Supporting Information

Tuning the Properties of Metal Organic Framework Nodes as Supports of Single-Site Catalysts

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Section 1. Experimental Results

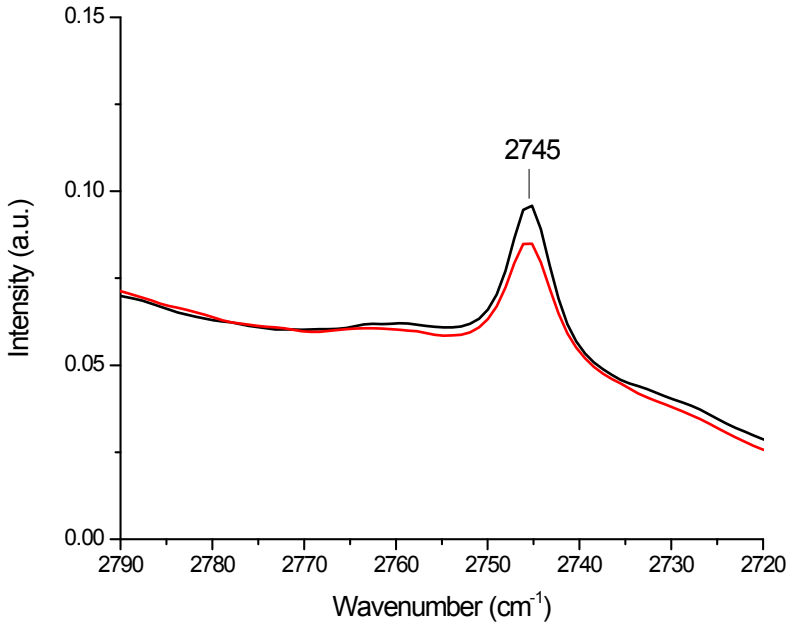


Figure S1. IR Spectra in the H Bonded H_2O/OH Region Characterizing of Bare Al-NU-1000 (Black) And the Samples Formed by Adsorption of $Ir(C_2H_4)_2(acac)$ on Them (Red).

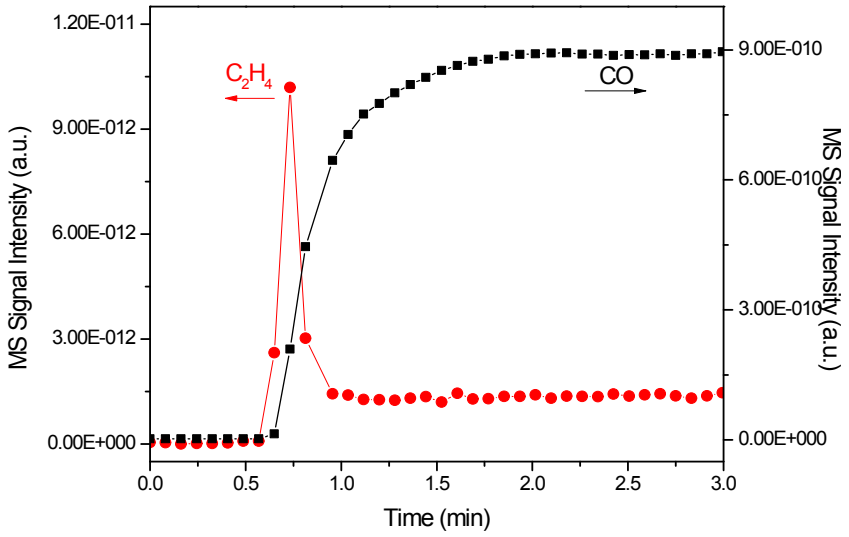


Figure S2. Mass Spectra Charactering the Effluent Gas after the NU-1000 Supported $Ir(C_2H_4)_2$ Complex Had Been Treated in 10% CO/He for 3 Min. The Data Indicate the Replacing of C_2H_4 Ligands on Iridium by CO.

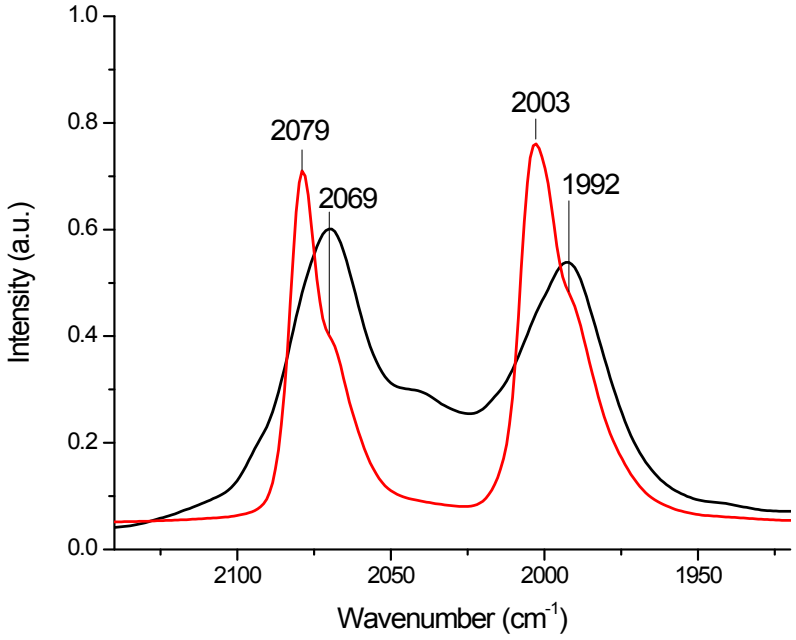


Figure S3. IR spectra in the ν_{CO} Region Characterizing $Ir(C_2H_4)_2$ Supported on NU-1000 (Black) And on Al-NU-1000 (Red) After Contact with a Pulse of CO in Helium At 298 K And 1 Bar for 3 Min.

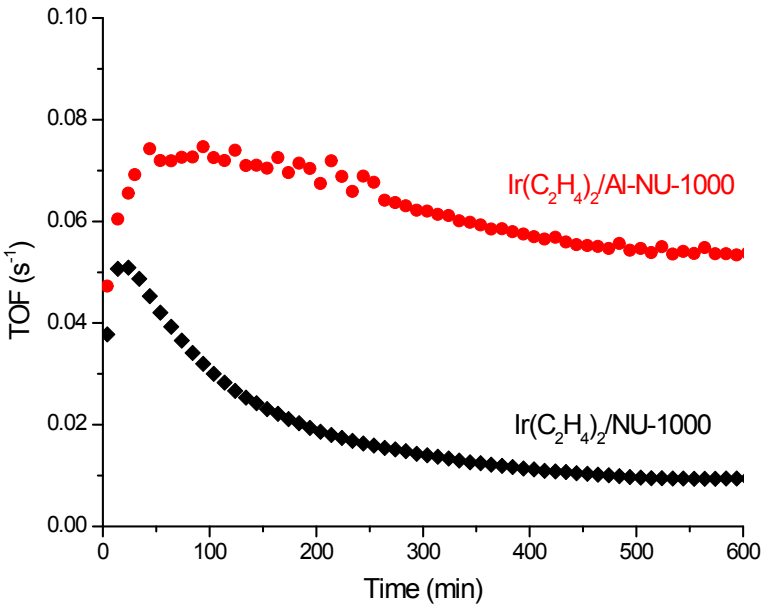


Figure S4. Long-term Activities During Ethylene Hydrogenation.

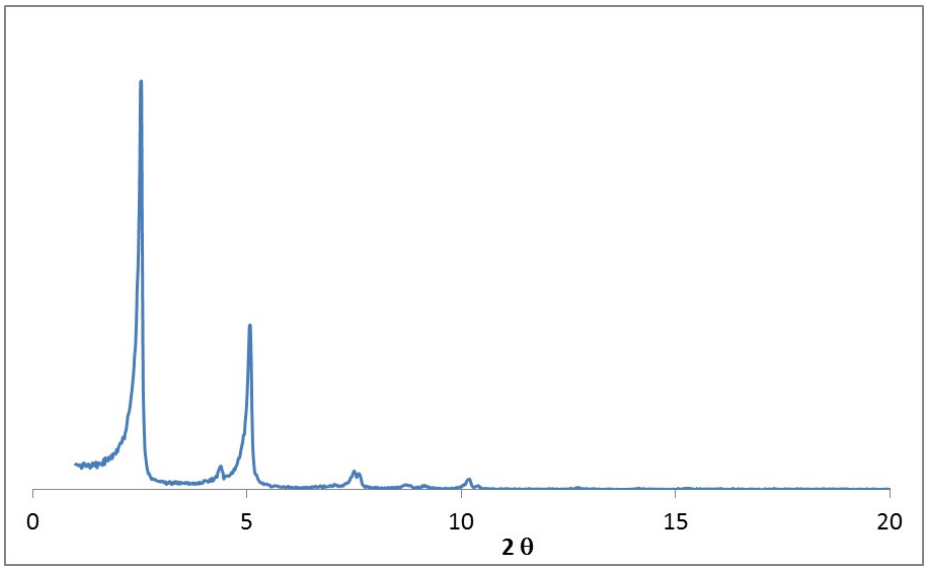


Figure S5. PXRD pattern of $Ir(CO)_2$@Al-NU-1000.

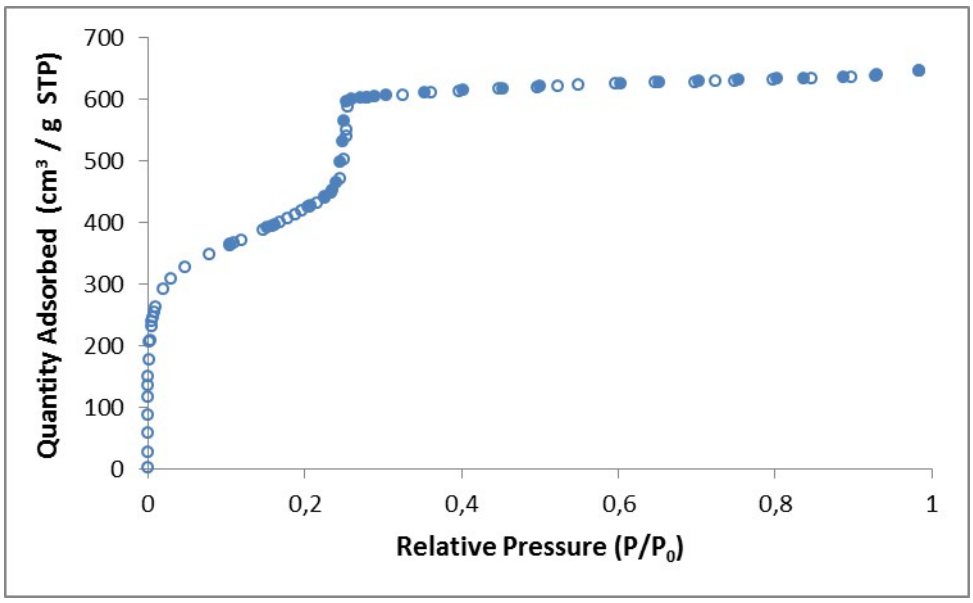


Figure S6. Adsorption (open circles) and desorption (solid circles) branches of the nitrogen physisorption isotherm of Al-NU-1000. Isotherms were collected on a Micromeritics TriStar II at 77 K. Before measurement, the sample was activated on a Micromeritics Smart VacPrep at 120 °C for 12 h.

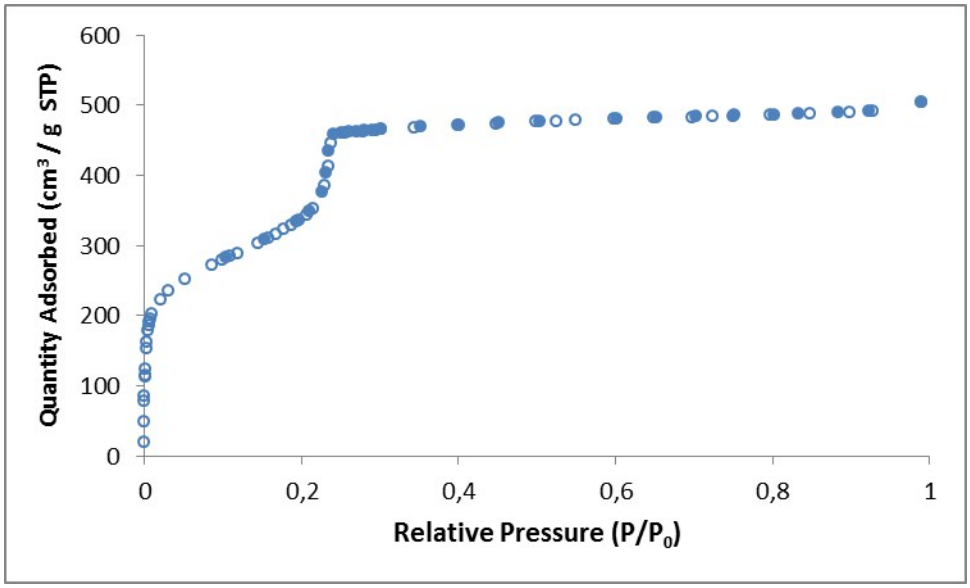


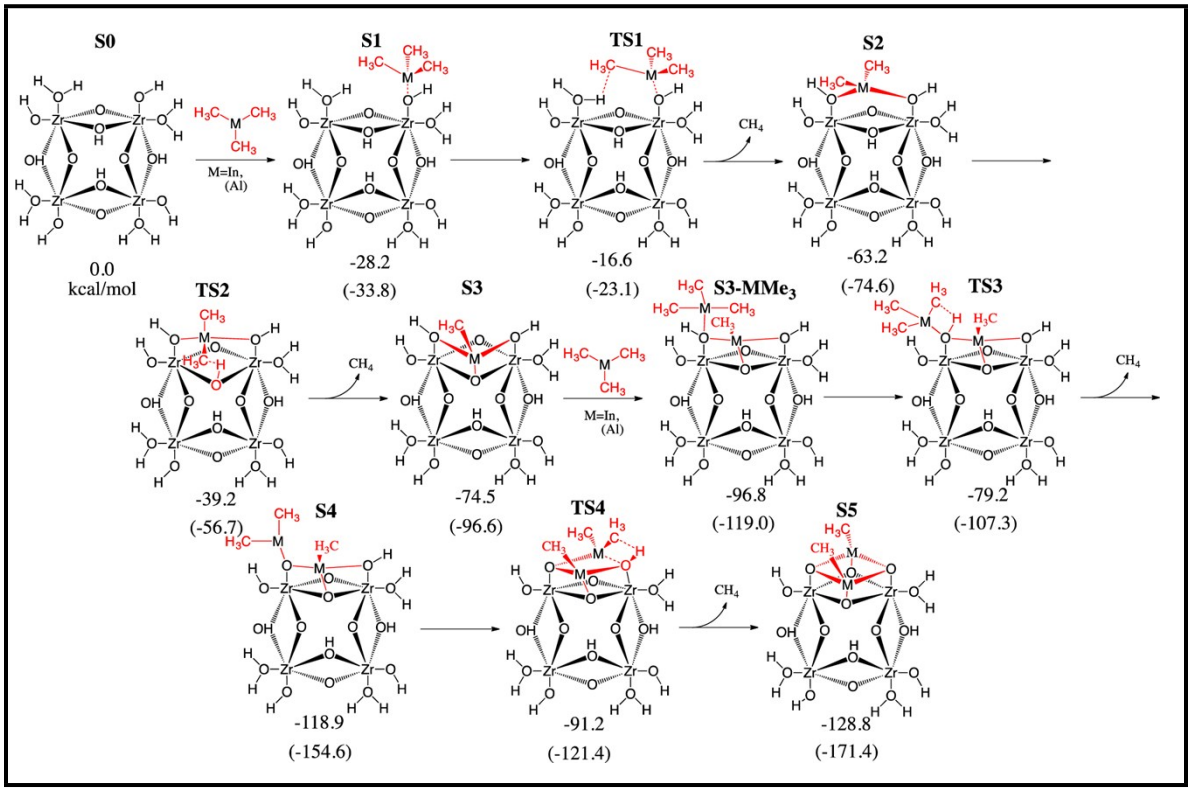
Figure S7. Adsorption (open circles) and desorption (solid circles) branches of the nitrogen physisorption isotherm of $Ir(CO)_2$@Al-NU-1000. Isotherms were collected on a Micromeritics TriStar II at 77 K. Before measurement, the sample was activated on a Micromeritics Smart VacPrep at 120 °C for 12 h.

Section 2. Computational Results

Section 2.1. Searching for Energetically Viable Ir@Al-NU-1000 Complexes

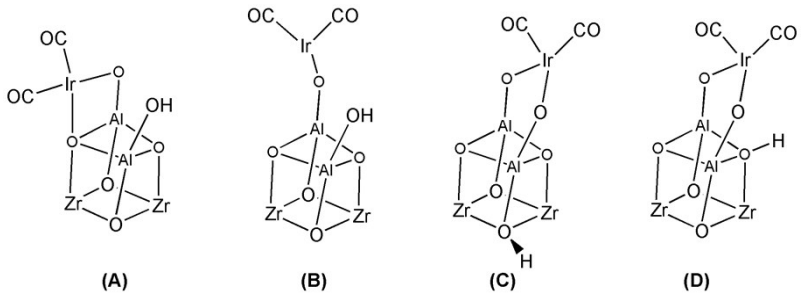
2.1.1. Dehydrated Al-NU-1000 Complexes

We have previously shown that NU-1000 metal organic framework (MOF) nodes can be coated with Aluminum atoms by starting from two equivalents of $Al(CH_3)_3$ precursors and releasing four equivalents of methane as byproduct (Scheme S1).[1] The overall process has been shown to be highly exothermic with a computed change in enthalpy of -128.8 kcal/mol.



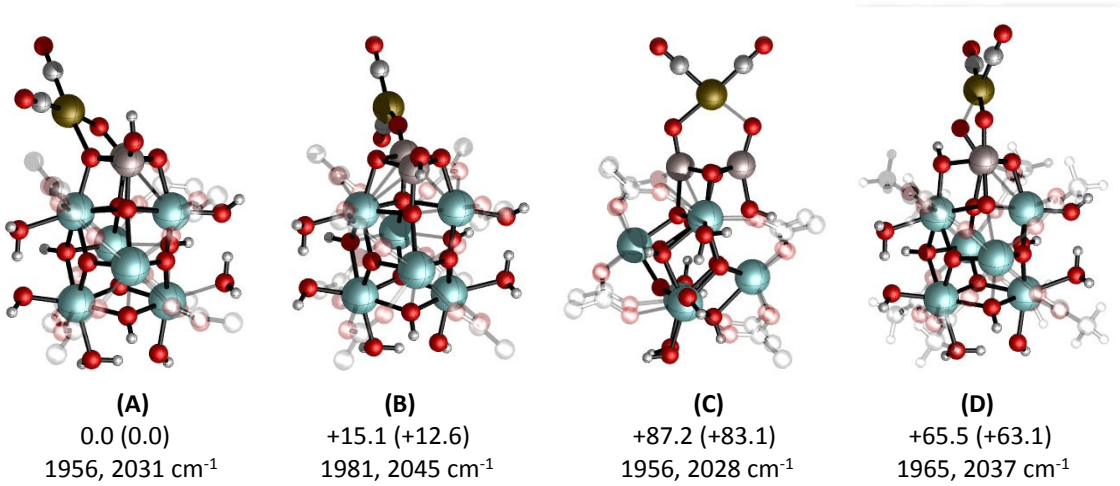
Scheme S1. M06-L Computed Relative Enthalpies (in kcal/mol) for Decorating NU-1000 with Al and In (in Parenthesis) Atoms.

