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885099000	-2.451401000
C	4.388901000	-3.187701000	-2.459999000
C	-4.292996000	-3.161898000	-2.734601000
C	4.106398000	-4.252600000	-3.328501000
C	-3.986007000	-4.236299000	-3.582698000
C	5.138201000	-5.020699000	-3.859400000
C	-4.998197000	-5.035203000	-4.107602000
C	6.482800000	-4.751200000	-3.537701000
C	-6.351100000	-4.782201000	-3.807099000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000

C	5.673398000	2.762021000	-2.369377000
C	-5.668800000	2.628898000	-2.684602000
C	4.341386000	3.021279000	-2.724818000
C	-4.324796000	2.871995000	-3.008004000
C	4.069911000	4.017822000	-3.673477000
C	-4.019407000	3.907098000	-3.904898000
C	5.105904000	4.760729000	-4.231154000
C	-5.032997000	4.692703000	-4.448901000
C	6.444697000	4.526426000	-3.861672000
C	-6.384200000	4.462602000	-4.123398000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223402000	-2.332303000	-2.105802000
C	-3.315201000	-2.089499000	2.441200000
C	-3.322899000	2.330097000	2.211502000
C	3.188498000	2.436999000	2.193702000
C	3.242001000	2.242003000	-2.085995000
C	3.280299000	-2.402401000	-1.851692000
C	-3.245500000	2.084795000	-2.346702000
C	3.174599000	-2.211101000	2.426598000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524399000
H	-4.737200000	-5.873099000	-4.749001000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876901000	5.534094000	-4.959807000
H	-4.774300000	5.498299000	-5.131202000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101095000	-2.666617000	2.881888000
H	3.964843000	3.004751000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768396000	2.911977000
O	-3.663691000	1.472104000	1.337405000
O	-3.609996000	1.255399000	-1.456698000
O	-3.654006000	-1.258597000	1.542902000
O	-2.127309000	-2.310197000	2.835694000
O	1.970295000	-2.521806000	2.683601000
O	2.089987000	-2.742705000	-2.140588000
O	3.548196000	-1.286120000	1.640813000
O	3.614207000	-1.448424000	-1.083692000
O	3.557206000	1.485680000	1.438511000
O	3.591823000	1.320280000	-1.285287000
O	2.046395000	2.547834000	-2.386389000
O	1.986504000	2.771306000	2.435713000
O	-2.020212000	-2.554525000	-2.444708000
O	-3.604005000	-1.474697000	-1.248397000
O	-2.134296000	2.562397000	2.592313000
O	-2.045088000	2.316711000	-2.694295000



H	-1.940625000	-2.860006000	0.219967000
H	-1.031335000	1.820431000	4.272928000
H	-0.132148000	0.519702000	4.126317000
H	-0.278653000	1.738843000	-4.735757000
H	0.006245000	4.090078000	-0.471723000
H	0.664852000	4.475886000	1.600169000
H	0.626183000	4.411136000	-1.914927000
H	1.872227000	0.167289000	2.972660000
H	-1.935887000	2.894521000	-0.113545000
H	-0.815564000	-1.484747000	4.539380000
H	-0.349952000	-2.314500000	-4.451041000
H	0.852671000	-4.194933000	1.913589000
H	0.524096000	-4.546725000	-1.481897000
H	0.010152000	-4.021730000	0.570615000
O	-1.115032000	0.122592000	1.543361000
O	-0.000262000	-3.884784000	1.584983000
O	1.041558000	1.496400000	-0.003540000
O	1.318579000	0.156992000	2.184741000
O	-0.074208000	-1.089985000	4.068411000
O	-0.152584000	1.528509000	3.997919000
O	0.162965000	-1.864264000	-3.769883000
O	1.044653000	-1.448642000	0.193828000
O	-1.418967000	-2.050061000	0.220688000
O	-0.055122000	-3.946874000	-1.000324000
O	-0.066416000	3.994278000	1.199259000
O	-0.063105000	3.910061000	-1.458055000
O	-1.420181000	2.082319000	-0.059087000
O	0.189733000	1.389425000	-3.969583000
O	1.263166000	-0.111581000	-2.168762000
O	-1.137594000	-0.091893000	-1.427193000
Zr	2.459868000	0.003791000	0.117906000
Zr	-0.081200000	-1.619725000	2.025843000
Zr	-0.036006000	1.963997000	1.730569000
Zr	-0.028871000	1.615667000	-1.821967000
Zr	-2.546891000	0.001654000	0.058073000
Zr	0.000371000	-1.914992000	-1.584851000
N	2.697193000	4.315926000	-4.118348000
N	-2.643041000	4.211765000	-4.337754000
N	-2.602863000	-4.573539000	-3.966050000
N	2.762302000	-4.481390000	-3.880940000
O	-2.127531000	-3.960963000	-4.916717000
O	-2.071134000	-5.484539000	-3.349122000
O	2.125410000	-5.439904000	-3.477085000
O	2.428032000	-3.723632000	-4.794330000
O	-2.186597000	3.529425000	-5.247513000
O	-2.100369000	5.166658000	-3.800167000
O	2.095838000	5.194077000	-3.505118000
O	2.293826000	3.704389000	-5.095533000
Fe	1.134928000	-0.264192000	-4.139314000
O	1.079465000	-0.316702000	-5.770766000
C	3.986074000	-0.014476000	-4.932505000
C	5.432291000	-0.248682000	-4.588441000
H	3.764248000	-0.125580000	-5.998604000
H	3.663911000	0.993600000	-4.643402000
H	5.581999000	-0.137447000	-3.510324000
H	5.754088000	-1.255294000	-4.877086000