Hydrolyzing Al decorated NU-1000 (Al-NU-1000) nodes leads to the formation of the hydroxylated Al-NU-1000 in which the methyl groups on the Al atoms are replaced with hydroxyl. These OH groups can subsequently provide ideal binding sites for transition metal catalysts such as Iridium (I) complexes to bind. To keep the neutrality of the overall system, we remove one proton after deposition of the Ir(I) complexes (For different dehydrated Ir(I) isomers considered in this work see Scheme S2).



Scheme S2. Four Different Dehydrated Ir@Al-NU-1000 Isomers Initially Considered in This Work.

Optimized structures of the (**A**)-(**D**) as well as their relative energies and scaled frequencies (scaling factor = 0.956) are shown in Figure S5 below.



(A)	**(B)**	**(C)**	**(D)**
0.0 (0.0)	+15.1 (+12.6)	+87.2 (+83.1)	+65.5 (+63.1)
1956, 2031 cm^{-1}	1981, 2045 cm^{-1}	1956, 2028 cm^{-1}	1965, 2037 cm^{-1}

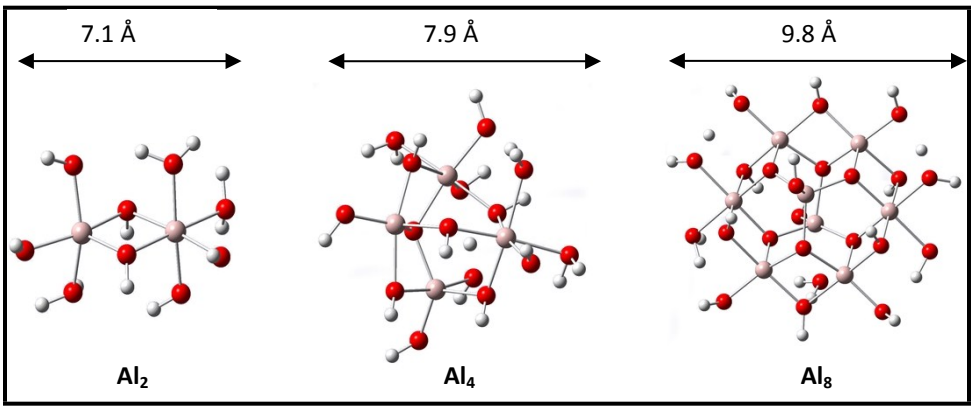
Figure S8. Optimized Structures of Different Dehydrated Ir@Al-NU-1000 Isomers Considered in This Work. The Relative Stabilities, Δ*H* (Δ*G* in Parenthesis) Are Given in kcal/mol. All Frequencies (in cm^{-1}) Are Scaled by 0.956. Color Code: Carbon: Gray, Oxygen: Red, Hydrogen: White, Aluminum: AntiqueWhite, Zirconium: Cyan, Iridium: Citron.

As can be seen from Figure S8, none of the dehydrated isomers yield frequencies close to the experimentally obtained values for the $Ir(CO)_2$@Al-NU-1000. In the next section we turn our focus on different hydrated isomers of these systems.

2. Saturated Ir@Al-NU-1000 with Hydroxo/Aqua Groups

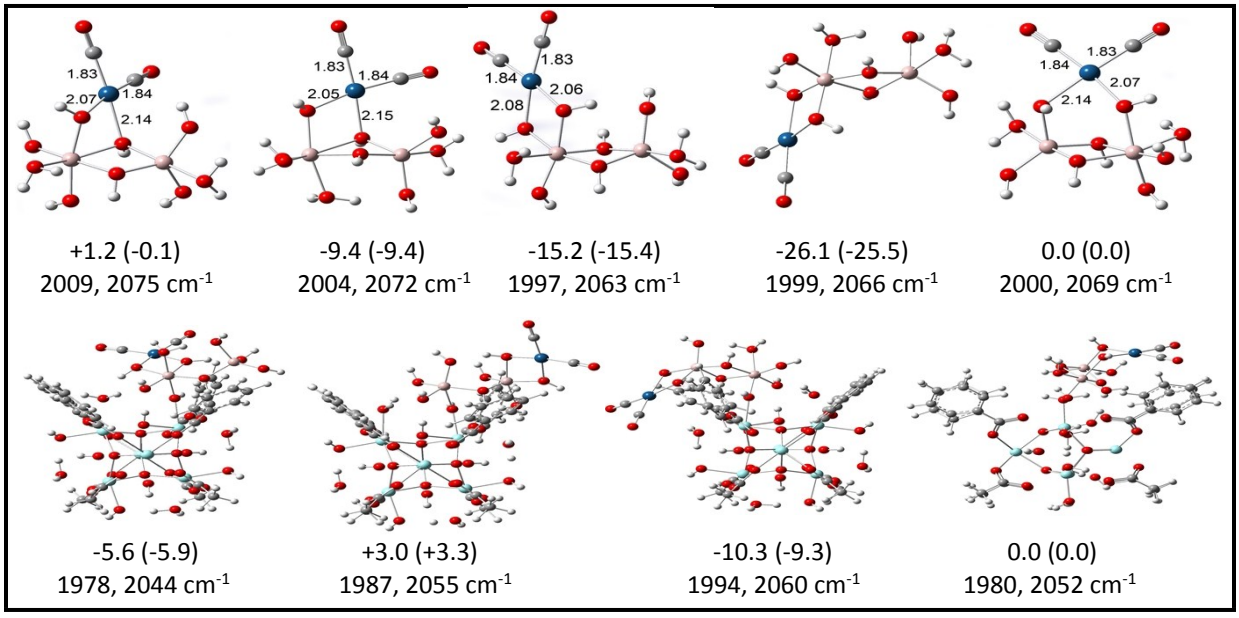
As mentioned above, the computed scaled carbonyl frequencies of both (**A**) and (**B**) isomers are far lower than the experimentally observed ones (i.e., 2003 and 2079 cm^{-1}). It has been shown before that saturation of Al clusters with hydroxyl/aqua groups can lead to more Lewis acidic Al sites/more Lewis basic oxygen atoms and ultimately higher carbonyl frequencies.[2] Due to the resemblance of the experimental frequencies of the Ir@Al-NU-1000 to the ones previously obtained for Ir@γ-Al_2O_3,[3] different Al_n clusters (n = 2, 4, and 8) were cut from the crystal

structure of the γ-Al_2O_3 and saturated with OH/OH_2 groups.[4] The optimized structures of these clusters are given below.



Following are all possible isomers on each Al cluster both with and without the NU-1000 node. Relative enthalpies (free energies) in kcal/mol as well as scaled carbonyl frequencies (scaling factor = 0.956) are also given for each optimized structure. For these calculations, the pyrene linkers were truncated to benzoates instead of acetates, on the upper side of the node, to capture all possible electrostatic interactions between Al clusters and linkers.

Ir@Al_2-NU-1000



+1.2 (-0.1)
2009, 2075 cm^{-1}

-9.4 (-9.4)
2004, 2072 cm^{-1}

-15.2 (-15.4)
1997, 2063 cm^{-1}

-26.1 (-25.5)
1999, 2066 cm^{-1}

0.0 (0.0)
2000, 2069 cm^{-1}

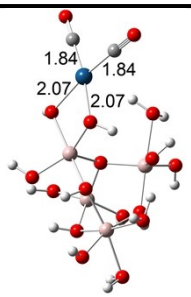
-5.6 (-5.9)
1978, 2044 cm^{-1}

+3.0 (+3.3)
1987, 2055 cm^{-1}

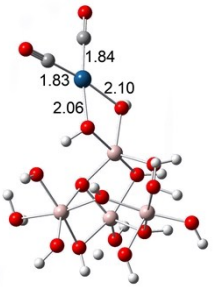
-10.3 (-9.3)
1994, 2060 cm^{-1}

0.0 (0.0)
1980, 2052 cm^{-1}

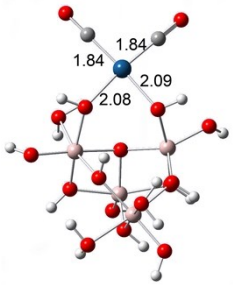
Ir@Al_4-NU-1000



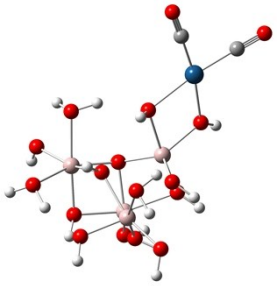
+2.8 (+3.0)
2008, 2073 cm^{-1}



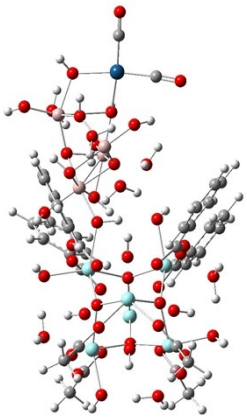
-1.5 (+0.5)
1997, 2064 cm^{-1}



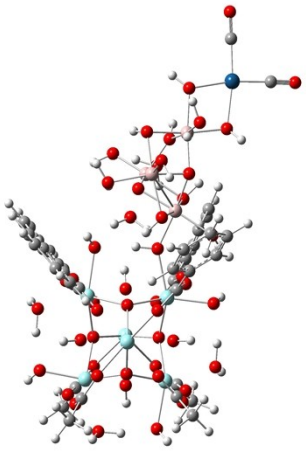
0.0 (0.0)
1999, 2066 cm^{-1}



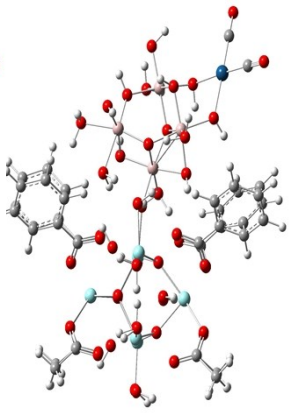
+0.4 (+2.5)
2009, 2075 cm^{-1}



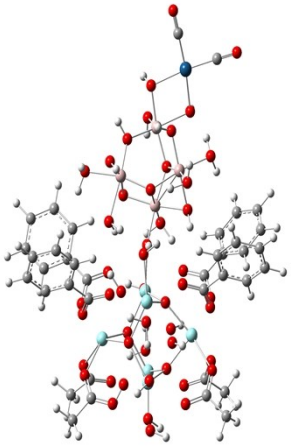
+2.7 (+2.5)
1992, 2062 cm^{-1}



-8.9 (-9.3)
1999, 2065 cm^{-1}

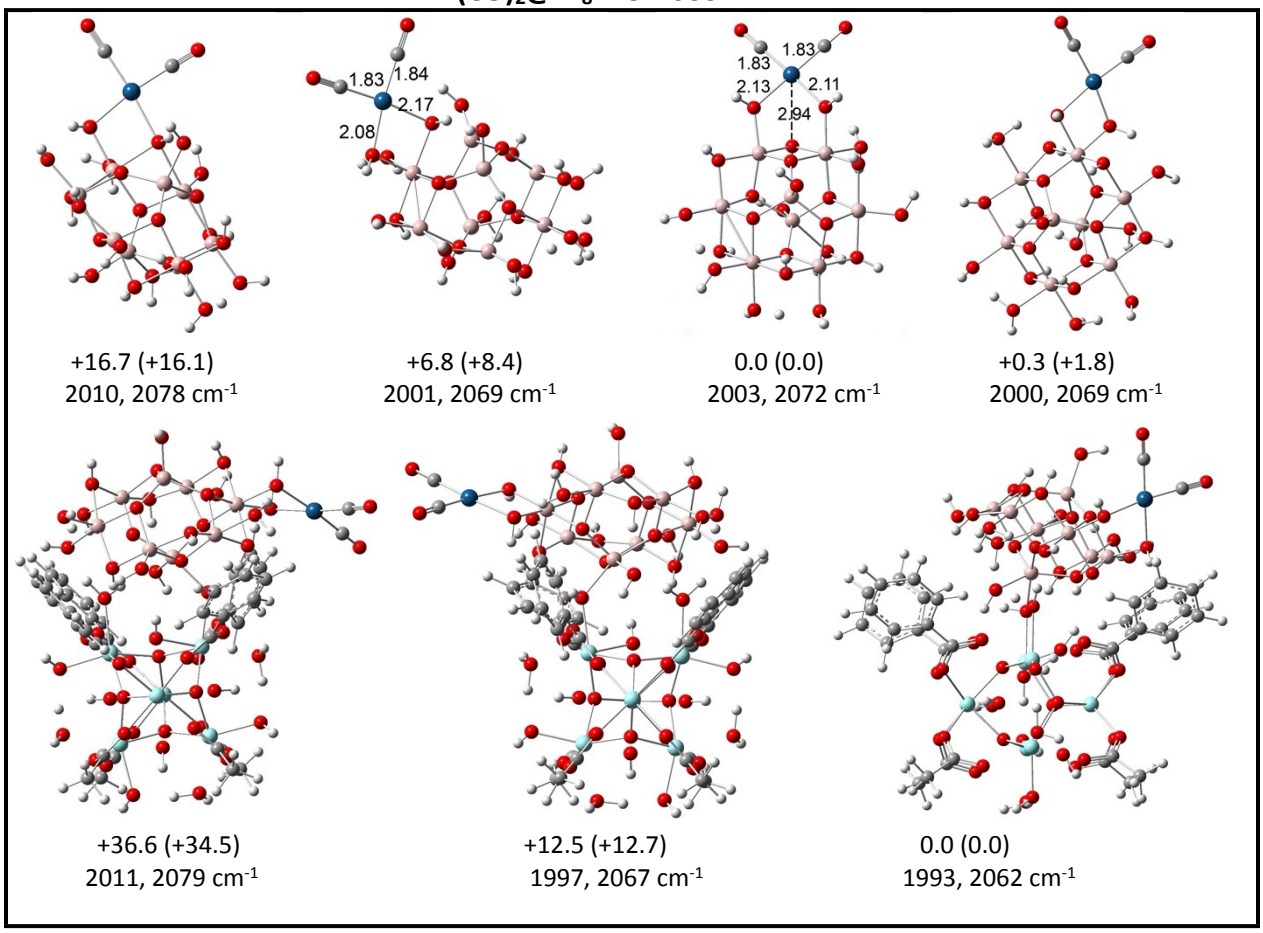


0.0 (0.0)
1994, 2064 cm^{-1}



+0.3 (+0.3)
1992, 2062 cm^{-1}

$Ir(CO)_2@Al_8$-NU-1000



In this search, we are ideally looking for any stable isomer that can reproduce the experimentally observed carbonyl frequencies.

The following points can be drawn from the above computations:

(i) In agreement with Gates and Dixon,[5] the bi-dentated isomer was found to be the most stable isomer for all the studied Al_n (n = 2, 4, and 8) clusters. All the mono-dentated isomers were converted to their corresponding bi-dentated ones during the optimization process.

(ii) By comparing these clusters to the previously studied dehydrated ones one can see a blue shift of ≈ 25 cm^{-1} in CO frequencies.

(iii) Node substitution changes the relative stabilities between the isomers by up to ≈ 16 kcal/mol and the CO frequencies by 5-10 cm^{-1}.

Unfortunately, none of the above studied Al_n systems can fulfill both stability and frequency conditions. For instance, in the $Ir(CO)_2@Al_8$-NU-1000 case one of the isomers has scaled carbonyl frequencies rather close to the experimentally observed ones but it is at the same time 36.6 kcal/mol in enthalpy less stable than the most stable isomer found for these systems.
In the next step, we focus on systematically exploring all possible ways of modulating Al clusters to fulfill both stability and frequency conditions.

To this end, four different classes of Ir@Al_n-NU-1000 (n = 2, 4, and 8) compounds were considered for further investigations:

(1) Cationic Ir@Al-NU-1000 generated by removing one OH group or addition of one extra proton.

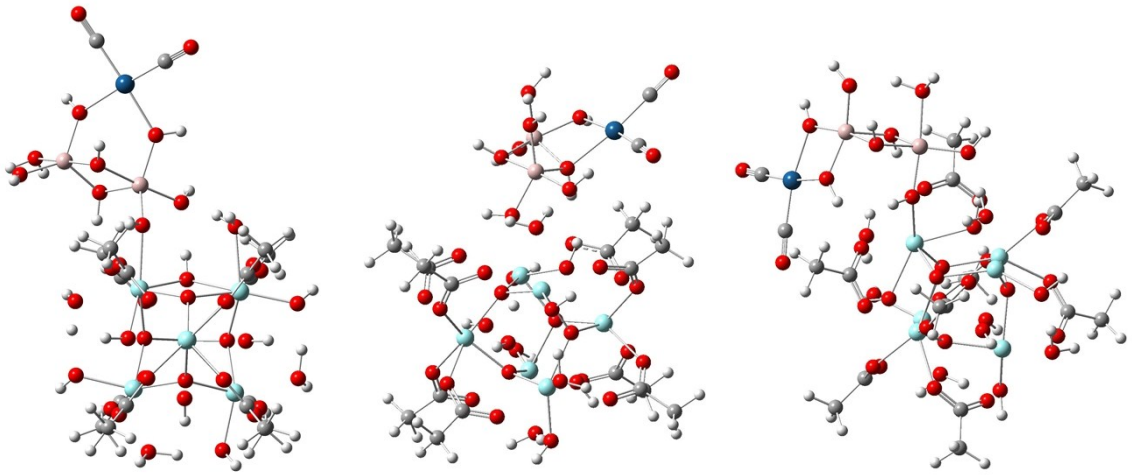
(2) Mixed Al-OH/Zr-OH coordination (i.e. coordinating the $Ir(CO)_2$ unit to Al-OH and Zr-OH sites simultaneously).

(3) Indirect coordination (i.e. $Ir(CO)_2$ Coordinates to one face of the NU-1000 node and Al_n (n = 2, 4, and 8) cluster to the other).

(4) Under coordination (lowering the coordination number of the Al atoms by removing one water molecule).

(1) Cationic Ir@Al-NU-1000

Three examples of the cationic species for Al_2 cluster on the NU-1000 node are shown below. Relative enthalpies (free energies) in kcal/mol as well as scaled carbonyl frequencies (scaling factor = 0.956) in cm^{-1} are also given.



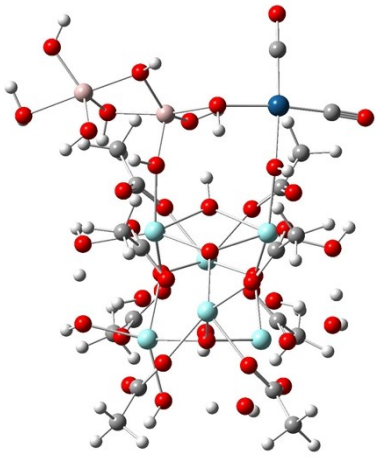
0.0 (0.0)
2018, 2083 cm^{-1}

+19.3 (+18.3)
2010, 2082 cm^{-1}

-8.2 (-6.2)
2004, 2068 cm^{-1}

Figure S9. Optimized Cationic $Ir(CO)_2$@Al_2-NU-1000 Structures.

(2) Mixed Al-OH/Zr-OH coordination



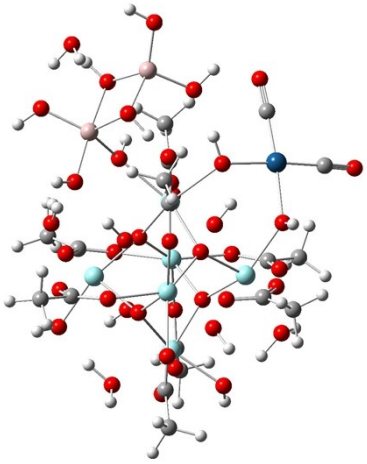
1988, 2055 cm^{-1}

Figure S10. Optimized Mixed Al-OH/Zr-OH $Ir(CO)_2@Al_2$-NU-1000 Structure.

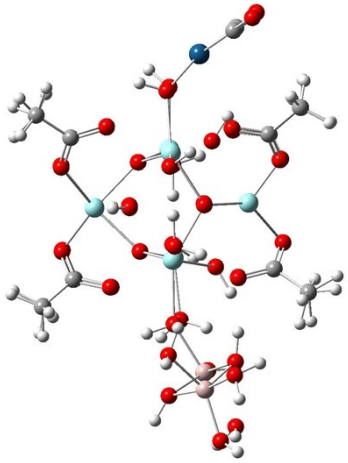
Since the frequencies did not change in the right direction, we did not pursue this further for other Al clusters.

(3) Indirect coordination

$Ir(CO)_2@Al_2$-NU-1000



-22.5 (-22.3)
1985, 2053 cm^{-1}



0.0 (0.0)
1989, 2058 cm^{-1}

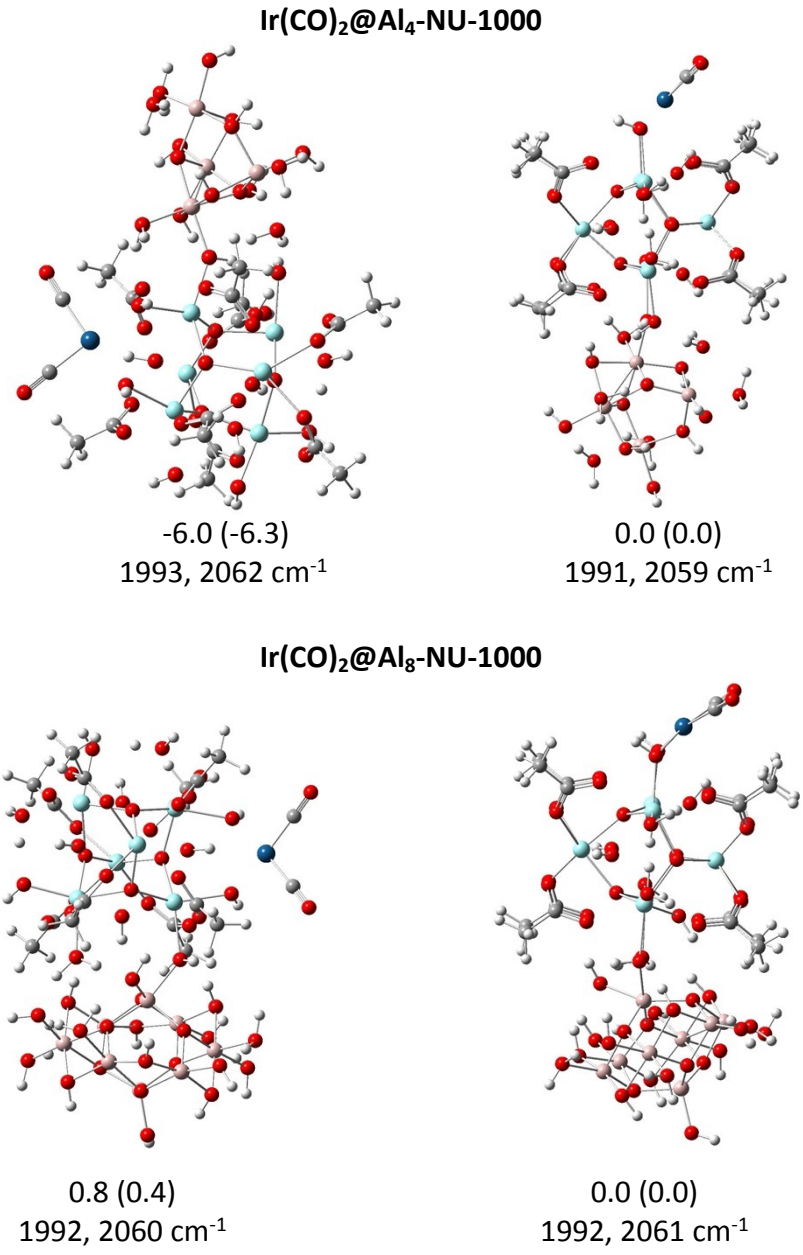
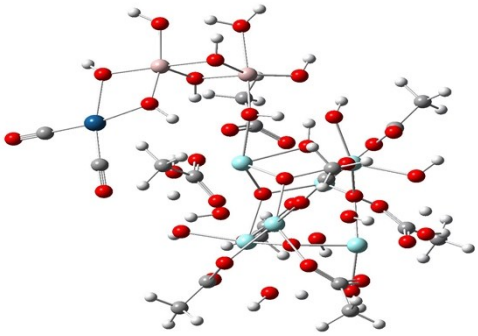


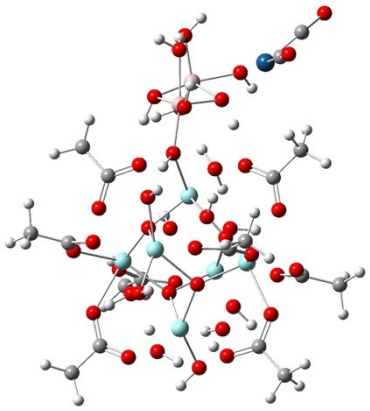
Figure S11. Optimized $Ir(CO)_2@Al_n$-NU-1000 (n = 2, 4, and 8) Structures with Indirect Coordination.

(4) Under Coordination

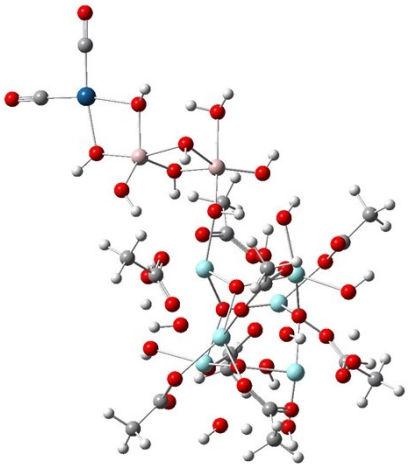
Ir@Al_2-NU-1000



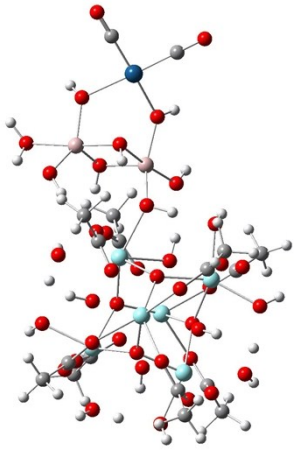
1990, 2057 cm^{-1}
0.0 (0.0)



2003, 2070 cm^{-1}
+9.8 (+8.3)

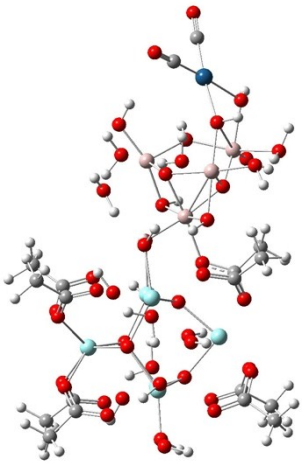


2002, 2067 cm^{-1}
+10.8 (+8.5)

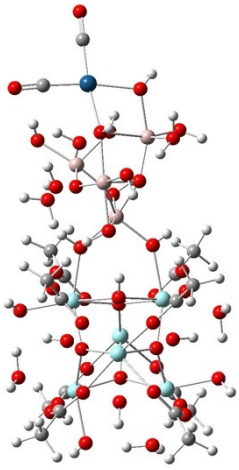


1997, 2066 cm^{-1}
+11.4 (+8.7)

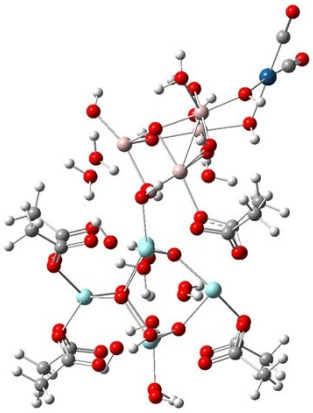
Ir@Al_4-NU-1000



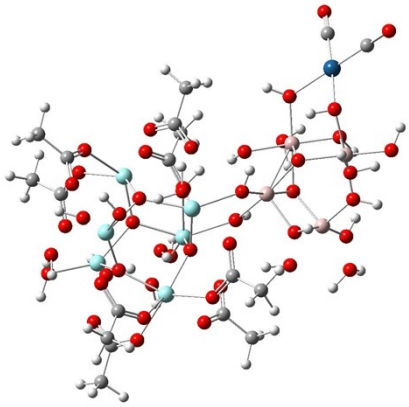
1987, 2053 cm^{-1}
0.0 (0.0)



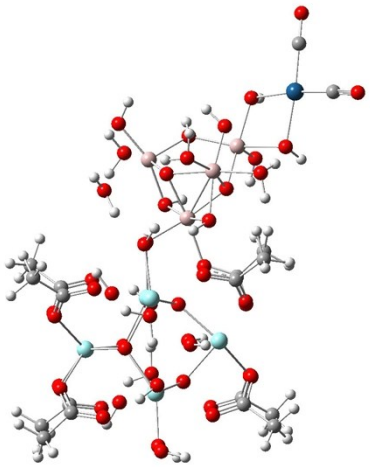
1983, 2051 cm^{-1}
-3.3 (-4.3)



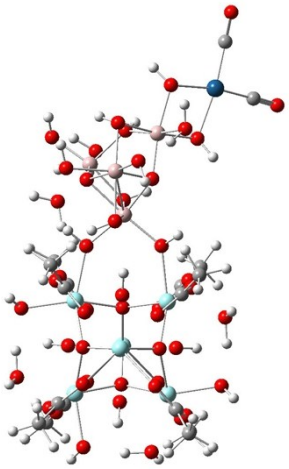
1987, 2056 cm^{-1}
-3.8 (-1.5)



1980, 2051 cm^{-1}
-4.4 (-6.6)

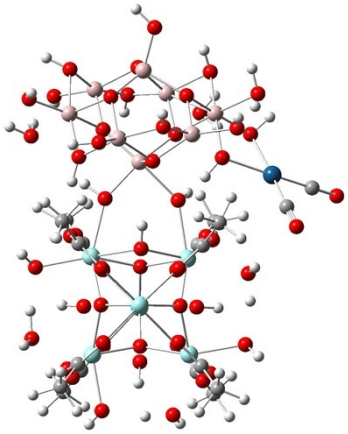


1983, 2051 cm^{-1}
-1.3 (+0.3)

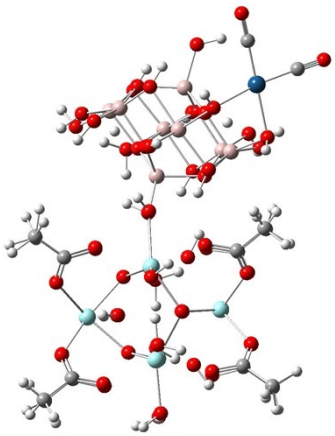


1987, 2054 cm^{-1}
-14.7 (-15.6)

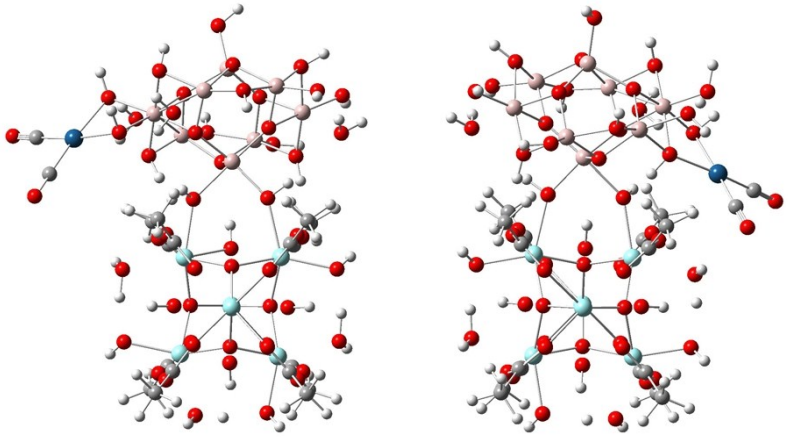
Ir@Al_8-NU-1000



1999, 2066 cm^{-1}
+25.0 (+23.9)



1984, 2052 cm^{-1}
0.0 (0.0)



2000, 2067 cm^{-1} +29.4 (+27.0)

1990, 2063 cm^{-1} +27.7 (+26.1)

Figure S12. Optimized Under Coordinated $Ir(CO)_2@Al_n$-NU-1000 (n = 2, 4, and 8) Structures.

Considering both relative energies between different isomers and closeness of the computed carbonyl stretching frequencies to the experimentally obtained ones, as well as EXAFS data reported in our previous work,[6] the $Ir(CO)_2@Al_8$-NU-1000 cluster isomers (specifically **Al_8-NU-1000 (opposite)** isomer in Figure S13 below) were selected for further investigations.

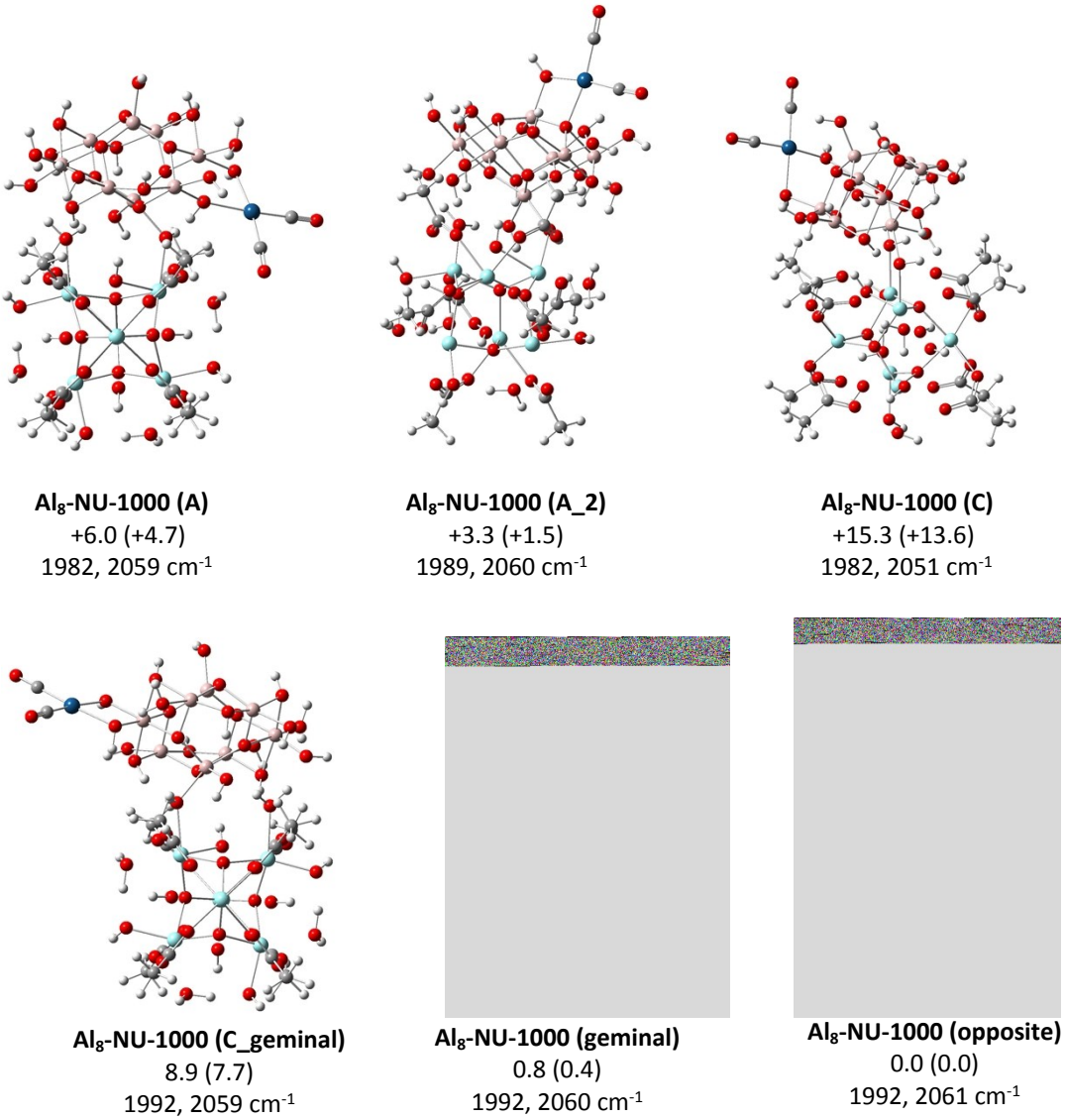


Figure S13. Optimized selected $Ir(CO)_2@Al_8$-NU-1000 isomers at the M06-L density functional. Relative enthalpies (free energies in parenthesis) in kcal/mol as well as scaled (0.956) carbonyl stretching frequencies (in cm^{-1}) are also given.

Also, New computations were performed in order to test the performance of other commonly used density functionals, the results of which are presented in Tables S1 and S2 of the supplementary information (SI). To summarize, the computed trend for relative stabilities between different isomers remain relatively constant for most of the studied **$Ir(CO)_2@Al_8$-NU-1000** species except for the **Al_8-NU-1000 (C)** isomer (Figure S13, SI). Although our M06 and M06-2X computed enthalpies (free energies) show that this isomer is 4.4 (5.9) kcal/mol and 3.8 (4.4) kcal/mol more stable than the **Al_8-NU-1000 (opposite)** one used in our mechanistic studies, however we have shown in our previous study that the latter isomer has the most resemblance to the available experimental EXAFS data and therefore we gave our final verdict to this species.[6]

Table S1. Computed relative electronic energy differences (kcal/mol) between selected Al_8-NU-1000 isomers using the M06-L, M06, and M06-2X density functionals at the M06-L optimized geometries. See Figure S13 for the M06-L optimized geometries and Table S6 for all the XYZ Cartesian coordinates.

Species	M06-L//M06-L	M06//M06-L	M06-2X//M06-L
Al_8-NU-1000 (A)	+7.0	+5.3	+4.9
Al_8-NU-1000 (A_2)	+3.8	+3.8	+4.7
Al_8-NU-1000 (C)	+16.2	-1.3	-1.7
Al_8-NU-1000 (C_geminal)	+9.0	+6.7	+8.4
Al_8-NU-1000 (geminal)	+0.8	+0.8	+0.6
Al_8-NU-1000 (opposite)	0.0	0.0	0.0

Table S2. Effects of geometric relaxation on the computed relative enthalpies (free energies in parenthesis) (kcal/mol) between selected Al_8-NU-1000 isomers using the M06-L, M06, and M06-2X density functionals at the M06-L optimized geometries. See Figure S13 for the M06-L optimized geometries and Tables S6-S8 for all the XYZ Cartesian coordinates.

Species	M06-L//M06-L	M06//M06	M06-2X//M06-2X
Al_8-NU-1000 (A)	+6.0 (+4.7)	+4.3 (+2.7)	+.2.8 (+2.8)
Al_8-NU-1000 (A_2)	+3.3 (+1.5)	+2.7 (+1.4)	+4.2 (+3.2)
Al_8-NU-1000 (C)	+15.3 (+13.6)	-4.4 (-5.9)	-3.8 (-4.4)
Al_8-NU-1000 (C_geminal)	+8.9 (+7.7)	+6.5 (+5.1)	+7.9 (+7.6)
Al_8-NU-1000 (geminal)	+0.8 (+0.4)	+0.4 (-0.4)	+0.5 (+0.7)
Al_8-NU-1000 (opposite)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)

The catalytic ethylene hydrogenation pathways starting from $Ir(C_2H_4)_2H_2$ on different supports (Al_8-NU-1000, NU-1000 and UiO-66 site-1) are given in the text (Figure 3). Also, the energetically preferred dimerization pathway is illustrated inside the text (Figure 4). Another commonly proposed pathway for ethylene dimerization reaction was also studied and is illustrated in Figure S13 below.