H	6.069537000	0.475023000	-5.105477000
O	3.145751000	-0.916763000	-4.171961000
H	3.086599000	-1.778102000	-4.629762000

Fe-NU-1000-NO<sub>2</sub> (TS1\_4)

Free Energy: -5105.711015

Electronic Energy: -5105.9844341

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000

H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.940711000	-2.856409000	0.217865000
H	-1.026292000	1.825408000	4.271514000
H	-0.133491000	0.520125000	4.121973000
H	-0.423424000	1.716180000	-4.680978000
H	0.012413000	4.112460000	-0.471092000
H	0.663681000	4.479477000	1.603818000
H	0.636261000	4.425213000	-1.920937000
H	1.865879000	0.165561000	2.978731000
H	-1.938117000	2.902785000	-0.102491000
H	-0.812808000	-1.487672000	4.531811000
H	-0.248060000	-2.241194000	-4.513399000
H	0.848192000	-4.203324000	1.915200000
H	0.515922000	-4.557719000	-1.491973000
H	0.011327000	-4.027045000	0.570172000
O	-1.113839000	0.124324000	1.539895000
O	0.001810000	-3.881513000	1.581076000
O	1.044484000	1.483471000	-0.009823000
O	1.321608000	0.156520000	2.184080000
O	-0.074101000	-1.089575000	4.059322000
O	-0.150251000	1.528655000	3.992707000
O	0.159133000	-1.773049000	-3.775540000
O	1.046072000	-1.430796000	0.173232000
O	-1.414081000	-2.049460000	0.213967000
O	-0.052701000	-3.949096000	-1.006036000
O	-0.061034000	3.992604000	1.197319000
O	-0.057266000	3.931026000	-1.457054000
O	-1.418426000	2.092074000	-0.062048000
O	0.132453000	1.421767000	-3.951063000
O	1.312578000	-0.103682000	-2.225831000
O	-1.095326000	-0.082413000	-1.421859000
Zr	2.480734000	0.011712000	0.130263000
Zr	-0.078962000	-1.617486000	2.018844000
Zr	-0.033534000	1.963895000	1.727869000
Zr	-0.028624000	1.658343000	-1.822081000
Zr	-2.538549000	0.002092000	0.051530000
Zr	0.006054000	-1.932211000	-1.592351000
N	2.693758000	4.399385000	-4.042593000

N	-2.643892000	4.203117000	-4.347071000
N	-2.602612000	-4.581962000	-3.958555000
N	2.737862000	-4.601477000	-3.750379000
O	-2.128202000	-3.993280000	-4.923796000
O	-2.070603000	-5.476628000	-3.318174000
O	2.176983000	-5.492605000	-3.122187000
O	2.305039000	-4.022198000	-4.736747000
O	-2.199413000	3.511902000	-5.256469000
O	-2.089908000	5.155565000	-3.817668000
O	2.120083000	5.174233000	-5.276357000
O	2.259437000	3.978532000	-5.101060000
Fe	1.175834000	-0.206514000	-4.093638000
O	1.134754000	-0.284195000	-5.806397000
C	4.076949000	-0.652515000	-4.781448000
C	5.284744000	-0.191355000	-4.008793000
H	3.697796000	-1.611708000	-4.396236000
H	4.335881000	-0.835108000	-5.834226000
H	5.644485000	0.762958000	-4.405199000
H	5.037339000	-0.054019000	-2.950871000
H	6.094190000	-0.924021000	-4.088265000
O	3.052621000	0.340358000	-4.735212000
H	2.266075000	0.134240000	-5.656395000

Fe-NU-1000-NO<sub>2</sub> (Int\_4)

Free Energy: -5105.746857

Electronic Energy: -5106.0244168

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000

C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.949465000	-2.857996000	0.225550000
H	-1.027016000	1.828121000	4.266806000
H	-0.130628000	0.525560000	4.122658000
H	-0.049553000	1.755994000	-4.720578000
H	0.004749000	4.094368000	-0.475137000
H	0.665307000	4.478877000	1.590356000
H	0.636457000	4.411929000	-1.917852000
H	1.867846000	0.171265000	2.973270000
H	-1.944535000	2.897170000	-0.105281000
H	-0.812148000	-1.481443000	4.538248000
H	0.219648000	-2.478251000	-4.357528000
H	0.850946000	-4.197792000	1.923424000
H	0.513106000	-4.569140000	-1.480856000
H	0.006769000	-4.031695000	0.584523000
O	-1.116014000	0.123498000	1.542021000
O	-0.001354000	-3.886557000	1.593803000
O	1.036164000	1.485867000	-0.015038000
O	1.319860000	0.158609000	2.181302000