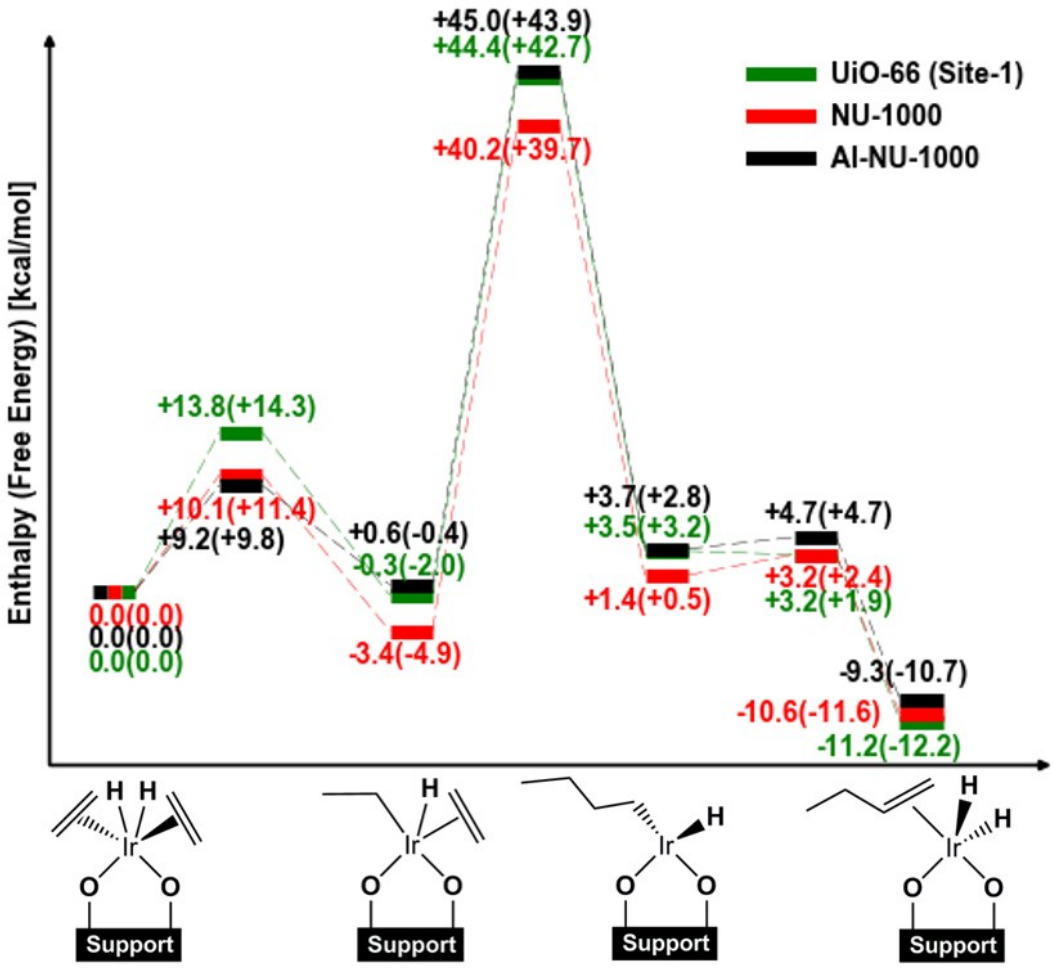


Figure S14. Computed Mechanistic Pathway for Ethylene Dimerization on Different Supports. For Clarity, Only Intermediate Species Are Shown.

However, by comparing this pathway to the one presented in Figure 4 one can see that this pathway is not energetically favorable.

Table S3. XYZ Cartesian coordinates of all optimized structures on the Al_8-NU-1000 support (all energies are in Hartree).

Isolated Al_8 Cluster

Electronic Energy: -3682.6664063
Enthalpy: -3682.277034
Free Energy: -3682.377202

Al	1.09891400	-2.34410300	0.83683000
Al	2.58003100	-0.14876000	0.47510400
Al	0.03320800	-0.62715800	-1.66534000
Al	-0.31361400	0.35747500	1.67917700
Al	1.47670900	2.11290500	-0.35812200
Al	-1.67896900	-2.24038700	0.58971800
Al	-1.24057500	2.16836700	-0.84132100
Al	-2.77028100	0.06230200	-0.27342600
H	2.55959000	0.55382900	-1.84274100
H	-0.01470900	-3.14896300	-1.66367300
H	-0.74510100	1.52549900	3.68309500
H	-3.68529400	-3.49293700	0.81881200
H	-0.43115800	-2.61482200	-3.07920900
H	-0.22801300	0.42617100	-3.75742600
H	-0.07132800	4.13952000	0.16908800
H	2.58457300	3.91113900	0.78078800
H	-2.83502200	-0.52823300	2.08279900
H	-3.87558200	-1.25307600	-2.02410300
H	-1.95720600	0.53124900	-2.52566900
H	-3.87708200	-2.04311800	-0.69107100
H	-2.95562100	3.78346800	-1.37715300
H	-3.67390700	2.27029500	-0.07340000
H	-4.91141500	1.33916400	-0.44755500
H	4.79439500	0.89696700	0.95262600
H	1.96710600	-0.85641200	2.69113200
H	-0.29197200	-4.41794700	0.20485800
H	3.55146500	-2.34799200	0.19517500
H	3.61724600	1.94679700	1.03300700
H	2.85107900	-3.84086400	1.44214200
H	4.04807600	-1.49668200	-1.00822000
O	1.37095300	-1.18261900	-0.53248400
O	2.86936200	0.96825500	-1.03107100
O	-0.27719600	-3.45835200	0.18479700
O	-0.64659800	0.62900100	3.36017100
O	-0.34334200	-1.47469900	1.59780200
O	1.25348000	1.00335600	1.07947400
O	0.26658400	-2.58595700	-2.41132400
O	-3.01739400	-3.35125600	0.14207100
O	-0.51446700	-0.40449300	-3.36962200
O	2.82218500	3.14656400	0.25124600
O	-1.49379000	-1.17111500	-0.84555600
O	0.25031800	1.24025500	-1.45266900

O	0.11070100	3.36750200	-0.37040000
O	-1.54198300	1.12906100	0.61496900
O	-2.99773900	-1.01568100	1.26406300
O	-4.13281300	-1.15471200	-1.09682500
O	-2.43901300	1.07111400	-1.85929300
O	-2.58850100	3.36262200	-0.59557500
O	-4.14685300	1.38478900	0.13839300
O	2.31428900	-1.31976900	1.91911900
O	3.91355900	1.01453400	1.32878600
O	2.42394600	-3.55038600	0.63128400
O	3.99196700	-1.46440300	-0.04452100

Al_8-NU-1000

Electronic Energy: -6929.6493612

Enthalpy: -6928.656483

Free Energy: -6928.858478

C	1.68441900	3.94341500	-3.15514000
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C	2.37165700	3.70494900	2.55374400
C	0.00185000	-4.64437900	-3.17737000
C	-5.46152400	-3.56982100	3.03745400
C	-4.20580600	5.17837100	-2.39073300
C	-6.09808400	-3.34300700	-2.42691100
C	-3.54711000	4.91457400	3.31258500
C	1.27407100	2.82442300	2.03809500
C	0.75416700	3.00364000	-2.46953500
C	-3.54118900	3.93046700	-1.89896000
C	-5.03722900	-2.44266000	-1.88258700
C	-4.54348500	-2.62142800	2.33674300
C	-0.02842400	-3.67128600	1.74594600
C	-3.03318900	3.71325000	2.58679300
C	-0.52889700	-3.45027300	-2.44888800
H	-1.86868900	-1.86908400	2.79187800
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H	-2.58982200	0.44534800	-3.97562800
H	-2.87040300	0.98983400	4.58079400
H	-5.71385300	0.96229800	0.78433400
H	-6.40247000	0.51830500	-1.22815700
H	-5.94858500	0.06940900	2.06977300
H	-2.57179600	-1.62584300	-2.85734900
H	-4.18309100	2.64829400	0.39248100
H	-0.51896300	0.67194100	-4.55440500
H	-1.03053800	-0.03613600	3.98737600
H	0.43602100	0.55786600	4.00816800
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O	-2.56908000	4.06745000	-1.09703400
O	-2.21123100	3.90981600	1.64630900
O	0.11535500	3.45844900	-1.47228600

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O	1.81864000	-0.51670600	-2.43732600
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O	0.55145400	-2.56826100	1.99555900
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O	-1.11156400	-3.77347300	1.11261300
O	-4.12228800	-3.00135600	-1.20844600
O	-3.76519800	-3.12667800	1.47663300
O	-4.57248700	-1.39586100	2.64411800
O	-5.10493400	-1.20182600	-2.10761500
O	-3.44108900	-0.57154600	0.19290000
O	-2.38732000	-1.10201100	-2.07109400
O	-1.03807600	0.04920300	-4.03293400
O	-3.55406000	0.67481800	-3.74731900
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O	-0.57770500	-1.22671500	-0.23773200
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Zr	-3.79387100	0.60143500	-1.47192100
Zr	-3.26983300	0.47247100	2.04340900
Zr	-1.27190100	2.64930600	0.03729400
Zr	0.12883800	-0.31372200	1.47522400
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Al	7.06242500	0.31162300	-0.23122100
Al	4.68852400	2.28473400	-1.02864700
Al	6.22937500	-2.52652200	0.89653900
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H	9.11245100	1.48235400	-0.17735000
H	6.66505400	-4.36450000	2.39605700
H	1.82997500	-2.44796100	-0.13682100
H	5.66882500	3.89577600	0.59970300
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H	8.06847200	-1.13859600	1.93596200
H	4.31384900	-1.99772600	3.90438000
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H	4.10698600	-0.43316100	-4.99051900
O	4.47672200	-0.82254200	-1.46389100
O	3.64920600	1.61558300	-2.39672000
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O	8.77073100	0.59553300	-0.29436400
O	6.94150600	-1.48373600	-0.47993500
O	6.07959000	1.20008200	-1.44625800
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O	5.26952300	3.62788400	-2.11529500
O	4.83504100	-1.45599700	1.30944400
O	3.76753600	1.16705300	0.25767500
O	4.96592500	3.23969400	0.55887900
O	6.32219100	0.77453400	1.33801900
O	7.28521800	-1.64698200	2.18067300
O	5.27867200	-1.98254900	3.87290100
O	4.22618500	0.61240500	2.93705100
O	5.74679200	2.70412700	3.11435800
O	6.69323300	0.50645500	3.93595200
O	6.41891000	-1.02284700	-3.13651800
O	5.73551700	1.76379100	-3.98175600
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H	3.39070900	0.20612600	2.62933000
H	-4.86509800	-4.24205100	3.66846800
H	-6.19039500	-3.05116500	3.66822200
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H	-6.79706100	-2.81051500	-3.07932800
H	-3.49929200	6.01357100	-2.44038400
H	-4.68999000	5.02061900	-3.36026600
H	-4.99254700	5.45487600	-1.67469400
H	-2.79089500	5.70581700	3.35197900
H	-4.40609500	5.31534500	2.75606900
H	-3.89592600	4.66078600	4.31898500
H	3.06459900	3.93051300	1.73022700
H	1.97272700	4.66916600	2.89263800
H	2.91040200	3.21830200	3.37670300
H	1.62934900	-4.99528700	1.73612400
H	0.84909100	-4.83584000	3.30109500
H	0.06000000	-5.80607800	2.01531700
H	1.03105300	-4.83540200	-2.84193800
H	-0.59839200	-5.54034000	-2.99085500
H	0.05751200	-4.43788800	-4.25264300

H	2.38789900	3.41175300	-3.80216300
H	1.10040200	4.65782300	-3.75282100
H	2.22895000	4.53604000	-2.40987400
H	5.71266800	2.56552000	-3.34848400

$Ir(CO)_2@Al_8$-NU-1000

Electronic Energy: -7260.0935486

Enthalpy: -7259.083675

Free Energy: -7259.298270

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.87657000	-1.87426300	2.78452900
H	1.51229300	1.35993900	-0.23621500
H	-3.67437500	1.60341300	-3.99756800
H	-2.57541300	0.45634400	-3.98240100
H	-2.88929200	0.97082400	4.59093200
H	-6.38323900	0.32828000	-1.14158300
H	-5.95820400	0.13682300	2.16421000
H	-2.57681500	-1.61911500	-2.86866400
H	-4.09241400	2.71168700	0.39080000
H	-0.50740700	0.65805400	-4.56833300
H	-1.04998100	-0.03153600	3.98457600
H	0.42330900	0.55156100	4.02088500
H	2.27910000	-1.61117900	1.87865200
O	-1.74636500	1.25637000	-1.41322500
O	-2.55063700	4.06169800	-1.12422600
O	-2.21552600	3.91171100	1.63921200
O	0.11524500	3.45657500	-1.47258300
O	0.64811900	1.82512200	-2.90296900
O	1.81961200	-0.50811600	-2.37852000
O	-0.05190100	-2.32886500	-2.75718600
O	0.54743900	-2.56778100	1.99780400
O	-1.42136100	-3.63473500	-1.56442500
O	-1.11119000	-3.77550900	1.11115300
O	-4.11040300	-3.00326200	-1.23143100
O	-3.77826300	-3.12474200	1.46089700

O	-4.56603600	-1.40078300	2.65081300
O	-5.11804000	-1.19351400	-2.07999200
O	-3.43567100	-0.56768300	0.17906700
O	-2.38579700	-1.10020700	-2.08066000
O	-1.03408000	0.04910400	-4.03791100
O	-3.54123500	0.67937600	-3.74511800
O	-0.07853100	-0.23631200	3.76567400
O	-0.57851800	-1.22390000	-0.24158100
O	0.61593300	0.98598300	-0.25118000
O	1.23352300	1.62027100	2.40159600
O	2.24417000	-0.69636300	1.55561200
O	0.46442400	3.35403400	1.21982600
O	-5.79482900	1.05123500	-0.88977500
O	-5.45367400	0.91940300	1.90817100
O	-3.49275600	1.95829200	0.29592100
O	-4.03582000	2.81321000	-2.23889900
O	-3.47358400	2.57980600	2.92725100
O	-2.63967000	0.24281800	4.01130900
O	-1.84946400	-1.29499100	2.01633500
O	-1.38872500	1.13630000	1.46146800
Zr	-2.35389300	-2.32014700	-0.04940500
Zr	-0.32497500	-0.12741700	-2.09038100
Zr	-3.74876700	0.60221800	-1.47105100
Zr	-3.31563200	0.46857100	2.05197700
Zr	-1.26073900	2.64076100	0.04848800
Zr	0.11044200	-0.30566800	1.48125000
H	2.12137400	-1.26166200	-1.76985600
Al	5.67140000	-2.08099500	-1.68105300
Al	5.07493900	0.28483700	-2.90748700
Al	3.64083200	-0.72808700	0.18103200
Al	7.05606000	0.25057800	-0.18350500
Al	4.73217700	2.09346000	-0.99909900
Al	6.24072100	-2.54536000	0.94344600
Al	4.85760500	1.86269200	1.69486100
Al	5.76237600	-0.48014500	2.60860600
H	2.88773500	1.10349800	-2.22493100
H	4.93628900	-4.18915600	-0.47630400
H	9.14307100	1.29370500	0.19346600
H	5.59716200	-2.75990500	3.39273600
H	1.87545300	-2.50586700	-0.10878300
H	5.67921100	3.90315600	0.45302800
H	4.66848000	3.95844800	-2.75489800
H	8.01951600	-1.02720100	1.77943100
H	4.45132400	-1.96261000	4.12748000
H	5.07652900	3.31430500	3.64674700
H	7.30611000	-0.95412400	-3.02659800
H	3.58453800	-2.92620600	-2.19624700
H	6.60128400	1.36010400	-4.40788200
H	4.12425900	-2.24047200	-3.47968600
H	3.88965900	-0.41123900	-4.89821500
O	4.48697500	-0.77804800	-1.42625100
O	3.69434200	1.61494700	-2.39411300
O	5.63349600	-3.53221500	-0.55326500

O	8.77977500	0.42802500	0.00143500
O	6.92173900	-1.53844100	-0.44967500
O	6.17174500	1.13911000	-1.44626800
O	2.64511500	-2.16694200	-0.58327100
O	6.02210500	-3.83577500	2.17611400
O	5.39568800	3.47379000	-2.34478700
O	4.82062900	-1.49293900	1.33241900
O	3.77678200	1.15857800	0.31786500
O	4.97858300	3.24692400	0.39055000
O	6.27675100	0.79963500	1.34455000
O	7.29605300	-1.52576300	2.19387100
O	5.39110500	-1.91306000	3.91521900
O	4.24593100	0.60113000	2.96551500
O	5.62190900	2.85639500	3.00399600
O	6.63070500	0.62010400	3.99554700
O	6.37903500	-1.19718700	-3.12693900
O	5.70606300	1.50883300	-4.09348500
O	4.33864500	-2.98115100	-2.82813900
O	3.84892100	-0.66603300	-3.97085700
H	3.40188000	0.20880700	2.66502500
H	-4.86622700	-4.32223500	3.57070000
H	-6.11797400	-3.06004300	3.74938500
H	-6.06115600	-4.12025600	2.30149100
H	-5.63613800	-4.17103500	-2.97781000
H	-6.64627200	-3.79791600	-1.59118200
H	-6.80233300	-2.81094100	-3.07411700
H	-3.46983300	5.96675600	-2.58386000
H	-4.81842200	4.99196600	-3.27877800
H	-4.87011200	5.54944700	-1.59716100
H	-2.74850700	5.64822000	3.47133800
H	-4.30352800	5.40416100	2.68238400
H	-4.02113600	4.64611700	4.26208500
H	5.65661900	2.81128000	-3.08267000
H	6.79225300	-4.31352100	2.49381500
H	3.07713800	3.91049900	1.73375800
H	1.97732100	4.68088600	2.86263800
H	2.89609800	3.23135700	3.39224000
H	2.38722000	3.40867700	-3.80218000
H	1.10203500	4.65332800	-3.75948100
H	2.22008000	4.54445300	-2.40876400
H	1.05144300	-4.80035600	-2.89201800
H	-0.56652100	-5.55158900	-2.95041600
H	0.00129700	-4.45566000	-4.25762900
H	0.83636400	-4.84064400	3.30373300
H	0.06558400	-5.80718700	2.00481700
H	1.63505800	-4.98961700	1.74683700
H	7.58729100	0.62669800	3.87020400
H	6.32432000	1.56133200	3.75513600
Ir	-6.47740100	2.26836100	0.68251400
C	-6.95522700	3.30052500	2.12353100
C	-7.30436000	3.42479000	-0.48129700
O	-7.22530300	3.94696600	3.04189300
O	-7.80708800	4.14799800	-1.22932100

H	2.45378100	-0.54668700	-3.16646600

Catalytic Hydrogenation Mechanism (Figure 3)