O	-0.072334000	-1.086067000	4.065265000
O	-0.149283000	1.533408000	3.991225000
O	0.169987000	-1.720095000	-3.761945000
O	1.044385000	-1.445854000	0.189529000
O	-1.420151000	-2.052995000	0.221335000
O	-0.053250000	-3.955136000	-1.000406000
O	-0.062098000	3.993032000	1.187499000
O	-0.061579000	3.917468000	-1.463690000
O	-1.421855000	2.088550000	-0.065161000
O	0.201076000	1.258601000	-3.936274000
O	1.328441000	-0.123122000	-2.120904000
O	-1.098776000	-0.086835000	-1.418979000
Zr	2.476262000	0.011018000	0.122551000
Zr	-0.080070000	-1.617583000	2.024919000
Zr	-0.034624000	1.963499000	1.722614000
Zr	-0.031596000	1.642850000	-1.838564000
Zr	-2.540350000	0.002104000	0.053739000
Zr	0.001515000	-1.934220000	-1.576089000
N	2.693979000	4.351945000	-4.079876000
N	-2.643003000	4.215823000	-4.335383000
N	-2.598914000	-4.595413000	-3.933328000
N	2.737548000	-4.585781000	-3.758853000
O	-2.123076000	-4.066434000	-4.931341000
O	-2.063609000	-5.442833000	-3.233256000
O	2.182030000	-5.509173000	-3.176625000
O	2.291571000	-3.953134000	-4.708861000
O	-2.190532000	3.548816000	-5.257914000
O	-2.096365000	5.159518000	-3.781679000
O	2.102076000	5.180057000	-3.389751000
O	2.271505000	3.826382000	-5.097726000
Fe	1.483088000	-0.280224000	-3.960233000
O	1.459065000	-0.516417000	-5.745576000
C	4.114239000	-0.462304000	-4.969043000
C	5.489999000	0.134705000	-4.757149000
H	4.148351000	-1.560336000	-4.867980000
H	3.738394000	-0.248759000	-5.979668000
H	5.481877000	1.212433000	-4.944643000
H	5.822525000	-0.026505000	-3.726517000
H	6.212524000	-0.331301000	-5.434185000
O	3.245556000	0.082746000	-4.006046000
H	0.572063000	-0.810974000	-5.997617000

Fe-NU-1000-NO<sub>2</sub> (TS2\_4)

Free Energy: -5105.730684

Electronic Energy: -5106.0031756

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000

C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000

O	-2.045100000	2.316700000	-2.694300000
H	-1.949598000	-2.855280000	0.228346000
H	-1.031761000	1.823598000	4.277795000
H	-0.129733000	0.525514000	4.131237000
H	-0.396672000	1.600254000	-4.635131000
H	0.002147000	4.093925000	-0.475247000
H	0.662625000	4.483832000	1.593757000
H	0.641031000	4.405155000	-1.914944000
H	1.874812000	0.173211000	2.972434000
H	-1.941909000	2.898221000	-0.108938000
H	-0.812917000	-1.480298000	4.547705000
H	-0.487266000	-2.070781000	-4.332081000
H	0.854304000	-4.189529000	1.928435000
H	0.431555000	-4.603044000	-1.489049000
H	-0.000740000	-4.035801000	0.595695000
O	-1.115499000	0.126555000	1.549122000
O	-0.004899000	-3.889566000	1.605915000
O	1.036804000	1.510763000	0.002767000
O	1.316583000	0.161377000	2.187793000
O	-0.072306000	-1.085158000	4.075881000
O	-0.152321000	1.534068000	4.002773000
O	0.145603000	-1.710580000	-3.703646000
O	1.044131000	-1.461679000	0.212079000
O	-1.423287000	-2.048406000	0.225620000
O	-0.076637000	-3.959646000	-0.983646000
O	-0.070516000	4.000217000	1.198626000
O	-0.062683000	3.915754000	-1.462670000
O	-1.421482000	2.088513000	-0.063176000
O	0.190179000	1.254404000	-3.955232000
O	1.380042000	-0.115919000	-2.046325000
O	-1.093984000	-0.082893000	-1.410152000
Zr	2.454685000	0.012290000	0.118317000
Zr	-0.079541000	-1.618435000	2.033908000
Zr	-0.036367000	1.970675000	1.734120000
Zr	-0.017413000	1.635774000	-1.825120000
Zr	-2.534353000	0.004602000	0.059447000
Zr	0.002113000	-1.936358000	-1.565727000
N	2.696195000	4.388432000	-4.058351000
N	-2.643854000	4.200835000	-4.349602000
N	-2.602993000	-4.563826000	-3.977723000
N	2.733858000	-4.689993000	-3.650577000
O	-2.145891000	-3.949312000	-4.936187000
O	-2.053056000	-5.466488000	-3.364666000
O	2.245163000	-5.534515000	-2.915145000
O	2.221875000	-4.252141000	-4.678269000
O	-2.197799000	3.502923000	-5.253641000
O	-2.091541000	5.158748000	-3.828825000
O	2.108831000	5.166433000	-3.307199000
O	2.278988000	3.957693000	-5.120600000
Fe	1.491190000	-0.243337000	-3.939049000
O	2.289470000	-1.395245000	-5.272133000
C	4.060755000	0.300796000	-5.153416000
C	5.378323000	-0.006373000	-4.485318000
H	3.509977000	-0.776100000	-5.474277000
H	4.130917000	0.812884000	-6.130191000
H	5.962996000	0.912080000	-4.351323000



H	5.201247000	-0.432342000	-3.493244000
H	5.980331000	-0.705943000	-5.073686000
O	3.100273000	0.784276000	-4.370852000
H	2.216994000	-2.362037000	-5.172375000

Fe-NU-1000-NO<sub>2</sub> (Prod\_4)