$Ir(C_2H_4)_2@Al_8$-NU-1000

Electronic Energy: -7190.6433158

Enthalpy: -7189.541475

Free Energy: -7189.758824

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.87718300	-1.87338100	2.78307500
H	1.50707900	1.36316100	-0.23584400
H	-3.67098500	1.60539200	-3.98975900
H	-2.58221200	0.45249300	-3.98157100
H	-2.88744700	0.97312400	4.58789000
H	-6.38112900	0.36043600	-1.31192400
H	-5.92697500	0.15782300	2.33978000
H	-2.57326100	-1.62129300	-2.86563100
H	-4.16881300	2.68559600	0.39812000
H	-0.50948300	0.66019700	-4.56397900
H	-1.06168900	-0.03041700	3.98304100
H	0.41273700	0.55460200	4.02256800
H	2.26597500	-1.61074000	1.87732400
O	-1.75435200	1.26090200	-1.40474800
O	-2.55794900	4.06523500	-1.11606600
O	-2.22747500	3.91653500	1.63020100
O	0.11406800	3.45749400	-1.47346500
O	0.64691800	1.82538400	-2.90324100
O	1.81479400	-0.50583100	-2.37142000
O	-0.05188500	-2.32867200	-2.75631100
O	0.54555100	-2.56748000	1.99979300
O	-1.42225800	-3.63537800	-1.56517700
O	-1.11123200	-3.77622400	1.11109200
O	-4.11506200	-3.00205500	-1.22430800
O	-3.78324600	-3.12356600	1.45621700
O	-4.55645900	-1.40636100	2.66610000
O	-5.11081500	-1.19781100	-2.09895000

O	-3.44373200	-0.57206800	0.18032600
O	-2.38584000	-1.10081400	-2.07789100
O	-1.03617600	0.04994900	-4.03518200
O	-3.54742300	0.67732400	-3.74740300
O	-0.08782700	-0.23315400	3.76509700
O	-0.57935500	-1.22291400	-0.24019000
O	0.61105600	0.98914800	-0.25014100
O	1.23151000	1.62078000	2.40298200
O	2.23672500	-0.69549200	1.55456400
O	0.46307200	3.35468200	1.22119400
O	-5.79991800	1.04903100	-0.96492900
O	-5.44791800	0.91645700	1.98266300
O	-3.54098600	1.95613300	0.30153900
O	-4.02409700	2.81543600	-2.25502300
O	-3.45518400	2.58011400	2.94317000
O	-2.64404300	0.23931700	4.01319900
O	-1.85235900	-1.29455700	2.01452100
O	-1.40071300	1.14143400	1.45474800
Zr	-2.35589200	-2.31936900	-0.04851000
Zr	-0.33219700	-0.12285900	-2.08552900
Zr	-3.76207400	0.59696500	-1.46926500
Zr	-3.33175400	0.46558500	2.05248700
Zr	-1.27048300	2.64374100	0.04938900
Zr	0.10152300	-0.29967800	1.48193600
H	2.11442300	-1.26197600	-1.76554800
Al	5.66179700	-2.08891700	-1.67627400
Al	5.07127300	0.27780700	-2.90391400
Al	3.63310800	-0.73174200	0.18424000
Al	7.05154900	0.23921200	-0.17865500
Al	4.73310500	2.08718600	-0.99548600
Al	6.22924300	-2.55444800	0.94818800
Al	4.85625100	1.85629900	1.69818100
Al	5.75432100	-0.48832100	2.61263100
H	2.88698700	1.10124800	-2.22121700
H	4.91811000	-4.19197800	-0.47045900
H	9.13933000	1.27874400	0.19931000
H	5.58293000	-2.76733800	3.39680100
H	1.86750000	-2.50800200	-0.10800800
H	5.68528100	3.89467800	0.45644100
H	4.67016500	3.94898200	-2.75267400
H	8.01065700	-1.04014500	1.78515200
H	4.43608100	-1.96711100	4.12576000
H	5.07257700	3.30257700	3.65260300
H	7.30009100	-0.96575500	-3.01939100
H	3.57294600	-2.92848200	-2.18911300
H	6.60346400	1.34879900	-4.40016900
H	4.11333600	-2.24473800	-3.47382000
H	3.88651900	-0.41729800	-4.89494600
O	4.48186400	-0.78206800	-1.42186900
O	3.69441800	1.61149000	-2.39091600
O	5.62004900	-3.54012300	-0.54821100
O	8.77596000	0.41317200	0.00684700
O	6.91415100	-1.54973500	-0.44473700

O	6.17143500	1.13063000	-1.44219900
O	2.63969700	-2.17222200	-0.58072600
O	6.00784100	-3.84445900	2.18109700
O	5.39888400	3.46688300	-2.34218100
O	4.81208900	-1.49844800	1.33597600
O	3.77591900	1.15519900	0.32101700
O	4.98277800	3.24052400	0.39399000
O	6.27422100	0.79058800	1.34976000
O	7.28648500	-1.53753300	2.19974200
O	5.37731800	-1.92031100	3.91912900
O	4.24037700	0.59624700	2.96850400
O	5.62035200	2.84870600	3.00897700
O	6.62501400	0.61000100	4.00042400
O	6.37292700	-1.20747100	-3.12214000
O	5.70730600	1.49993200	-4.08958900
O	4.32636600	-2.98577000	-2.82215000
O	3.84416200	-0.67046200	-3.96726200
H	3.39555800	0.20616700	2.66665700
H	-4.86547700	-4.32294500	3.56898800
H	-6.11571200	-3.06038400	3.75176800
H	-6.06384000	-4.11937900	2.30300500
H	-5.63516600	-4.16844200	-2.98110900
H	-6.64505300	-3.80190300	-1.59260100
H	-6.80322100	-2.81052700	-3.07283700
H	-3.46065100	5.93241000	-2.67074000
H	-4.88364500	4.98017900	-3.22731500
H	-4.79010000	5.60929800	-1.56529100
H	-2.74207000	5.63809400	3.48778000
H	-4.28619100	5.41982000	2.67435300
H	-4.03159200	4.64623200	4.25703000
H	5.65936900	2.80293000	-3.07888700
H	6.77779500	-4.32161100	2.50013400
H	3.07966500	3.90787300	1.73523900
H	1.97750700	4.68186100	2.85967100
H	2.89383700	3.23268400	3.39443800
H	2.38876400	3.40845600	-3.80044000
H	1.10199000	4.65127400	-3.76184100
H	2.21855800	4.54638500	-2.40923700
H	1.05083900	-4.80172000	-2.89052000
H	-0.56769900	-5.55120500	-2.95170400
H	0.00318000	-4.45516200	-4.25755900
H	0.82653000	-4.84457400	3.30570300
H	0.06996300	-5.80797800	1.99654700
H	1.63960100	-4.98481000	1.75552100
H	7.58118900	0.61532500	3.87185000
H	6.31971900	1.55153500	3.75970500
H	2.44493800	-0.54765000	-3.16127000
Ir	-6.65304900	2.08651400	0.68728200
C	-6.84894200	3.45390800	2.25559600
C	-7.86524900	2.47438600	2.33609800
C	-8.21648000	2.62724500	-0.58048800
C	-7.18839300	3.59482200	-0.65721000
H	-7.08963000	4.47775600	1.94629000

H	-5.96701100	3.36487000	2.90136400
H	-8.90133400	2.72639600	2.08321300
H	-7.77569400	1.65985400	3.06613400
H	-9.15609300	2.85518800	-0.06438600
H	-8.32672200	1.88737000	-1.38384600
H	-7.32436800	4.58543400	-0.20775900
H	-6.48983900	3.56809700	-1.50247500

$Ir(C_2H_4)H_2@Al_8$-NU-1000

Electronic Energy: -7113.2699744

Enthalpy: -7112.207984

Free Energy: -7112.422070

C	1.68443300	3.94340300	-3.15513700
C	0.64900700	-4.90820900	2.22467400
C	2.37166100	3.70494600	2.55373900
C	0.00186100	-4.64437400	-3.17736900
C	-5.46156200	-3.56978900	3.03744800
C	-4.20582200	5.17836400	-2.39072800
C	-6.09811000	-3.34299300	-2.42688300
C	-3.54708500	4.91456900	3.31261100
C	1.27407600	2.82445900	2.03810600
C	0.75415100	3.00365800	-2.46954400
C	-3.54120300	3.93045800	-1.89883700
C	-5.03720900	-2.44270700	-1.88244900
C	-4.54350800	-2.62142700	2.33649900
C	-0.02839500	-3.67129100	1.74597300
C	-3.03317900	3.71325900	2.58669100
C	-0.52888800	-3.45031000	-2.44889000
H	-1.88490400	-1.87725100	2.77948900
H	1.50528800	1.36254200	-0.23500200
H	-3.66532500	1.60817400	-3.99294500
H	-2.57855800	0.45274100	-3.98484700
H	-2.86265100	1.02323000	4.54366500
H	-6.37999900	0.37887800	-1.33296300
H	-5.93811300	0.63073000	2.71813100
H	-2.57240900	-1.62221200	-2.86902100
H	-4.15695600	2.69059100	0.40869600
H	-0.50747100	0.66133200	-4.56323900
H	-1.07293200	-0.03294200	3.97605400
H	0.39881400	0.55661500	4.02285800
H	2.26707900	-1.61025900	1.87755600
O	-1.75523600	1.26036000	-1.40541400
O	-2.55797400	4.06317200	-1.11600600
O	-2.23628100	3.91541000	1.62105400
O	0.11398400	3.45719700	-1.47320400
O	0.64704000	1.82532000	-2.90304100
O	1.81434100	-0.50633300	-2.37070600
O	-0.05223200	-2.32870400	-2.75655500
O	0.54593000	-2.56747300	1.99907300
O	-1.42173400	-3.63639300	-1.56497300

O	-1.11126000	-3.77717100	1.11150000
O	-4.11218100	-3.00304800	-1.22999600
O	-3.79554600	-3.12308500	1.44127200
O	-4.53327500	-1.41207800	2.68153500
O	-5.11030100	-1.19765100	-2.09967600
O	-3.44308000	-0.57282900	0.17593700
O	-2.38546400	-1.10143300	-2.08138900
O	-1.03518000	0.05047800	-4.03611700
O	-3.54425100	0.67947200	-3.75176300
O	-0.09820200	-0.23293600	3.76393200
O	-0.58117000	-1.22405000	-0.24113700
O	0.60910300	0.98880000	-0.24956500
O	1.23022200	1.62101800	2.40366200
O	2.23597900	-0.69511500	1.55474300
O	0.46206900	3.35455500	1.22173600
O	-5.79280500	1.04645700	-0.95596400
O	-5.46814300	0.94327700	1.93694300
O	-3.54673100	1.94945600	0.30060200
O	-4.02617000	2.81606200	-2.25506200
O	-3.44550000	2.57910900	2.94970200
O	-2.66158600	0.24906300	4.00606200
O	-1.85204400	-1.29883700	2.01098700
O	-1.40458800	1.13679500	1.45381200
Zr	-2.35949300	-2.32512000	-0.04865800
Zr	-0.33261200	-0.12438300	-2.08539900
Zr	-3.76118000	0.59527000	-1.47546200
Zr	-3.33699400	0.45794100	2.03940200
Zr	-1.27042500	2.64166900	0.04981000
Zr	0.10015400	-0.30339700	1.48041400
H	2.11397400	-1.26249300	-1.76471400
Al	5.66140600	-2.08855600	-1.67581200
Al	5.07059100	0.27766800	-2.90438800
Al	3.63263200	-0.73090600	0.18421300
Al	7.05072300	0.24045200	-0.17907600
Al	4.73192100	2.08766100	-0.99660600
Al	6.22916200	-2.55289000	0.94882600
Al	4.85503700	1.85800800	1.69713900
Al	5.75357300	-0.48616900	2.61242300
H	2.88596400	1.10149000	-2.22199800
H	4.91876700	-4.19169700	-0.46934300
H	9.13839600	1.28021500	0.19940600
H	5.58312700	-2.76493600	3.39750600
H	1.86756300	-2.50825600	-0.10740300
H	5.68351500	3.89597100	0.45456900
H	4.66907100	3.94884900	-2.75457800
H	8.01013400	-1.03767600	1.78507300
H	4.43620000	-1.96503800	4.12671100
H	5.07206300	3.30529900	3.65090100
H	7.29958800	-0.96597700	-3.01949500
H	3.57258400	-2.92853500	-2.18810400
H	6.60218300	1.34820200	-4.40161600
H	4.11293800	-2.24547700	-3.47319700
H	3.88521500	-0.41826900	-4.89479400

O	4.48135800	-0.78172500	-1.42182500
O	3.69348600	1.61149000	-2.39193100
O	5.62021200	-3.53932300	-0.54716600
O	8.77504500	0.41461300	0.00704700
O	6.91370300	-1.54856800	-0.44454600
O	6.17045400	1.13125300	-1.44295000
O	2.63936400	-2.17184800	-0.58031700
O	6.00823400	-3.84244600	2.18226200
O	5.39771900	3.46699100	-2.34367100
O	4.81155900	-1.49719500	1.33625100
O	3.77462300	1.15604900	0.32029600
O	4.98111700	3.24166900	0.39239700
O	6.27293300	0.79225100	1.34891300
O	7.28604500	-1.53505800	2.19984500
O	5.37729200	-1.91777400	3.91955600
O	4.23945800	0.59838200	2.96797300
O	5.61950700	2.85099000	3.00730800
O	6.62420100	0.61281300	3.99962900
O	6.37237100	-1.20758000	-3.12202300
O	5.70622300	1.49946300	-4.09053300
O	4.32600900	-2.98609200	-2.82113100
O	3.84336500	-0.67120000	-3.96702500
H	3.39437500	0.20842200	2.66677400
H	-4.86702700	-4.33962300	3.54620200
H	-6.09749600	-3.06202600	3.76905900
H	-6.08421900	-4.09792900	2.30423900
H	-5.63471300	-4.16657700	-2.98338300
H	-6.64340100	-3.80399800	-1.59265200
H	-6.80482600	-2.80997200	-3.07062400
H	-3.46235700	5.94097800	-2.65078700
H	-4.86850500	4.98242300	-3.23991200
H	-4.80835900	5.59612400	-1.57140400
H	-2.78485100	5.69952600	3.36955300
H	-4.39086800	5.32804700	2.74159600
H	-3.91355700	4.65802700	4.31192000
H	5.65849300	2.80288900	-3.08007000
H	6.77834500	-4.31910700	2.50165800
H	3.07947900	3.90860600	1.73526400
H	1.97720400	4.68160800	2.86010800
H	2.89388400	3.23235800	3.39420900
H	2.38786400	3.40847800	-3.80141600
H	1.10203500	4.65233200	-3.76067800
H	2.21954900	4.54534800	-2.40911400
H	1.05006800	-4.80330500	-2.88849400
H	-0.56915200	-5.55070700	-2.95342500
H	0.00559200	-4.45437700	-4.25740900
H	0.82740600	-4.84430300	3.30556000
H	0.06935900	-5.80775400	1.99732300
H	1.63921200	-4.98540100	1.75479400
H	7.58040300	0.61786000	3.87123500
H	6.31906800	1.55428200	3.75837500
H	2.44466200	-0.54806700	-3.16053400
Ir	-6.67851100	2.09615400	0.68244400

C	-8.27005400	2.55078400	-0.60272900
C	-7.30644500	3.58329600	-0.66559900
H	-9.22545700	2.71197700	-0.09395900
H	-8.32044000	1.80903800	-1.40957200
H	-7.51090900	4.56428200	-0.22615300
H	-6.59498800	3.59673700	-1.50043900
H	-7.70122400	2.27933300	1.85746200
H	-6.78546300	3.29496600	1.69030600

$Ir(C_2H_4)_2H_2$@Al_8-NU-1000 (isomer-1)

Electronic Energy: -7191.8195008

Enthalpy: -7190.698807

Free Energy: -7190.916544

C	1.68445300	3.94340500	-3.15510700
C	0.64900400	-4.90821500	2.22466200
C	2.37166100	3.70495400	2.55372700
C	0.00185100	-4.64437500	-3.17737500
C	-5.46146600	-3.56984800	3.03749300
C	-4.20579000	5.17838300	-2.39072600
C	-6.09807400	-3.34300600	-2.42693000
C	-3.54713700	4.91458200	3.31255300
C	1.27402500	2.82437100	2.03806100
C	0.75414500	3.00358000	-2.46953900
C	-3.54114700	3.93051300	-1.89899900
C	-5.03726000	-2.44255300	-1.88274700
C	-4.54344900	-2.62145500	2.33700200
C	-0.02842500	-3.67128800	1.74594500
C	-3.03327000	3.71320800	2.58679400
C	-0.52889400	-3.45023900	-2.44891200
H	-1.89059300	-1.88640800	2.77236700
H	1.50033400	1.36441800	-0.23365400
H	-3.66383200	1.61233500	-3.98151300
H	-2.58909500	0.44873200	-3.98297100
H	-2.85911100	0.98652700	4.57795100
H	-6.31848000	0.49512700	-1.66405800
H	-5.47238600	1.83264300	2.67997300
H	-2.58797300	-1.62174800	-2.85457700
H	-4.22803800	2.58400500	0.43000700
H	-0.51546300	0.65969600	-4.56415500
H	-1.06226400	-0.03721300	3.97717000
H	0.41373300	0.54486000	4.01908900
H	2.26276000	-1.60749100	1.87557400
O	-1.75568300	1.25961700	-1.40698400
O	-2.57239000	4.06491200	-1.09525500
O	-2.22398900	3.90797700	1.63731900
O	0.10999600	3.45747900	-1.47580100
O	0.64862900	1.82470200	-2.90252900
O	1.81304100	-0.50621600	-2.36605700
O	-0.05211200	-2.32846400	-2.75543500
O	0.54679800	-2.56762800	1.99600400

O	-1.42408600	-3.63530200	-1.56644500
O	-1.11208300	-3.77755500	1.11162300
O	-4.11818000	-3.00322200	-1.22228100
O	-3.80728700	-3.12310900	1.43096600
O	-4.53327900	-1.41428100	2.68092700
O	-5.10023200	-1.20279800	-2.12139300
O	-3.49846100	-0.58469600	0.18638400
O	-2.39085800	-1.09899000	-2.07077800
O	-1.04033400	0.04790300	-4.03530600
O	-3.55355200	0.67890900	-3.75236300
O	-0.08713400	-0.24294300	3.76220100
O	-0.59099200	-1.21980200	-0.24063400
O	0.60479900	0.98944700	-0.24879300
O	1.22937900	1.62149400	2.40566300
O	2.23341000	-0.69275500	1.55146000
O	0.46266600	3.35309000	1.22004700
O	-5.82274900	1.09359600	-1.08968200
O	-5.41700900	1.06597300	2.09908900
O	-3.53290100	1.93560700	0.28985800
O	-4.00366600	2.81923000	-2.28107000
O	-3.46811200	2.58460300	2.94907500
O	-2.63250500	0.24613400	4.00543100
O	-1.85653000	-1.30646800	2.00512700
O	-1.40959400	1.13413800	1.45716700
Zr	-2.36398400	-2.32195400	-0.04807900
Zr	-0.33596100	-0.12367800	-2.08633700
Zr	-3.77314500	0.60289700	-1.47319400
Zr	-3.34934500	0.45073600	2.05090000
Zr	-1.27513600	2.63651500	0.04711600
Zr	0.09514500	-0.30155000	1.48192900
H	2.11154100	-1.26364800	-1.76158500
Al	5.65963100	-2.08936500	-1.67270200
Al	5.06962100	0.27611000	-2.90338900
Al	3.63088500	-0.73029700	0.18535500
Al	7.04964200	0.24013400	-0.17725300
Al	4.73212800	2.08742000	-0.99652700
Al	6.22721600	-2.55218300	0.95210400
Al	4.85395700	1.85936200	1.69707000
Al	5.75091800	-0.48453600	2.61412500
H	2.88551600	1.10252200	-2.22135800
H	4.91555500	-4.19027900	-0.46470500
H	9.13676100	1.27994500	0.20224500
H	5.57962800	-2.76266700	3.40033800
H	1.87247800	-2.51514500	-0.10392200
H	5.68485400	3.89607900	0.45345800
H	4.66882100	3.94640300	-2.75653900
H	8.00776000	-1.03648600	1.78820200
H	4.43105400	-1.96235600	4.12591600
H	5.06960800	3.30710200	3.65023500
H	7.29825700	-0.96829700	-3.01659700
H	3.57060400	-2.92845900	-2.18159900
H	6.60246000	1.34417000	-4.40061900
H	4.10985100	-2.24752700	-3.46868700

H	3.88275900	-0.42075800	-4.89253600
O	4.48065000	-0.78132600	-1.41986700
O	3.69374600	1.61121700	-2.39188800
O	5.61847000	-3.53954200	-0.54314300
O	8.77407000	0.41411300	0.00964600
O	6.91250100	-1.54900500	-0.44179700
O	6.17068300	1.13068100	-1.44218800
O	2.64148400	-2.17554200	-0.57906000
O	6.00611100	-3.84107000	2.18635000
O	5.39838400	3.46631700	-2.34513900
O	4.80985600	-1.49588700	1.33818000
O	3.77443000	1.15724300	0.32049600
O	4.98184300	3.24242900	0.39168100
O	6.27202900	0.79316500	1.35049200
O	7.28379600	-1.53388400	2.20319000
O	5.37286400	-1.91538800	3.92182400
O	4.23682500	0.60048900	2.96808600
O	5.61801100	2.85266200	3.00754800
O	6.62127600	0.61486200	4.00133600
O	6.37112400	-1.20997900	-3.11969600
O	5.70642900	1.49657000	-4.09030100
O	4.32314800	-2.98742200	-2.81604700
O	3.84172700	-0.67307000	-3.96458500
H	3.39180600	0.21110000	2.66573000
H	-6.24714100	-3.89132300	2.33923100
H	-4.91632700	-4.47539100	3.32930500
H	-5.93140900	-3.11221800	3.91398000
H	-5.63941000	-4.08205500	-3.09626800
H	-6.55266200	-3.91399400	-1.60669400
H	-6.87271500	-2.79286000	-2.97088900
H	-3.49720600	6.01165900	-2.44739500
H	-4.69432600	5.01989100	-3.35809800
H	-4.98749100	5.46432800	-1.67207600
H	-2.76198600	5.67044400	3.42782200
H	-4.33970600	5.37862400	2.70739600
H	-3.97079400	4.65249700	4.28753500
H	5.65926300	2.80125900	-3.08050900
H	6.77667900	-4.31609400	2.50707600
H	3.07995100	3.90824000	1.73555000
H	1.97742500	4.68190700	2.85950400
H	2.89332100	3.23261100	3.39468800
H	2.38969700	3.40815200	-3.79914400
H	1.10187900	4.65006300	-3.76311600
H	2.21744800	4.54776900	-2.40947400
H	1.05227200	-4.79916000	-2.89452500
H	-0.56535400	-5.55186900	-2.94858000
H	-0.00139700	-4.45641700	-4.25781300
H	0.83874500	-4.83993200	3.30329900
H	0.06438100	-5.80687100	2.00670000
H	1.63403200	-4.99098300	1.74484500
H	7.57736000	0.61976200	3.87205300
H	6.31619900	1.55621100	3.75932200
H	2.44258500	-0.54876000	-3.15622100

Ir	-7.17584100	1.16722500	0.73164100
H	-8.13130600	1.49553400	1.93969200
H	-8.46198800	0.88688300	-0.13940100
C	-7.88706600	3.00823500	-0.12229600
C	-6.75428900	3.27637600	0.66538000
H	-8.88859200	3.25661700	0.23440400
H	-7.78138700	2.95774300	-1.20920500
H	-6.85200100	3.73523600	1.65387500
H	-5.80284300	3.45652400	0.15424800
C	-6.92875700	-0.98411800	0.56960800
C	-7.64687200	-0.71618800	1.73705100
H	-5.84753400	-1.15177700	0.59600700
H	-7.44003000	-1.34013000	-0.32958800
H	-7.11873300	-0.68348400	2.69355400
H	-8.72526100	-0.88072500	1.78331400

$Ir(C_2H_4)_2H_2@Al_8$-NU-1000 (isomer-2)

Electronic Energy: -7191.8060947

Enthalpy: -7190.685915

Free Energy: -7190.904908

C	1.68444300	3.94340400	-3.15512200
C	0.64901100	-4.90821700	2.22464700
C	2.37165600	3.70495100	2.55374200
C	0.00186600	-4.64437800	-3.17736000
C	-5.46148600	-3.56979600	3.03753800
C	-4.20578200	5.17833800	-2.39084900
C	-6.09811000	-3.34294800	-2.42695500
C	-3.54711300	4.91452600	3.31266200
C	1.27405100	2.82449000	2.03812700
C	0.75414700	3.00370300	-2.46962200
C	-3.54106200	3.93042300	-1.89871800
C	-5.03723900	-2.44265000	-1.88205600
C	-4.54359300	-2.62147200	2.33628100
C	-0.02843100	-3.67127100	1.74596100
C	-3.03323900	3.71314100	2.58653600
C	-0.52889200	-3.45022700	-2.44890700
H	-1.88011500	-1.88780500	2.78308300
H	1.49518900	1.36760000	-0.23460900
H	-3.60929000	1.64150400	-3.93445900
H	-2.57816900	0.44488700	-3.97079900
H	-2.86602400	0.98955700	4.59592000
H	-6.36998200	1.31911900	-1.64938800
H	-5.57532800	1.89507000	2.24874200
H	-2.59281900	-1.62879100	-2.85368700
H	-4.22968300	2.57576600	0.33999500
H	-0.50995800	0.65110600	-4.56284100
H	-1.04518900	-0.03013900	3.98723800
H	0.43229700	0.54494400	4.01615100
H	2.26579500	-1.60887000	1.87596500
O	-1.75733900	1.25104000	-1.41487100

O	-2.55852400	4.05994800	-1.11632000
O	-2.20651600	3.90632600	1.65160700
O	0.11033800	3.45601200	-1.47518600
O	0.64941600	1.82447200	-2.90282800
O	1.81928500	-0.50661100	-2.36393200
O	-0.04620900	-2.33003500	-2.75126500
O	0.54738300	-2.56847400	1.99673700
O	-1.42359100	-3.63779400	-1.56716000
O	-1.11146300	-3.77931000	1.11177700
O	-4.12840000	-3.00375600	-1.20144000
O	-3.79435900	-3.12649900	1.44442500
O	-4.52234500	-1.41822800	2.69515500
O	-5.07955600	-1.20360800	-2.13018900
O	-3.45747100	-0.57805500	0.18911800
O	-2.38203400	-1.11105600	-2.07017800
O	-1.03357700	0.03722400	-4.03512700
O	-3.53645400	0.69723000	-3.73593100
O	-0.07356700	-0.24234200	3.76716600
O	-0.58575600	-1.22562700	-0.23834600
O	0.60092700	0.98984500	-0.24918000
O	1.23060500	1.62158200	2.40542900
O	2.23578600	-0.69405600	1.55222700
O	0.46451600	3.35227800	1.21807100
O	-5.80050300	1.16943100	-0.88643900
O	-5.42216300	0.97461300	2.01617100
O	-3.50471700	1.94599600	0.29461900
O	-4.03215100	2.81746600	-2.25743600
O	-3.49635200	2.58733900	2.92722900
O	-2.61785100	0.26007800	4.01842600
O	-1.84943500	-1.30577900	2.01731400
O	-1.40540300	1.13206300	1.46159700
Zr	-2.36471500	-2.33236300	-0.04542800
Zr	-0.33095700	-0.13212200	-2.08470400
Zr	-3.76034800	0.57954000	-1.45366500
Zr	-3.34333300	0.44796900	2.06925200
Zr	-1.27226700	2.62883500	0.05060900
Zr	0.09614200	-0.30585200	1.48302500
H	2.11880000	-1.26449000	-1.76018500
Al	5.66596100	-2.08585600	-1.66952100
Al	5.07483100	0.27983000	-2.89910700
Al	3.63423400	-0.72981000	0.18772500
Al	7.05258600	0.24378600	-0.17163800
Al	4.73417900	2.08954500	-0.99163200
Al	6.23160400	-2.54992700	0.95547200
Al	4.85421700	1.85986700	1.70188300
Al	5.75227000	-0.48377700	2.61835300
H	2.88916800	1.10413800	-2.21848900
H	4.92118500	-4.18697300	-0.46273100
H	9.13811000	1.28568600	0.20961600
H	5.58202800	-2.76248300	3.40296500
H	1.87729500	-2.51577900	-0.10512300
H	5.68567700	3.89773900	0.45997400
H	4.66924600	3.94868900	-2.75045600

H	8.01013600	-1.03331800	1.79396100
H	4.43210900	-1.96346800	4.12779100
H	5.06643200	3.30532600	3.65670400
H	7.30486000	-0.96149500	-3.01021300
H	3.57885700	-2.92886600	-2.18377600
H	6.60826400	1.35037500	-4.39369300
H	4.11947400	-2.24395800	-3.46815900
H	3.88993700	-0.41617400	-4.88965200
O	4.48564800	-0.77913000	-1.41678900
O	3.69723800	1.61338900	-2.38815200
O	5.62462800	-3.53674600	-0.54079200
O	8.77684600	0.41947800	0.01600900
O	6.91748800	-1.54538600	-0.43721800
O	6.17401000	1.13443300	-1.43681800
O	2.64772400	-2.17642600	-0.57818800
O	6.01079200	-3.83984900	2.18874100
O	5.39962400	3.46991600	-2.33895600
O	4.81322300	-1.49499800	1.34103700
O	3.77677400	1.15786200	0.32404700
O	4.98305900	3.24378100	0.39733700
O	6.27378000	0.79515500	1.35606600
O	7.28646200	-1.53171500	2.20821700
O	5.37415000	-1.91575600	3.92488500
O	4.23706700	0.59975500	2.97165100
O	5.61635200	2.85296000	3.01382800
O	6.62066200	0.61544700	4.00702100
O	6.37828200	-1.20452500	-3.11514900
O	5.71149900	1.50164100	-4.08493600
O	4.33325700	-2.98433800	-2.81613800
O	3.84891900	-0.66979500	-3.96205900
H	3.39267200	0.20996300	2.66795100
H	-4.86756000	-4.20248200	3.71131900
H	-6.21824300	-3.04782400	3.63280700
H	-5.93911500	-4.24556300	2.31757800
H	-5.64296800	-4.23206900	-2.87845400
H	-6.72084900	-3.69762800	-1.59347700
H	-6.73921800	-2.83176100	-3.15227300
H	-3.49809900	6.01208700	-2.44929700
H	-4.69628600	5.01996900	-3.35729300
H	-4.98611500	5.46163900	-1.66992800
H	-2.76579700	5.67514900	3.42126000
H	-4.34801800	5.37088700	2.71312800
H	-3.96410900	4.65159000	4.29027500
H	5.66175800	2.80552500	-3.07452700
H	6.78174500	-4.31382300	2.51008300
H	3.08081200	3.90654200	1.73592700
H	1.97814300	4.68270400	2.85799900
H	2.89212200	3.23333500	3.39584500
H	2.39052300	3.40780900	-3.79797200
H	1.10250000	4.64940700	-3.76452200
H	2.21668400	4.54857000	-2.40957200
H	1.03679500	-4.82675100	-2.85563900
H	-0.59127700	-5.54295700	-2.98113700

H	0.04394400	-4.44204000	-4.25418600
H	0.84365100	-4.83804600	3.30227100
H	0.06238000	-5.80655900	2.01075100
H	1.63182700	-4.99349700	1.74067300
H	7.57677300	0.62125800	3.87799300
H	6.31488600	1.55667800	3.76517400
H	2.44914700	-0.54733600	-3.15386500
Ir	-6.97231100	0.17517500	0.62261900
C	-7.85862100	-0.42129800	2.44040600
C	-8.25775500	-1.31993600	1.43236100
C	-8.73386800	1.50810300	0.18347400
C	-7.85326100	2.22335100	0.97950200
H	-8.57415000	0.31516200	2.82485300
H	-7.04214000	-0.67299700	3.12385800
H	-9.27215300	-1.26949000	1.02538400
H	-7.80408800	-2.31089700	1.35778400
H	-9.63141600	1.04879200	0.60953200
H	-8.78507300	1.68071000	-0.89482900
H	-8.03208600	2.34533100	2.05142200
H	-7.15569900	2.93433500	0.52554800
H	-6.00594700	-1.09918100	0.50306900
H	-7.68172300	-0.54040600	-0.59590600

TS1(di-ethyl)@Al_8-NU-1000 (isomer-1)

Electronic Energy: -7191.790895

Enthalpy: -7190.672510

Free Energy: -7190.890296

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.87733000	-1.87082200	2.78164600
H	1.51094900	1.36002800	-0.23833500
H	-3.67736300	1.60607700	-3.97820800
H	-2.59342900	0.45104300	-3.97587700
H	-2.87378700	0.97483900	4.58832700
H	-6.31844700	0.39376100	-1.55126500
H	-5.82037000	0.22640900	2.63269300

H	-2.57602400	-1.61608600	-2.85968500
H	-4.25602700	2.61907000	0.43425800
H	-0.51934000	0.66339400	-4.55973800
H	-1.06195900	-0.03361100	3.98404200
H	0.41363900	0.55199600	4.02456700
H	2.26283700	-1.61083300	1.87372800
O	-1.76026800	1.26703100	-1.39341100
O	-2.56086400	4.06897600	-1.11281400
O	-2.24387500	3.92451100	1.61494500
O	0.11558000	3.45810900	-1.47229800
O	0.64326600	1.82636900	-2.90452300
O	1.80915600	-0.50448300	-2.37196400
O	-0.05389700	-2.32795100	-2.75671000
O	0.54709500	-2.56777900	1.99695100
O	-1.42232700	-3.63524600	-1.56451400
O	-1.11328500	-3.77595200	1.11391800
O	-4.11752800	-3.00123500	-1.22162300
O	-3.79544700	-3.12158200	1.44388100
O	-4.53728800	-1.41473900	2.68777500
O	-5.10846900	-1.20066000	-2.10927700
O	-3.46800700	-0.57913800	0.18676700
O	-2.38858200	-1.09766200	-2.07066000
O	-1.04459500	0.05288600	-4.02985800
O	-3.55828200	0.67571200	-3.74239000
O	-0.08678300	-0.23419700	3.76268000
O	-0.58352100	-1.21966300	-0.23932300
O	0.61393100	0.98843300	-0.25130400
O	1.23254000	1.62047200	2.40119900
O	2.23600300	-0.69551600	1.55090600
O	0.46100700	3.35644100	1.22394200
O	-5.82055100	1.06153900	-1.06071300
O	-5.42016200	0.93090900	2.10940600
O	-3.57944500	1.94426600	0.31302600
O	-4.01219800	2.81659700	-2.26577700
O	-3.41916700	2.57885500	2.96362800
O	-2.63646700	0.23403500	4.01992700
O	-1.85087000	-1.29413300	2.01160200
O	-1.40245100	1.14671600	1.44786000
Zr	-2.35894000	-2.31744100	-0.04659900
Zr	-0.33795300	-0.11794400	-2.08104000
Zr	-3.76888000	0.59990100	-1.45951300
Zr	-3.33084400	0.46673700	2.05928000
Zr	-1.27675000	2.65367300	0.05329500
Zr	0.10061200	-0.29577300	1.48092200
H	2.10818200	-1.26191500	-1.76774600
Al	5.65590000	-2.09169600	-1.68283700
Al	5.06528400	0.27488000	-2.91066000
Al	3.62995000	-0.73352400	0.17969500
Al	7.04888100	0.23592400	-0.18715000
Al	4.73093000	2.08461600	-1.00176000
Al	6.22718600	-2.55684100	0.94075500
Al	4.85607000	1.85441300	1.69163500
Al	5.75443800	-0.49029700	2.60520400

H	2.88293700	1.09992100	-2.22537000
H	4.91276900	-4.19362400	-0.47564100
H	9.13690800	1.27432300	0.19081900
H	5.58327600	-2.76895100	3.38985000
H	1.86522000	-2.51028900	-0.11013600
H	5.68438300	3.89268200	0.44892600
H	4.66538200	3.94443400	-2.75994700
H	8.00978300	-1.04246900	1.77529100
H	4.43636100	-1.96851000	4.11798600
H	5.07313900	3.29828300	3.64697100
H	7.29349800	-0.97009100	-3.02710000
H	3.56540300	-2.92895700	-2.19116300
H	6.59747100	1.34409200	-4.40761200
H	4.10437200	-2.24705000	-3.47757200
H	3.87877500	-0.42080000	-4.90007700
O	4.47775700	-0.78362100	-1.42712700
O	3.69044800	1.60984600	-2.39613900
O	5.61552900	-3.54276500	-0.55445200
O	8.77368500	0.40880900	-0.00223000
O	6.91081900	-1.55295300	-0.45326300
O	6.16861500	1.12787500	-1.45010100
O	2.63635300	-2.17406800	-0.58429000
O	6.00786900	-3.84668200	2.17428900
O	5.39553500	3.46420000	-2.34978100
O	4.81090000	-1.50027400	1.32980700
O	3.77469800	1.15356300	0.31584100
O	4.98180500	3.23856400	0.38717400
O	6.27370200	0.78851300	1.34198000
O	7.28616600	-1.53978800	2.19100900
O	5.37786500	-1.92201000	3.91236600
O	4.24132400	0.59470400	2.96286500
O	5.62128900	2.84705700	3.00178400
O	6.62746200	0.60802300	3.99186400
O	6.36622500	-1.21140500	-3.12984700
O	5.70146800	1.49630300	-4.09710200
O	4.31762600	-2.98788400	-2.82575500
O	3.83675500	-0.67299800	-3.97214000
H	3.39598400	0.20484800	2.66190700
H	-6.08162300	-3.06701700	3.78645700
H	-6.10168300	-4.08061800	2.30601600
H	-4.86901200	-4.35449300	3.52520300
H	-6.66139400	-3.78222300	-1.59203100
H	-6.79138800	-2.81476000	-3.08943600
H	-5.63641600	-4.18218300	-2.96096700
H	-4.61952200	5.72698600	-1.53355000
H	-3.46756500	5.84760100	-2.85083800
H	-5.00959700	4.96228400	-3.10172600
H	-2.72565600	5.60160100	3.54972700
H	-4.22709000	5.46843200	2.65019000
H	-4.08785500	4.64086300	4.22379900
H	5.65552900	2.79970300	-3.08605000
H	6.77909600	-4.32148100	2.49377100
H	3.07997900	3.90731200	1.73530500

H	1.97765100	4.68206000	2.85912400
H	2.89371600	3.23279500	3.39456900
H	2.38467700	3.40943500	-3.80570500
H	1.10153900	4.65591800	-3.75591300
H	2.22347300	4.54131200	-2.40866000
H	-0.56748800	-5.55122900	-2.95120500
H	0.00244100	-4.45529600	-4.25758600
H	1.05099600	-4.80167500	-2.89110300
H	0.82859100	-4.84352800	3.30530600
H	0.06885700	-5.80782000	1.99866800
H	1.63862700	-4.98607600	1.75368300
H	7.58327400	0.61329600	3.86058200
H	6.32173200	1.54943300	3.75115600
H	2.43594100	-0.54839500	-3.16379400
Ir	-7.03905700	1.57720000	0.73460200
C	-7.95164100	2.98022200	-0.51578700
H	-8.05536400	1.75451400	1.93222300
C	-8.47559300	0.13182100	0.01798500
C	-7.47484200	-0.55123900	0.73675400
H	-6.89041800	2.87941000	1.62837500
H	-8.91815200	3.37903500	-0.18975400
H	-7.94543000	2.64607100	-1.55860800
C	-6.74127500	3.58428800	-0.00836900
H	-9.46416600	0.29406100	0.45348600
H	-8.47316300	0.13460700	-1.07805500
H	-7.68061400	-0.90457200	1.75166800
H	-6.65439100	-1.06705200	0.22635300
H	-6.79872900	4.48469500	0.61225000
H	-5.85902300	3.55630400	-0.65817000