Free Energy: -5105.770318

Electronic Energy: -5106.0443404

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000

H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.943363000	-2.861902000	0.232060000
H	-1.040927000	1.816245000	4.277019000
H	-0.129919000	0.524489000	4.136908000
H	-0.425753000	1.731940000	-4.596758000
H	0.001898000	4.076836000	-0.473978000
H	0.663014000	4.479499000	1.597450000
H	0.634082000	4.393408000	-1.909271000
H	1.889314000	0.172907000	2.964223000
H	-1.935784000	2.885065000	-0.122395000
H	-0.820425000	-1.479833000	4.556500000
H	-0.675639000	-2.320149000	-4.145329000
H	0.856714000	-4.185168000	1.933412000
H	0.503493000	-4.559640000	-1.468808000
H	0.006232000	-4.031100000	0.596130000
O	-1.112158000	0.122430000	1.550042000
O	-0.005565000	-3.893679000	1.611207000
O	1.042543000	1.525781000	0.014477000
O	1.313715000	0.160089000	2.192503000
O	-0.075615000	-1.088982000	4.087892000
O	-0.157234000	1.532796000	4.009523000
O	0.128308000	-1.988163000	-3.727686000
O	1.049343000	-1.482734000	0.235181000
O	-1.423621000	-2.051089000	0.232053000
O	-0.062841000	-3.959131000	-0.972500000
O	-0.076992000	4.001691000	1.208188000
O	-0.064467000	3.898576000	-1.459908000
O	-1.419529000	2.074034000	-0.060075000
O	0.196714000	1.353307000	-3.967817000
O	1.314925000	-0.122419000	-2.038704000
O	-1.139893000	-0.102251000	-1.430829000
Zr	2.427027000	0.004406000	0.106732000
Zr	-0.080118000	-1.623271000	2.044719000
Zr	-0.036296000	1.970907000	1.738596000
Zr	-0.009445000	1.593177000	-1.822355000
Zr	-2.535788000	0.003459000	0.062786000
Zr	0.011147000	-1.922061000	-1.552636000

N	2.697104000	4.335870000	-4.104187000
N	-2.645257000	4.197637000	-4.354296000
N	-2.614324000	-4.523151000	-4.043090000
N	2.751090000	-4.568184000	-3.817353000
O	-2.175031000	-3.798085000	-4.935401000
O	-2.059568000	-5.500061000	-3.567904000
O	2.116360000	-5.425585000	-3.220303000
O	2.423626000	-4.006393000	-4.856477000
O	-2.205303000	3.498161000	-5.261222000
O	-2.089475000	5.156502000	-3.840203000
O	2.103486000	5.196913000	-3.459877000
O	2.288864000	3.765657000	-5.103619000
Fe	1.178497000	-0.358503000	-4.093527000
O	0.794623000	-0.943122000	-6.288686000
C	4.222518000	-1.041115000	-4.685082000
C	5.114366000	-0.010736000	-4.106798000
H	4.656314000	-1.960387000	-5.116488000
H	1.314508000	-1.758436000	-6.258096000
H	4.957404000	0.953024000	-4.606124000
H	4.838569000	0.136669000	-3.052281000
H	6.168224000	-0.285994000	-4.176510000
O	2.991189000	-0.929368000	-4.685470000
H	-0.114602000	-1.246486000	-6.389959000

Fe-NU-1000-OH-O

Free Energy: -4433.692456

Electronic Energy: -4433.9130324

C	5.726500000	-2.889193000	-2.160209000
C	-5.638900000	-2.885101000	-2.451398000
C	4.388919000	-3.187698000	-2.460008000
C	-4.293001000	-3.161903000	-2.734597000
C	4.106369000	-4.252609000	-3.328505000
C	-3.985998000	-4.236301000	-3.582700000
C	5.138212000	-5.020694000	-3.859384000
C	-4.998201000	-5.035199000	-4.107600000
C	6.482799000	-4.751209000	-3.537689000
C	-6.351100000	-4.782199000	-3.807101000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673401000	2.761992000	-2.369408000
C	-5.668799000	2.628906000	-2.684592000
C	4.341409000	3.021297000	-2.724805000
C	-4.324797000	2.872005000	-3.007994000
C	4.069886000	4.017805000	-3.673301000
C	-4.019404000	3.907097000	-3.904901000
C	5.105905000	4.760701000	-4.231190000
C	-5.032999000	4.692698000	-4.448906000
C	6.444699000	4.526409000	-3.861691000
C	-6.384201000	4.462593000	-4.123408000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223402000	-2.332311000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322899000	2.330100000	2.211499000
C	3.188500000	2.437000000	2.193701000
C	3.241999000	2.242005000	-2.085998000

C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084803000	-2.346704000
C	3.174599000	-2.211099000	2.426599000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900901000	-5.847192000	-4.524411000
H	-4.737200000	-5.873101000	-4.748999000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876901000	5.534092000	-4.959809000
H	-4.774299000	5.498307000	-5.131192000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101095000	-2.666617000	2.881887000
H	3.964843000	3.004750000	2.662584000
H	-4.111859000	2.914439000	2.636931000
H	3.948377000	-2.768397000	2.911977000
O	-3.663703000	1.472100000	1.337398000
O	-3.610000000	1.255401000	-1.456700000
O	-3.654002000	-1.258599000	1.542898000
O	-2.127299000	-2.310203000	2.835698000
O	1.970301000	-2.521802000	2.683597000
O	2.089996000	-2.742681000	-2.140604000
O	3.548199000	-1.286096000	1.640799000
O	3.614196000	-1.448402000	-1.083694000
O	3.557201000	1.485693000	1.438500000
O	3.591789000	1.320308000	-1.285296000
O	2.046405000	2.547778000	-2.386393000
O	1.986502000	2.771303000	2.435695000
O	-2.020199000	-2.554484000	-2.444700000
O	-3.604000000	-1.474704000	-1.248396000
O	-2.134298000	2.562406000	2.592297000
O	-2.045087000	2.316682000	-2.694298000
H	-1.958623000	-2.855944000	0.218863000
H	-1.014660000	1.831501000	4.315234000
H	-0.136495000	0.514830000	4.146626000
H	-0.299661000	1.608475000	-4.745844000
H	-0.039085000	4.067890000	-0.395539000
H	0.636568000	4.482166000	1.605655000
H	0.825593000	4.307692000	-1.698093000
H	1.865886000	0.164688000	2.984786000
H	-1.963667000	2.883342000	-0.094133000
H	-0.807958000	-1.491575000	4.558397000
H	-0.021793000	-2.302618000	-4.571884000
H	0.839742000	-4.209847000	1.915654000
H	0.677540000	-4.503539000	-1.373148000
H	-0.020207000	-4.027117000	0.592395000
O	-1.115634000	0.117886000	1.529777000
O	-0.011707000	-3.886039000	1.595183000
O	1.036359000	1.490181000	0.006455000

O	1.316659000	0.154678000	2.193218000
O	-0.080387000	-1.086400000	4.074646000
O	-0.152129000	1.523190000	4.009303000
O	0.198711000	-1.781541000	-3.794321000
O	1.044175000	-1.450668000	0.197277000
O	-1.417306000	-2.058621000	0.217715000
O	-0.052682000	-3.971893000	-1.041195000
O	-0.084957000	3.984465000	1.206235000
O	-0.011426000	3.928584000	-1.403656000
O	-1.425655000	2.084614000	-0.056152000
O	0.221747000	1.377434000	-3.971789000
O	1.327868000	-0.112015000	-2.114767000
O	-1.108411000	-0.089404000	-1.432775000
Zr	2.495521000	0.005734000	0.127197000
Zr	-0.084949000	-1.616923000	2.038997000
Zr	-0.043177000	1.952512000	1.752426000
Zr	-0.031256000	1.630947000	-1.779150000
Zr	-2.570137000	-0.002133000	0.049761000
Zr	0.009883000	-1.922702000	-1.547599000
Fe	1.251748000	-0.240918000	-3.980738000
O	1.830187000	-0.362674000	-5.491722000
O	2.861301000	-4.604076000	-3.711818000
H	2.255318000	-3.964073000	-3.288072000
O	-2.723986000	-4.577598000	-3.913832000
H	-2.134847000	-3.961527000	-3.432791000
O	2.825940000	4.314801000	-4.109090000
H	2.224357000	3.669503000	-3.689749000
O	-2.763418000	4.230213000	-4.274202000
H	-2.166164000	3.641199000	-3.772452000

Fe-NU-1000-OH (Ads\_4)

Free Energy: -4588.676627

Electronic Energy: -4588.9776038

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451399000
C	4.388903000	-3.187699000	-2.460002000
C	-4.293000000	-3.161903000	-2.734597000
C	4.106394000	-4.252601000	-3.328502000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138202000	-5.020698000	-3.859398000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872001000	-3.007999000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000

C	-6.680500000	3.408600000	-3.237600000
C	-3.223401000	-2.332309000	-2.105797000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322901000	2.330102000	2.211500000
C	3.188500000	2.436998000	2.193701000
C	3.241998000	2.241995000	-2.086000000
C	3.280300000	-2.402392000	-1.851709000
C	-3.245502000	2.084807000	-2.346700000
C	3.174601000	-2.211100000	2.426601000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663704000	1.472101000	1.337399000
O	-3.610005000	1.255403000	-1.456699000
O	-3.654000000	-1.258598000	1.542899000
O	-2.127298000	-2.310199000	2.835697000
O	1.970300000	-2.521796000	2.683595000
O	2.090003000	-2.742682000	-2.140594000
O	3.548201000	-1.286093000	1.640799000
O	3.614190000	-1.448399000	-1.083704000
O	3.557200000	1.485692000	1.438499000
O	3.591789000	1.320303000	-1.285298000
O	2.046407000	2.547769000	-2.386385000
O	1.986501000	2.771293000	2.435697000
O	-2.020184000	-2.554502000	-2.444698000
O	-3.604002000	-1.474701000	-1.248397000
O	-2.134300000	2.562402000	2.592300000
O	-2.045094000	2.316705000	-2.694308000
H	-1.953580000	-2.857614000	0.222056000
H	-1.022798000	1.825970000	4.301826000
H	-0.137245000	0.514016000	4.141983000
H	-0.357167000	1.578499000	-4.720160000
H	-0.043776000	4.052121000	-0.409288000
H	0.638543000	4.477008000	1.600484000
H	0.830231000	4.285524000	-1.699564000
H	1.866696000	0.165280000	2.984628000
H	-1.959621000	2.875851000	-0.098092000
H	-0.812390000	-1.490900000	4.553153000
H	-0.443186000	-2.139009000	-4.443438000

H	0.842367000	-4.204030000	1.912198000
H	0.658722000	-4.504816000	-1.379592000
H	-0.013381000	-4.018639000	0.582414000
O	-1.116548000	0.116743000	1.533154000
O	-0.009764000	-3.883686000	1.590661000
O	1.040517000	1.486379000	0.003047000
O	1.317208000	0.154476000	2.193487000
O	-0.079938000	-1.089027000	4.074137000
O	-0.154668000	1.522588000	4.006713000
O	0.206682000	-1.908407000	-3.771556000
O	1.047410000	-1.447861000	0.198120000
O	-1.419700000	-2.055534000	0.220864000
O	-0.054256000	-3.964402000	-1.026698000
O	-0.086823000	3.982164000	1.204773000
O	-0.012442000	3.913136000	-1.414707000
O	-1.424731000	2.075546000	-0.054996000
O	0.222665000	1.410464000	-3.970561000
O	1.270651000	-0.118302000	-2.161978000
O	-1.142050000	-0.097608000	-1.436541000
Zr	2.485660000	0.001071000	0.123932000
Zr	-0.084793000	-1.617882000	2.035666000
Zr	-0.042492000	1.949856000	1.746226000
Zr	-0.031871000	1.597216000	-1.790711000
Zr	-2.573853000	-0.002027000	0.053916000
Zr	0.004071000	-1.908184000	-1.556980000
O	2.861140000	-4.580071000	-3.734707000
H	2.247905000	-3.963370000	-3.279907000
O	-2.724054000	-4.581751000	-3.911661000
H	-2.130701000	-3.981729000	-3.416120000
O	2.827262000	4.298155000	-4.120161000
H	2.222287000	3.669042000	-3.675828000
O	-2.763036000	4.230146000	-4.272586000
H	-2.165924000	3.641126000	-3.769229000
Fe	1.158836000	-0.271397000	-4.111865000
O	1.037838000	-0.336734000	-5.742893000
C	4.003503000	0.233720000	-4.878093000
C	5.443469000	0.089864000	-4.474699000
H	3.833289000	0.154346000	-5.956446000
H	3.587869000	1.194270000	-4.555600000
H	5.526515000	0.126794000	-3.385027000
H	5.867156000	-0.857320000	-4.823407000
H	6.034167000	0.909874000	-4.893546000
O	3.199565000	-0.773860000	-4.196877000
H	3.254494000	-1.594444000	-4.708338000