TS1(di-ethyl)@Al_8-NU-1000 (isomer-2)

Electronic Energy: -7191.8030383

Enthalpy: -7190.684186

Free Energy: -7190.900975

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900

H	-1.88537000	-1.87607000	2.77675300
H	1.49851800	1.36444300	-0.24335900
H	-3.64725000	1.60671200	-3.97189300
H	-2.58637100	0.43669400	-3.97247500
H	-2.86908800	0.98181700	4.59353300
H	-5.93176900	2.03460800	-1.69724500
H	-5.81082800	0.13283700	2.51718700
H	-2.58357700	-1.63803800	-2.85238800
H	-4.25286000	2.58545700	0.41090100
H	-0.51412600	0.65531500	-4.56427800
H	-1.05546500	-0.03324300	3.98454800
H	0.41955000	0.55103000	4.01617600
H	2.26636900	-1.61170700	1.87062300
O	-1.76992600	1.25680400	-1.40561400
O	-2.56718300	4.05704500	-1.10765800
O	-2.22779600	3.91786900	1.63022000
O	0.11116600	3.45717000	-1.47420600
O	0.64411100	1.82621300	-2.90449600
O	1.80903700	-0.50354000	-2.36758100
O	-0.05036900	-2.32893300	-2.75358400
O	0.54697300	-2.56749900	1.99762700
O	-1.42113100	-3.63785200	-1.56415700
O	-1.11249700	-3.77600300	1.11299400
O	-4.12132900	-3.00898000	-1.21169300
O	-3.78926900	-3.12329500	1.45204300
O	-4.53842600	-1.41427900	2.68845200
O	-5.10053500	-1.20358400	-2.10050700
O	-3.49534300	-0.58503500	0.18622500
O	-2.38621000	-1.11324700	-2.07016400
O	-1.03656600	0.04075300	-4.03634500
O	-3.54746500	0.67350600	-3.73921300
O	-0.08222600	-0.23726200	3.76244700
O	-0.59044100	-1.22082700	-0.23834300
O	0.60323000	0.98899000	-0.25315000
O	1.23370000	1.62012300	2.40185700
O	2.23729700	-0.69659600	1.54745200
O	0.46200800	3.35356200	1.22138800
O	-5.79618800	1.24898800	-1.15498000
O	-5.42564100	0.90474900	2.08337200
O	-3.54315300	1.94008400	0.31667200
O	-4.02088800	2.82297500	-2.27964800
O	-3.44944600	2.58313400	2.95241700
O	-2.63287200	0.24296500	4.02257000
O	-1.85495900	-1.29471600	2.01039400
O	-1.39822500	1.14036700	1.45432800
Zr	-2.36652100	-2.32328300	-0.05256800
Zr	-0.34277000	-0.12457100	-2.08523400
Zr	-3.78448000	0.58578900	-1.45682100
Zr	-3.32613900	0.46524900	2.06145700
Zr	-1.27613700	2.63841700	0.04994600
Zr	0.10154200	-0.30298400	1.47947600
H	2.10802400	-1.26274600	-1.76613200
Al	5.65740100	-2.09082200	-1.68588700

Al	5.06437100	0.27558700	-2.91340800
Al	3.63241200	-0.73362200	0.17744400
Al	7.04997600	0.23760300	-0.19045500
Al	4.73107600	2.08498100	-1.00378800
Al	6.23015700	-2.55563300	0.93762800
Al	4.85690100	1.85463500	1.68937500
Al	5.75721500	-0.48951100	2.60252300
H	2.88264700	1.10037600	-2.22624600
H	4.91604800	-4.19285800	-0.47822200
H	9.13761700	1.27673800	0.18754500
H	5.58811300	-2.76822200	3.38728400
H	1.87241000	-2.51768300	-0.11007400
H	5.68418100	3.89349400	0.44661900
H	4.66393600	3.94509900	-2.76181600
H	8.01230600	-1.04024400	1.77119700
H	4.44121800	-1.96849300	4.11632900
H	5.07195000	3.29616700	3.64590100
H	7.29330000	-0.96776900	-3.03132300
H	3.56715600	-2.92982800	-2.19212100
H	6.59492200	1.34493700	-4.41208000
H	4.10411000	-2.24678600	-3.47886800
H	3.87464500	-0.42095300	-4.90086100
O	4.47909400	-0.78303300	-1.42923100
O	3.69013900	1.61016800	-2.39759000
O	5.61870100	-3.54190600	-0.55726100
O	8.77477400	0.41105800	-0.00547700
O	6.91252800	-1.55128200	-0.45660200
O	6.16903200	1.12920700	-1.45302400
O	2.64110800	-2.17743700	-0.58517100
O	6.01180600	-3.84540300	2.17151100
O	5.39458100	3.46523100	-2.35209700
O	4.81336900	-1.49990900	1.32784900
O	3.77584400	1.15332500	0.31413100
O	4.98189700	3.23904900	0.38508900
O	6.27515900	0.78966500	1.33923800
O	7.28931200	-1.53807300	2.18743100
O	5.38253100	-1.92139000	3.91003200
O	4.24335700	0.59447800	2.96100300
O	5.62130700	2.84782200	2.99971200
O	6.63011600	0.60950100	3.98877400
O	6.36616300	-1.20990800	-3.13327000
O	5.69953400	1.49736000	-4.09992900
O	4.31895900	-2.98755400	-2.82746400
O	3.83478100	-0.67286500	-3.97275800
H	3.39802000	0.20477000	2.66017100
H	-6.14427700	-3.05559800	3.72153200
H	-6.03105000	-4.15697100	2.30585900
H	-4.86189300	-4.29018300	3.60937100
H	-6.72297100	-3.69688800	-1.59480200
H	-6.73813400	-2.83076400	-3.15257200
H	-5.64562200	-4.23389900	-2.87753800
H	-4.64742100	5.03452700	-3.38288700
H	-5.02592400	5.43009000	-1.70239700

H	-3.51267300	6.02607200	-2.39755500
H	-2.73079300	5.61326100	3.53225200
H	-4.24440200	5.45676900	2.65759300
H	-4.07016100	4.64299700	4.23524700
H	5.65436200	2.80080900	-3.08844900
H	6.78306700	-4.32092500	2.48982200
H	3.08221500	3.90345700	1.73625800
H	1.97893800	4.68387000	2.85502400
H	2.89105200	3.23445600	3.39711300
H	2.38839500	3.40812600	-3.80055800
H	1.10148900	4.65082500	-3.76187300
H	2.21886600	4.54680100	-2.40972100
H	-0.58056600	-5.54679900	-2.96729200
H	0.02500600	-4.44819600	-4.25598200
H	1.04349700	-4.81513700	-2.87166600
H	0.83199200	-4.84242600	3.30466200
H	0.06729100	-5.80740600	2.00113800
H	1.63713400	-4.98785300	1.75077700
H	7.58580800	0.61537900	3.85659900
H	6.32358900	1.55067700	3.74805300
H	2.43387700	-0.54807000	-3.16069000
Ir	-6.98656300	1.64182100	0.68878500
C	-8.08058400	2.07033600	2.38169000
C	-8.31875700	0.22466500	-0.27878800
C	-7.38509800	-0.47125300	0.49737700
H	-6.32295300	3.15460700	1.03109100
H	-7.87393400	1.39715700	3.22371300
H	-9.15143700	2.24624400	2.22720700
C	-7.17130800	3.19029500	2.20501500
H	-9.34592800	0.36029800	0.06950300
H	-8.17029900	0.29775000	-1.35884900
H	-7.66759400	-0.87134800	1.47754900
H	-6.50208100	-0.92313400	0.03452900
H	-6.31963800	3.25592600	2.89282800
H	-7.59168900	4.16832200	1.94674800
H	-7.99088700	2.46862000	-0.21514300

TS1(mono-ethyl)@Al_8-NU-1000

Electronic Energy: -7113.2495019

Enthalpy: -7112.188943

Free Energy: -7112.402752

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400

C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.88280600	-1.87954000	2.77514900
H	1.50371000	1.36258900	-0.23298800
H	-3.69168400	1.59071900	-4.01718700
H	-2.58883900	0.45071700	-3.99131500
H	-2.89746100	0.92509200	4.62822600
H	-6.40481000	0.31394800	-1.22942000
H	-5.98830600	0.17781100	2.06445800
H	-2.58162700	-1.62243800	-2.85542600
H	-3.78515400	2.95556700	0.34304100
H	-0.51204300	0.65530600	-4.56868100
H	-1.05533100	-0.04306300	3.99767400
H	0.41700900	0.54910200	4.03062300
H	2.25830000	-1.60771900	1.87217100
O	-1.76456500	1.27436900	-1.39641500
O	-2.57704100	4.06022500	-1.08683000
O	-2.26704200	3.91067300	1.59119800
O	0.12071500	3.46195100	-1.47003100
O	0.63823200	1.82771500	-2.90236100
O	1.79985100	-0.49836300	-2.35909400
O	-0.05469100	-2.32698900	-2.75880300
O	0.54508900	-2.56626400	2.00377800
O	-1.42432900	-3.62894200	-1.56501700
O	-1.11037400	-3.77002900	1.10926500
O	-4.12304100	-2.99665000	-1.20595300
O	-3.77576700	-3.12239600	1.46090000
O	-4.56521700	-1.40408700	2.65643600
O	-5.10402400	-1.20460500	-2.11707300
O	-3.45832400	-0.53105900	0.18615800
O	-2.39817600	-1.09195900	-2.07322400
O	-1.04209100	0.05122500	-4.03631400
O	-3.55586100	0.66780900	-3.76229300
O	-0.08231700	-0.23736700	3.76752300
O	-0.58521400	-1.21464300	-0.23784000
O	0.60220200	1.00073400	-0.24571300
O	1.22593200	1.62219500	2.40250000
O	2.22889800	-0.69244000	1.54879900
O	0.46657100	3.35888400	1.21946500
O	-5.81660100	1.06542600	-1.09954200
O	-5.42729600	0.95890100	2.00875100
O	-3.66063200	1.99371200	0.32134800
O	-4.00115000	2.81837100	-2.28328800
O	-3.40881100	2.57574100	2.97657900
O	-2.63396700	0.21303000	4.03466700
O	-1.85801400	-1.28850500	2.01575500
O	-1.40967000	1.14870800	1.45507300
Zr	-2.36873100	-2.29913300	-0.04642700

Zr	-0.34959200	-0.11776500	-2.08493400
Zr	-3.80343300	0.60625700	-1.49129800
Zr	-3.33492700	0.47281900	2.08938200
Zr	-1.23726100	2.63045000	0.04378500
Zr	0.09511600	-0.30083800	1.48594100
H	2.09698000	-1.25965500	-1.75792700
Al	5.64655800	-2.09020200	-1.68590400
Al	5.05517800	0.27721600	-2.91291800
Al	3.62603100	-0.73088900	0.17907900
Al	7.04290000	0.23727600	-0.19172900
Al	4.72554400	2.08768700	-1.00341900
Al	6.22137500	-2.55490800	0.93750500
Al	4.85222300	1.85721800	1.68984200
Al	5.75191200	-0.48790600	2.60283700
H	2.87721300	1.10099000	-2.21988800
H	4.90641300	-4.19314700	-0.47763800
H	9.13311300	1.27309800	0.18629600
H	5.58241900	-2.76655400	3.38836000
H	1.86390800	-2.51426700	-0.10689400
H	5.67960400	3.89481900	0.44712400
H	4.66404800	3.95112300	-2.76131700
H	8.00607900	-1.04064600	1.76900200
H	4.43865300	-1.96642400	4.12266100
H	5.07710400	3.30592200	3.64316600
H	7.28141200	-0.97003400	-3.03699000
H	3.55463900	-2.92686300	-2.18756000
H	6.58162400	1.34467200	-4.41825800
H	4.08936100	-2.24511200	-3.47586500
H	3.85608100	-0.41732200	-4.89674300
O	4.46993500	-0.78046700	-1.42819100
O	3.68163600	1.61402700	-2.39530900
O	5.60759100	-3.54064400	-0.55686900
O	8.76745800	0.40850000	-0.00617300
O	6.90261400	-1.55118600	-0.45792100
O	6.16134500	1.12965200	-1.45355900
O	2.63216200	-2.17373500	-0.58255700
O	6.00196100	-3.84369700	2.17174400
O	5.39100800	3.46568200	-2.35176600
O	4.80534600	-1.49776900	1.32925000
O	3.76702700	1.15710700	0.31511700
O	4.97618000	3.24151500	0.38530900
O	6.26752000	0.79029100	1.33735200
O	7.28220900	-1.53722800	2.18528100
O	5.37867700	-1.91903000	3.91078100
O	4.23821900	0.59772800	2.96174000
O	5.62062600	2.84926100	2.99796300
O	6.62587700	0.61050800	3.98768300
O	6.35322100	-1.20983700	-3.13466000
O	5.68842800	1.49829800	-4.10049200
O	4.30487700	-2.98561400	-2.82476400
O	3.81994500	-0.66914000	-3.96843500
H	3.39324700	0.20700300	2.66190700
H	-4.86452400	-4.28525800	3.61819800

H	-6.15127400	-3.05223800	3.71115700
H	-6.02174300	-4.16267000	2.30373500
H	-5.63572400	-4.17418400	-2.97317000
H	-6.65226300	-3.79493500	-1.59351000
H	-6.79586400	-2.81031100	-3.08034900
H	-3.46262500	5.88259100	-2.78530300
H	-4.96473500	4.96412800	-3.14979100
H	-4.68064400	5.68397300	-1.53811600
H	-4.46394000	5.24645900	2.80423100
H	-3.81514700	4.67314500	4.34627200
H	-2.83005300	5.74173600	3.27633600
H	5.64837700	2.80130700	-3.08905100
H	6.77120100	-4.32404200	2.48767800
H	3.07656500	3.91185100	1.73359100
H	1.97587300	4.67994400	2.86357500
H	2.89686300	3.23145100	3.39181900
H	2.37759900	3.41107000	-3.81440800
H	1.10086200	4.66401700	-3.74546900
H	2.23151100	4.53217500	-2.40736700
H	1.06034700	-4.78341000	-2.91808900
H	-0.54959500	-5.55658700	-2.92964600
H	-0.02888800	-4.46535800	-4.25898600
H	0.81251500	-4.84983200	3.30821900
H	0.07578700	-5.80870800	1.98503700
H	1.64552900	-4.97798700	1.76734500
H	7.58213400	0.61396700	3.85965500
H	6.32184600	1.55245100	3.74730900
H	2.42504300	-0.54433400	-3.15296100
Ir	-6.05214200	2.45646800	0.67331000
C	-8.06324600	2.74821000	0.61184600
H	-6.06929600	3.67419800	-0.40988500
H	-6.06552300	3.45781400	1.88852300
H	-8.53804600	3.18572700	1.49769800
H	-8.61605800	1.87708700	0.23213000
C	-7.47890600	3.64831300	-0.37444800
H	-7.56415000	4.72744600	-0.19343200
H	-7.61831000	3.40434400	-1.43643800

Ir(C_2H_5) (C_2H_4) H@Al_8-NU-1000

Electronic Energy: -7191.8205137

Enthalpy: -7190.697895

Free Energy: -7190.917192

C	1.68444400	3.94340200	-3.15512400
C	0.64900600	-4.90821500	2.22466000
C	2.37166400	3.70494300	2.55373900
C	0.00185900	-4.64437600	-3.17736700
C	-5.46154800	-3.56981600	3.03742900
C	-4.20581200	5.17836300	-2.39074400
C	-6.09809700	-3.34300200	-2.42689500
C	-3.54708600	4.91457200	3.31260500

C	1.27405300	2.82442400	2.03808100
C	0.75415000	3.00363900	-2.46956100
C	-3.54120500	3.93043200	-1.89896900
C	-5.03718800	-2.44268600	-1.88246900
C	-4.54354100	-2.62138500	2.33664000
C	-0.02841400	-3.67126600	1.74592500
C	-3.03318400	3.71322200	2.58683000
C	-0.52887500	-3.45023500	-2.44887700
H	-1.87509300	-1.87844900	2.78285900
H	1.50863100	1.36003800	-0.24065400
H	-3.66762700	1.60477200	-3.96674800
H	-2.59548100	0.44046500	-3.97480100
H	-2.85167100	1.00392800	4.57205000
H	-6.42748500	0.76785600	-1.59620100
H	-5.86553900	0.37812500	2.69316000
H	-2.58070900	-1.62449600	-2.85982600
H	-4.19635100	2.65685000	0.41669600
H	-0.52250900	0.66368900	-4.56091000
H	-1.05256900	-0.03712800	3.98279700
H	0.42069900	0.54955800	4.01803200
H	2.27215600	-1.61028900	1.87407400
O	-1.76038400	1.25500800	-1.39677200
O	-2.56119900	4.06050500	-1.10895700
O	-2.22677700	3.91664900	1.62941000
O	0.11420100	3.45708400	-1.47269300
O	0.64380300	1.82611200	-2.90425100
O	1.81251000	-0.50666000	-2.37457500
O	-0.05355000	-2.32840600	-2.75737700
O	0.54958300	-2.56844200	1.99386700
O	-1.41962900	-3.63772500	-1.56323000
O	-1.11347400	-3.77728700	1.11499400
O	-4.11350200	-3.00518400	-1.22634200
O	-3.79823300	-3.12046100	1.43948200
O	-4.52031800	-1.41851500	2.70103400
O	-5.10435300	-1.19775400	-2.09980700
O	-3.44834100	-0.57735100	0.18436900
O	-2.38489500	-1.10492400	-2.07361300
O	-1.04458000	0.04951900	-4.03206400
O	-3.55898100	0.67059000	-3.73950600
O	-0.07973000	-0.23891700	3.76230200
O	-0.58111700	-1.22540200	-0.24103600
O	0.61205100	0.98721900	-0.25315700
O	1.23234200	1.62061000	2.40201000
O	2.24087400	-0.69547200	1.55043000
O	0.46326900	3.35466800	1.22072300
O	-5.80128100	1.11984900	-0.95224200
O	-5.43534400	0.89526500	2.00018700
O	-3.55785400	1.94187900	0.31216400
O	-4.00256300	2.81705000	-2.28241200
O	-3.43632500	2.57823100	2.95589100
O	-2.63710200	0.24381000	4.02031700
O	-1.84524300	-1.29976600	2.01447000
O	-1.39715200	1.13827300	1.45114100