Fe-NU-1000-OH (TS1\_4)

Free Energy: -4588.658877

Electronic Energy: -4588.9546189

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000

C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000



O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.952733000	-2.852171000	0.217627000
H	-1.017442000	1.830658000	4.301606000
H	-0.139195000	0.513721000	4.137711000
H	-0.517876000	1.579518000	-4.631150000
H	-0.030132000	4.075403000	-0.398258000
H	0.640966000	4.480110000	1.609951000
H	0.821454000	4.315008000	-1.712100000
H	1.860199000	0.163439000	2.991209000
H	-1.959546000	2.886945000	-0.089226000
H	-0.810958000	-1.494369000	4.543497000
H	-0.407236000	-2.062842000	-4.487835000
H	0.840016000	-4.208935000	1.908774000
H	0.651482000	-4.508639000	-1.393655000
H	-0.012886000	-4.020726000	0.577453000
O	-1.115146000	0.119637000	1.529265000
O	-0.006905000	-3.879221000	1.583130000
O	1.045374000	1.475646000	-0.001103000
O	1.320322000	0.154285000	2.193249000
O	-0.080458000	-1.088977000	4.064295000
O	-0.152553000	1.522200000	4.002022000
O	0.203845000	-1.834767000	-3.779222000
O	1.049741000	-1.427966000	0.176091000
O	-1.414336000	-2.052917000	0.212995000
O	-0.057143000	-3.964740000	-1.036216000
O	-0.078100000	3.983122000	1.205389000
O	-0.011046000	3.935378000	-1.405261000
O	-1.422467000	2.087368000	-0.056742000
O	0.152784000	1.472810000	-3.949004000
O	1.313924000	-0.107401000	-2.227549000
O	-1.102921000	-0.085398000	-1.434067000
Zr	2.507719000	0.010951000	0.135130000
Zr	-0.082169000	-1.614548000	2.027182000
Zr	-0.039736000	1.950103000	1.744305000
Zr	-0.029414000	1.642375000	-1.789176000
Zr	-2.566186000	-0.000527000	0.047441000
Zr	0.009223000	-1.917291000	-1.567447000
O	2.864354000	-4.589929000	-3.730157000
H	2.250773000	-3.950220000	-3.315133000
O	-2.724914000	-4.582274000	-3.913300000
H	-2.130003000	-3.979294000	-3.424424000
O	2.828112000	4.303406000	-4.119119000
H	2.229775000	3.639543000	-3.723590000
O	-2.764103000	4.232217000	-4.274262000
H	-2.163077000	3.647776000	-3.771971000
Fe	1.158321000	-0.200064000	-4.085304000
O	1.010231000	-0.280000000	-5.796547000
C	4.023917000	-0.654010000	-4.835597000
C	5.201135000	-0.184286000	-4.025287000
H	3.646090000	-1.619388000	-4.461595000
H	4.307511000	-0.822520000	-5.883466000
H	5.572490000	0.769698000	-4.409972000
H	4.920881000	-0.046839000	-2.975991000

H	6.009805000	-0.919657000	-4.074561000
O	2.978778000	0.324920000	-4.815690000
H	2.157774000	0.104654000	-5.711716000

Fe-NU-1000-OH (Int\_4)

Free Energy: -4588.694658

Electronic Energy: -4588.9947954

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000

H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.959406000	-2.862724000	0.241253000
H	-1.020002000	1.840282000	4.303236000
H	-0.137080000	0.527046000	4.149104000
H	-0.398124000	1.359836000	-4.645380000
H	-0.040826000	4.055454000	-0.415235000
H	0.636851000	4.482011000	1.591835000
H	0.834638000	4.274502000	-1.711797000
H	1.865203000	0.175514000	2.993443000
H	-1.963022000	2.875170000	-0.097233000
H	-0.810672000	-1.484711000	4.567728000
H	-0.715317000	-1.589641000	-4.075827000
H	0.840093000	-4.199127000	1.957819000
H	0.611283000	-4.562197000	-1.367147000
H	-0.018173000	-4.041765000	0.630342000
O	-1.116119000	0.117515000	1.536521000
O	-0.014815000	-3.888637000	1.632890000
O	1.036493000	1.480373000	0.001775000
O	1.317932000	0.159009000	2.200799000
O	-0.080428000	-1.081955000	4.085995000
O	-0.153215000	1.533443000	4.007637000
O	0.155571000	-1.789706000	-3.708975000
O	1.055069000	-1.455383000	0.220762000
O	-1.421770000	-2.063137000	0.233730000
O	-0.061949000	-3.988990000	-0.989053000
O	-0.084500000	3.981834000	1.195417000
O	-0.012329000	3.913800000	-1.421283000
O	-1.424599000	2.076772000	-0.061199000
O	0.239086000	1.272604000	-3.931304000
O	1.352377000	-0.133847000	-2.066673000
O	-1.108352000	-0.101957000	-1.428945000
Zr	2.501674000	0.011672000	0.126277000
Zr	-0.082135000	-1.614190000	2.051595000
Zr	-0.040285000	1.951553000	1.744150000
Zr	-0.027833000	1.615453000	-1.800737000
Zr	-2.563859000	-0.000450000	0.053567000
Zr	0.013242000	-1.941335000	-1.507698000
O	2.863777000	-4.593175000	-3.728400000

H	2.248555000	-3.963869000	-3.300739000
O	-2.726231000	-4.580654000	-3.918617000
H	-2.126527000	-3.973549000	-3.440550000
O	2.827178000	4.300158000	-4.120372000
H	2.231219000	3.639739000	-3.714328000
O	-2.764656000	4.230875000	-4.275883000
H	-2.163232000	3.642821000	-3.778012000
Fe	1.490007000	-0.320624000	-3.905615000
O	1.490183000	-0.732109000	-5.665133000
C	4.122409000	-0.403193000	-4.894934000
C	5.480032000	0.220090000	-4.657846000
H	4.164289000	-1.491028000	-4.720393000
H	3.777424000	-0.258081000	-5.927879000
H	5.475152000	1.284474000	-4.906092000
H	5.769101000	0.117767000	-3.607951000
H	6.228980000	-0.281281000	-5.278062000
O	3.199662000	0.184541000	-4.003683000
H	0.931204000	-1.512807000	-5.786760000

Fe-NU-1000-OH (TS2\_4)

Free Energy: -4588.678904

Electronic Energy: -4588.973514

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000
C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000

H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.962596000	-2.854136000	0.231878000
H	-1.023967000	1.830646000	4.316022000
H	-0.136948000	0.520362000	4.153879000
H	-0.603345000	1.226315000	-4.476174000
H	-0.040594000	4.058925000	-0.403768000
H	0.636517000	4.485253000	1.601101000
H	0.835684000	4.283059000	-1.699518000
H	1.868158000	0.172950000	2.992017000
H	-1.962804000	2.878353000	-0.098812000
H	-0.810558000	-1.486532000	4.569380000
H	-0.716766000	-1.677343000	-4.118912000
H	0.842068000	-4.193599000	1.944611000
H	0.600089000	-4.561519000	-1.370497000
H	-0.022139000	-4.032639000	0.621346000
O	-1.115914000	0.120859000	1.538673000
O	-0.017540000	-3.889200000	1.626335000
O	1.038173000	1.508116000	0.021274000
O	1.314380000	0.160029000	2.203945000
O	-0.079924000	-1.083131000	4.088898000
O	-0.156512000	1.528752000	4.017954000
O	0.148957000	-1.768796000	-3.706997000
O	1.049946000	-1.466262000	0.231610000

O	-1.423367000	-2.055684000	0.228585000
O	-0.066896000	-3.980349000	-0.994605000
O	-0.090973000	3.990336000	1.209220000
O	-0.009352000	3.917489000	-1.410000000
O	-1.424892000	2.079970000	-0.057097000
O	0.205231000	1.248175000	-3.954458000
O	1.389946000	-0.120849000	-1.997764000
O	-1.103527000	-0.091577000	-1.427633000
Zr	2.479242000	0.010103000	0.127355000
Zr	-0.083958000	-1.615948000	2.050919000
Zr	-0.044402000	1.958114000	1.756823000
Zr	-0.011016000	1.615402000	-1.781491000
Zr	-2.561045000	0.000437000	0.054982000
Zr	0.013266000	-1.929664000	-1.524959000
O	2.856903000	-4.577726000	-3.732062000
H	2.249998000	-3.981084000	-3.242225000
O	-2.725826000	-4.580737000	-3.917048000
H	-2.127169000	-3.972884000	-3.437923000
O	2.829441000	4.294447000	-4.127170000
H	2.232863000	3.628496000	-3.731059000
O	-2.764812000	4.231142000	-4.275898000
H	-2.162546000	3.644538000	-3.776885000
Fe	1.522913000	-0.263124000	-3.884123000
O	2.379477000	-1.491433000	-5.106330000
C	4.125440000	0.223377000	-5.031835000
C	5.398084000	-0.027160000	-4.266499000
H	3.612230000	-0.882730000	-5.311855000
H	4.244219000	0.661124000	-6.038632000
H	5.987133000	0.895686000	-4.201615000
H	5.165348000	-0.347442000	-3.246466000
H	6.014767000	-0.790874000	-4.749495000
O	3.108631000	0.747524000	-4.348684000
H	2.215142000	-2.445844000	-5.084205000

Fe-NU-1000-OH (Prod\_4)

Free Energy: -4588.727259

Electronic Energy: -4589.0216379

C	5.726500000	-2.889200000	-2.160200000
C	-5.638900000	-2.885100000	-2.451400000
C	4.388900000	-3.187700000	-2.460000000
C	-4.293000000	-3.161900000	-2.734600000
C	4.106400000	-4.252600000	-3.328500000
C	-3.986000000	-4.236300000	-3.582700000
C	5.138200000	-5.020700000	-3.859400000
C	-4.998200000	-5.035200000	-4.107600000
C	6.482800000	-4.751200000	-3.537700000
C	-6.351100000	-4.782200000	-3.807100000
C	6.755800000	-3.657500000	-2.694900000
C	-6.649700000	-3.679700000	-2.983400000
C	5.673400000	2.762000000	-2.369400000
C	-5.668800000	2.628900000	-2.684600000
C	4.341400000	3.021300000	-2.724800000
C	-4.324800000	2.872000000	-3.008000000
C	4.069900000	4.017800000	-3.673300000
C	-4.019400000	3.907100000	-3.904900000
C	5.105900000	4.760700000	-4.231200000

C	-5.033000000	4.692700000	-4.448900000
C	6.444700000	4.526400000	-3.861700000
C	-6.384200000	4.462600000	-4.123400000
C	6.708200000	3.500400000	-2.934600000
C	-6.680500000	3.408600000	-3.237600000
C	-3.223400000	-2.332300000	-2.105800000
C	-3.315200000	-2.089500000	2.441200000
C	-3.322900000	2.330100000	2.211500000
C	3.188500000	2.437000000	2.193700000
C	3.242000000	2.242000000	-2.086000000
C	3.280300000	-2.402400000	-1.851700000
C	-3.245500000	2.084800000	-2.346700000
C	3.174600000	-2.211100000	2.426600000
H	5.937000000	-2.056700000	-1.495800000
H	-5.871700000	-2.048200000	-1.800500000
H	4.900900000	-5.847200000	-4.524400000
H	-4.737200000	-5.873100000	-4.749000000
H	7.786000000	-3.416500000	-2.445100000
H	-7.686200000	-3.452500000	-2.747200000
H	5.874800000	1.981600000	-1.642500000
H	-5.899000000	1.830200000	-1.986300000
H	4.876900000	5.534100000	-4.959800000
H	-4.774300000	5.498300000	-5.131200000
H	7.734600000	3.290500000	-2.644500000
H	-7.714900000	3.205600000	-2.972200000
H	-7.139900000	-5.409200000	-4.210200000
H	7.286100000	-5.356800000	-3.944800000
H	-7.172900000	5.077500000	-4.544800000
H	7.252000000	5.109100000	-4.293600000
H	-4.101094000	-2.666618000	2.881887000
H	3.964843000	3.004750000	2.662583000
H	-4.111859000	2.914440000	2.636930000
H	3.948377000	-2.768397000	2.911976000
O	-3.663700000	1.472100000	1.337400000
O	-3.610000000	1.255400000	-1.456700000
O	-3.654000000	-1.258600000	1.542900000
O	-2.127300000	-2.310200000	2.835700000
O	1.970300000	-2.521800000	2.683600000
O	2.090000000	-2.742700000	-2.140600000
O	3.548200000	-1.286100000	1.640800000
O	3.614200000	-1.448400000	-1.083700000
O	3.557200000	1.485700000	1.438500000
O	3.591800000	1.320300000	-1.285300000
O	2.046400000	2.547800000	-2.386400000
O	1.986500000	2.771300000	2.435700000
O	-2.020200000	-2.554500000	-2.444700000
O	-3.604000000	-1.474700000	-1.248400000
O	-2.134300000	2.562400000	2.592300000
O	-2.045100000	2.316700000	-2.694300000
H	-1.954671000	-2.861143000	0.229412000
H	-1.035850000	1.819805000	4.310103000
H	-0.136856000	0.518228000	4.155814000
H	-0.518981000	1.398146000	-4.527994000
H	-0.041982000	4.045871000	-0.398116000
H	0.633565000	4.482302000	1.602461000
H	0.828607000	4.288150000	-1.688831000

H	1.878734000	0.168654000	2.987340000
H	-1.965167000	2.871291000	-0.104057000
H	-0.822793000	-1.486765000	4.568837000
H	-0.775140000	-1.959567000	-4.068536000
H	0.843288000	-4.194343000	1.940345000
H	0.603159000	-4.547995000	-1.375659000
H	-0.017169000	-4.025315000	0.614218000
O	-1.114580000	0.118222000	1.539349000
O	-0.017414000	-3.891992000	1.623703000
O	1.039227000	1.522134000	0.032936000
O	1.310596000	0.157862000	2.209982000
O	-0.084535000	-1.088698000	4.095638000
O	-0.161895000	1.526493000	4.022565000
O	0.136939000	-1.984613000	-3.755882000
O	1.050219000	-1.482758000	0.244315000
O	-1.423579000	-2.057580000	0.230718000
O	-0.062096000	-3.970350000	-0.991580000
O	-0.101074000	3.993475000	1.216394000
O	-0.010612000	3.908914000	-1.403571000
O	-1.426216000	2.074347000	-0.056193000
O	0.254796000	1.396123000	-3.955005000
O	1.343422000	-0.117515000	-1.988272000
O	-1.133898000	-0.105626000	-1.436013000
Zr	2.447316000	0.008078000	0.121617000
Zr	-0.087723000	-1.620752000	2.055256000
Zr	-0.047504000	1.958472000	1.757101000
Zr	-0.011363000	1.590130000	-1.786398000
Zr	-2.561687000	-0.001617000	0.052526000
Zr	0.022758000	-1.911342000	-1.529978000
O	2.866038000	-4.581592000	-3.732895000
H	2.248676000	-3.951589000	-3.300041000
O	-2.724067000	-4.580311000	-3.916181000
H	-2.125951000	-3.986453000	-3.417360000
O	2.828383000	4.300755000	-4.118877000
H	2.221832000	3.663484000	-3.687687000
O	-2.763450000	4.228542000	-4.274614000
H	-2.163750000	3.639518000	-3.773093000
Fe	1.300891000	-0.337495000	-3.986256000
O	0.670960000	-0.680820000	-6.197595000
C	4.258845000	-1.189899000	-4.656972000
C	5.009241000	-0.142274000	-3.937901000
H	4.806647000	-2.024719000	-5.126509000
H	1.416451000	-0.671793000	-6.809160000
H	4.814955000	0.835765000	-4.395402000
H	4.632210000	-0.073431000	-2.906722000
H	6.083563000	-0.328404000	-3.924622000
O	3.026325000	-1.177182000	-4.777740000
H	0.488470000	-1.620764000	-6.053207000