Zr	-2.36029900	-2.32789200	-0.04934000
Zr	-0.33510500	-0.12572300	-2.08482200
Zr	-3.76379400	0.58988000	-1.45693600
Zr	-3.32096500	0.45488100	2.05586800
Zr	-1.27058400	2.64420600	0.05114400
Zr	0.10498900	-0.30396900	1.47730300
H	2.11309400	-1.26288700	-1.76939700
Al	5.66282100	-2.08705100	-1.68446000
Al	5.06769900	0.27803100	-2.91321200
Al	3.63528000	-0.73099000	0.17786900
Al	7.05187700	0.24419800	-0.19047600
Al	4.73013500	2.08843900	-1.00550000
Al	6.23542700	-2.54949900	0.93943900
Al	4.85668400	1.85989500	1.68809900
Al	5.75953700	-0.48280800	2.60294000
H	2.88347900	1.10035300	-2.22862800
H	4.92526300	-4.19094800	-0.47627600
H	9.13875600	1.28636100	0.18556200
H	5.59319700	-2.76144400	3.38907000
H	1.87189900	-2.51029600	-0.11036700
H	5.68051400	3.89875800	0.44403100
H	4.66322900	3.94873800	-2.76422700
H	8.01557200	-1.03147500	1.77250600
H	4.44610900	-1.96286400	4.11940600
H	5.07375400	3.30766000	3.64117000
H	7.29783600	-0.96327100	-3.03073000
H	3.57374000	-2.92863700	-2.19239500
H	6.59648100	1.34910100	-4.41294000
H	4.11137600	-2.24624200	-3.47898500
H	3.88063600	-0.42041800	-4.90164600
O	4.48205800	-0.78115200	-1.42916100
O	3.69054600	1.61086600	-2.39938700
O	5.62549000	-3.53740700	-0.55521500
O	8.77626000	0.42026600	-0.00619800
O	6.91656300	-1.54500500	-0.45527700
O	6.16913300	1.13354800	-1.45349800
O	2.64192800	-2.17240500	-0.58512700
O	6.01822000	-3.83880000	2.17380900
O	5.39301300	3.46799900	-2.35403300
O	4.81692000	-1.49548300	1.32851400
O	3.77547500	1.15620100	0.31298600
O	4.97898000	3.24343800	0.38282600
O	6.27553200	0.79590700	1.33835100
O	7.29280400	-1.52971100	2.18859300
O	5.38689900	-1.91438300	3.91114600
O	4.24453000	0.59995900	2.96033300
O	5.62137700	2.85447500	2.99693600
O	6.63072400	0.61790800	3.98857300
O	6.37079200	-1.20603500	-3.13208700
O	5.70087300	1.49991900	-4.10063700
O	4.32611900	-2.98627200	-2.82677300
O	3.83998600	-0.67257000	-3.97361600
H	3.39976000	0.20852500	2.66010100

H	-4.86131400	-4.26167500	3.64335800
H	-6.16776000	-3.05104700	3.69332800
H	-6.00275700	-4.18626500	2.30944300
H	-5.63589400	-4.18089900	-2.96240400
H	-6.65975200	-3.78192500	-1.59158000
H	-6.79189000	-2.81331400	-3.08716900
H	-3.73301700	5.49167300	-3.33291500
H	-5.26717600	5.00478800	-2.59961700
H	-4.07883800	5.99927000	-1.67697100
H	-2.73453500	5.36240900	3.90124000
H	-3.86319300	5.68235700	2.59584200
H	-4.37181300	4.66197300	3.98638700
H	5.65343600	2.80372500	-3.09038800
H	6.78959300	-4.31393800	2.49243000
H	3.08009600	3.90664800	1.73524800
H	1.97808200	4.68259600	2.85810400
H	2.89317800	3.23316500	3.39510500
H	2.38508400	3.40896800	-3.80481500
H	1.10150000	4.65520500	-3.75672500
H	2.22277600	4.54226600	-2.40890900
H	1.04983100	-4.80368500	-2.88779100
H	-0.56959600	-5.55047900	-2.95365000
H	0.00627600	-4.45441100	-4.25740500
H	0.84155200	-4.83857500	3.30271200
H	0.06315100	-5.80674800	2.00944600
H	1.63274500	-4.99259000	1.74252400
H	7.58668200	0.62429800	3.85842200
H	6.32387000	1.55882800	3.74742100
H	2.44079700	-0.54936500	-3.16574300
Ir	-6.89120900	1.81562100	0.71139300
C	-7.63797100	2.82973300	2.39863200
C	-8.26671500	1.57261100	2.25880300
C	-7.22473500	3.64943400	-0.23125000
C	-6.22741500	4.65591600	0.29646700
H	-8.19636500	3.74542900	2.18019600
H	-6.82540900	2.95670800	3.12508300
H	-9.30472900	1.50603200	1.91964000
H	-7.96670700	0.72917400	2.89600500
H	-8.25157800	4.02565500	-0.10908800
H	-7.07001400	3.47807400	-1.30954000
H	-6.36905800	4.87538300	1.36446500
H	-6.31234200	5.61767900	-0.23944400
H	-8.15704500	1.77317100	-0.20114900
H	-5.17679500	4.34022600	0.17002200

Ir(C_2H_5) H@Al_8-NU-1000

Electronic Energy: -7113.2106767

Enthalpy: -7112.146880

Free Energy: -7112.363541

C	1.68444400	3.94340200	-3.15512400

C	0.64900600	-4.90821500	2.22466000
C	2.37166400	3.70494300	2.55373900
C	0.00185900	-4.64437600	-3.17736700
C	-5.46154800	-3.56981600	3.03742900
C	-4.20581200	5.17836300	-2.39074400
C	-6.09809700	-3.34300200	-2.42689500
C	-3.54708600	4.91457200	3.31260500
C	1.27405300	2.82442400	2.03808100
C	0.75415000	3.00363900	-2.46956000
C	-3.54120500	3.93043200	-1.89896900
C	-5.03718800	-2.44268600	-1.88246900
C	-4.54354100	-2.62138500	2.33664000
C	-0.02841400	-3.67126600	1.74592500
C	-3.03318400	3.71322200	2.58683000
C	-0.52887500	-3.45023500	-2.44887700
H	-1.87860800	-1.87475900	2.77872400
H	1.50345800	1.36352000	-0.23686400
H	-3.67159900	1.60816800	-3.98639300
H	-2.58123300	0.45505100	-3.98059900
H	-2.88867600	0.95760500	4.60520600
H	-6.42921500	0.32657300	-1.44029200
H	-5.87984600	0.18936700	2.43400700
H	-2.58018400	-1.61551400	-2.86516400
H	-4.15427500	2.70462900	0.42167800
H	-0.51282300	0.66366400	-4.56054000
H	-1.06888600	-0.03121400	3.98562800
H	0.40945400	0.54990400	4.03058700
H	2.25654100	-1.60869000	1.87447100
O	-1.76015100	1.26001600	-1.40585200
O	-2.55345100	4.06090000	-1.12383200
O	-2.25331800	3.92087200	1.60537700
O	0.11501400	3.45611300	-1.47242800
O	0.64571400	1.82532000	-2.90392100
O	1.81568500	-0.50640100	-2.37141100
O	-0.05135300	-2.32831100	-2.75683900
O	0.54373900	-2.56704900	2.00004400
O	-1.42206200	-3.63367200	-1.56487900
O	-1.11171500	-3.77643200	1.11088200
O	-4.11509000	-3.00008400	-1.22467900
O	-3.78930400	-3.12130500	1.44782900
O	-4.54525900	-1.41253300	2.67958500
O	-5.10399100	-1.19681900	-2.10708100
O	-3.45299800	-0.56727500	0.17956900
O	-2.38451100	-1.09843400	-2.07712400
O	-1.03929300	0.05255900	-4.03237000
O	-3.54683400	0.68033700	-3.74391200
O	-0.09308500	-0.23326600	3.76426200
O	-0.58330500	-1.21971800	-0.24135900
O	0.60626200	0.99215700	-0.25150500
O	1.23069100	1.62090700	2.40057800
O	2.22912800	-0.69342100	1.55142400
O	0.46025400	3.35757100	1.22447800
O	-5.87481600	0.99571600	-1.01415900

O	-5.41930500	0.94392700	2.04766300
O	-3.56976600	1.95009600	0.30154500
O	-4.03764900	2.81373500	-2.24108800
O	-3.42465500	2.58086400	2.96329900
O	-2.63878500	0.23270600	4.02202400
O	-1.85592500	-1.29411800	2.01145400
O	-1.40713800	1.14669200	1.44861900
Zr	-2.35771200	-2.31866500	-0.04339500
Zr	-0.32735200	-0.12566600	-2.08514700
Zr	-3.74540700	0.59425400	-1.46494800
Zr	-3.35480900	0.46826900	2.07115900
Zr	-1.26836900	2.64383800	0.05643500
Zr	0.09261300	-0.29508900	1.48482300
H	2.11523100	-1.26309800	-1.76476400
Al	5.65844300	-2.09000600	-1.67199700
Al	5.07256400	0.27783100	-2.89960300
Al	3.62853800	-0.73100200	0.18604300
Al	7.04880400	0.23605000	-0.17202100
Al	4.73358500	2.08738400	-0.99157900
Al	6.22145000	-2.55720200	0.95302500
Al	4.85280000	1.85517200	1.70205600
Al	5.74611400	-0.49101800	2.61729800
H	2.88800900	1.10377500	-2.21898800
H	4.91143100	-4.19331700	-0.46818400
H	9.13768800	1.27308800	0.20851900
H	5.57078400	-2.77010800	3.40051400
H	1.86305700	-2.50698500	-0.10922000
H	5.68668100	3.89261200	0.46238000
H	4.67687100	3.95093400	-2.74813800
H	8.00336900	-1.04541400	1.79345800
H	4.42371900	-1.96900900	4.12808500
H	5.07084000	3.30273400	3.65663100
H	7.29953400	-0.96882500	-3.01398100
H	3.56987700	-2.92830500	-2.18818100
H	6.60606100	1.34755700	-4.39567700
H	4.11240300	-2.24470600	-3.47210300
H	3.88608900	-0.41303700	-4.89161600
O	4.47916700	-0.78203500	-1.41926100
O	3.69568600	1.61343700	-2.38844600
O	5.61360100	-3.54157400	-0.54469800
O	8.77300200	0.40819500	0.01554400
O	6.90945800	-1.55256000	-0.43876900
O	6.17093000	1.12863000	-1.43661200
O	2.63575600	-2.17180600	-0.58161100
O	5.99619000	-3.84737600	2.18493100
O	5.40318200	3.46600100	-2.33675700
O	4.80490600	-1.49955800	1.33876100
O	3.77315600	1.15617200	0.32296100
O	4.98290900	3.23991600	0.39862100
O	6.26950500	0.78757700	1.35524100
O	7.27768400	-1.54193400	2.20638800
O	5.36525600	-1.92294000	3.92261400
O	4.23282600	0.59552400	2.97060700

O	5.61717100	2.84578900	3.01399500
O	6.61574400	0.60540800	4.00677300
O	6.37195300	-1.20885200	-3.11693100
O	5.71026900	1.49965500	-4.08450500
O	4.32400000	-2.98569900	-2.82036900
O	3.84427700	-0.66811900	-3.96441600
H	3.38792400	0.20689800	2.66711000
H	-4.86346800	-4.30025000	3.59804800
H	-6.13556400	-3.05517800	3.72910000
H	-6.04074400	-4.14560700	2.30480000
H	-5.63328900	-4.16208600	-2.98890300
H	-6.63892000	-3.81015000	-1.59329500
H	-6.80831700	-2.80982200	-3.06658500
H	-3.46083500	5.94443500	-2.63608600
H	-4.85686000	4.98679000	-3.24973900
H	-4.82217100	5.58941800	-1.57940800
H	-2.79677700	5.71237400	3.34173500
H	-4.41333700	5.31012200	2.76261900
H	-3.88311400	4.66186500	4.32345200
H	5.66343000	2.80219800	-3.07373100
H	6.76463000	-4.32619900	2.50511000
H	3.07807200	3.91084600	1.73463800
H	1.97661800	4.68044400	2.86295300
H	2.89560300	3.23105800	3.39240600
H	2.38794500	3.40869100	-3.80148800
H	1.10204200	4.65236800	-3.76061200
H	2.21961100	4.54512700	-2.40901400
H	1.05073500	-4.80185000	-2.89027900
H	-0.56794500	-5.55103400	-2.95170700
H	0.00328300	-4.45508100	-4.25753100
H	0.81601400	-4.84852600	3.30763800
H	0.07460900	-5.80874500	1.98806900
H	1.64424900	-4.97956300	1.76471600
H	7.57236600	0.60853100	3.88153600
H	6.31311600	1.54770700	3.76567700
H	2.44894900	-0.54566000	-3.16004700
Ir	-6.83649200	1.82216600	0.50951300
C	-8.13846500	2.76339600	-0.74551400
C	-7.41893300	3.91798800	-1.42117900
H	-9.00250000	3.13480700	-0.15707200
H	-8.56457300	2.08910600	-1.51181500
H	-6.96982400	4.61500700	-0.69025700
H	-8.08640100	4.53383100	-2.04864000
H	-7.77093700	0.63761200	0.86856000
H	-6.60672800	3.55891700	-2.07224600

TS2@Al_8-NU-1000

Electronic Energy: -7191.8130521

Enthalpy: -7190.692261

Free Energy: -7190.911325

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.87801900	-1.87318600	2.78284500
H	1.50984000	1.36184800	-0.23478400
H	-3.66110200	1.61442600	-3.98166800
H	-2.58001900	0.45483200	-3.98211300
H	-2.88959600	0.97619500	4.58256600
H	-6.36096900	0.34350500	-1.26039500
H	-5.94479600	0.15700600	2.25932700
H	-2.56978600	-1.62035200	-2.86808200
H	-4.18510300	2.65146200	0.41814200
H	-0.50682600	0.66020300	-4.56328600
H	-1.06477700	-0.02913900	3.98075300
H	0.40885800	0.55711800	4.02212200
H	2.26720000	-1.61160500	1.87932500
O	-1.74950500	1.26131100	-1.40711400
O	-2.55584300	4.06430800	-1.11876000
O	-2.22218600	3.91709200	1.63489200
O	0.11411400	3.45719100	-1.47363200
O	0.64876900	1.82503200	-2.90324000
O	1.81794600	-0.50679700	-2.37282100
O	-0.05039300	-2.32918200	-2.75551800
O	0.54502100	-2.56756800	2.00102100
O	-1.42306400	-3.63566900	-1.56629900
O	-1.11011100	-3.77690800	1.10965200
O	-4.11464200	-3.00305700	-1.22583900
O	-3.77830800	-3.12588900	1.46178700
O	-4.56427600	-1.40353200	2.65700800
O	-5.11277900	-1.19709300	-2.09527400
O	-3.44234000	-0.57653200	0.17879000
O	-2.38395100	-1.10093800	-2.07933500
O	-1.03373800	0.04916600	-4.03560800
O	-3.54450800	0.68302200	-3.74833300
O	-0.09016800	-0.23198500	3.76580200
O	-0.57812800	-1.22394500	-0.24043800
O	0.61436300	0.98670400	-0.24995600
O	1.23234700	1.62075700	2.40320400
O	2.23836700	-0.69642800	1.55643800
O	0.46349500	3.35458500	1.22105900

O	-5.78523100	1.05665000	-0.95679900
O	-5.45310600	0.92759700	1.94747900
O	-3.52044800	1.95489200	0.30049400
O	-4.02920800	2.81732800	-2.25304500
O	-3.45800400	2.57985200	2.93956300
O	-2.64774400	0.24046100	4.00970000
O	-1.85254800	-1.29481700	2.01401300
O	-1.39754000	1.13962800	1.45661000
Zr	-2.35461700	-2.32000600	-0.04849800
Zr	-0.32923800	-0.12330800	-2.08534300
Zr	-3.75459600	0.59952700	-1.46899700
Zr	-3.33239100	0.46712000	2.04720200
Zr	-1.27202900	2.64524000	0.05118500
Zr	0.10212600	-0.30022100	1.48239600
H	2.11741200	-1.26234300	-1.76634900
Al	5.66409900	-2.08995900	-1.67312400
Al	5.07478900	0.27650600	-2.90159600
Al	3.63393300	-0.73242900	0.18600900
Al	7.05299000	0.23829900	-0.17513600
Al	4.73510800	2.08610800	-0.99370200
Al	6.23051900	-2.55505000	0.95147500
Al	4.85650700	1.85567200	1.70010200
Al	5.75413100	-0.48874100	2.61520900
H	2.88946300	1.10098800	-2.22147200
H	4.91966600	-4.19254400	-0.46747000
H	9.14000100	1.27817400	0.20473000
H	5.58226800	-2.76760300	3.39941300
H	1.86753200	-2.50685900	-0.10823000
H	5.68680100	3.89382800	0.45853600
H	4.67208600	3.94645000	-2.75153300
H	8.01105700	-1.04035500	1.78927600
H	4.43430500	-1.96744400	4.12630200
H	5.07073800	3.30039000	3.65527600
H	7.30386000	-0.96731100	-3.01390600
H	3.57529400	-2.92905500	-2.18730300
H	6.60911500	1.34719800	-4.39540600
H	4.11719500	-2.24606100	-3.47186700
H	3.89358000	-0.41907100	-4.89404300
O	4.48434500	-0.78299300	-1.41963800
O	3.69771200	1.61035800	-2.39008200
O	5.62201400	-3.54110300	-0.54499000
O	8.77740900	0.41242800	0.01155300
O	6.91632600	-1.55072200	-0.44122000
O	6.17396700	1.12968500	-1.43942900
O	2.64090400	-2.17234400	-0.57995500
O	6.00924900	-3.84518600	2.18438400
O	5.40145900	3.46590300	-2.34033300
O	4.81317800	-1.49913600	1.33796200
O	3.77748400	1.15443400	0.32238000
O	4.98441600	3.23961300	0.39572000
O	6.27506900	0.79008900	1.35275000
O	7.28690300	-1.53793300	2.20368200
O	5.37599200	-1.92070100	3.92162500

O	4.24026700	0.59574800	2.97023200
O	5.61977600	2.84834900	3.01140900
O	6.62442100	0.60970600	4.00336400
O	6.37690700	-1.20906600	-3.11852200
O	5.71220300	1.49836100	-4.08701200
O	4.32928300	-2.98691700	-2.81966300
O	3.84948800	-0.67209100	-3.96641400
H	3.39533700	0.20581700	2.66821000
H	-4.86446200	-4.29534000	3.60536100
H	-6.14296800	-3.05582000	3.72252000
H	-6.03256100	-4.15140300	2.30296200
H	-5.63528200	-4.16575000	-2.98524900
H	-6.64172400	-3.80598400	-1.59266400
H	-6.80594700	-2.80987200	-3.06938000
H	-3.48099000	5.98982000	-2.51900600
H	-4.76054300	5.00534200	-3.31903300
H	-4.92429900	5.50754800	-1.62588600
H	-2.74145400	5.63689700	3.48973800
H	-4.28466000	5.42012200	2.67304800
H	-4.03390200	4.64620400	4.25588400
H	5.66290800	2.80170300	-3.07640500
H	6.78001900	-4.31984500	2.50517400
H	3.08042400	3.90670400	1.73559600
H	1.97788100	4.68243100	2.85836200
H	2.89299300	3.23331400	3.39532000
H	2.39058100	3.40808000	-3.79818500
H	1.10238300	4.64932200	-3.76450600
H	2.21645500	4.54856100	-2.40948400
H	1.05033800	-4.80262500	-2.88915700
H	-0.56858700	-5.55097500	-2.95294300
H	0.00481800	-4.45463500	-4.25747100
H	0.82757400	-4.84431800	3.30551400
H	0.06957400	-5.80791500	1.99724000
H	1.63913800	-4.98529300	1.75459200
H	7.58049100	0.61531700	3.87401800
H	6.31884200	1.55110100	3.76220000
H	2.44844300	-0.54863200	-3.16209900
Ir	-6.61299300	2.14423000	0.67972500
C	-6.80182600	3.49708300	2.26804100
C	-7.86600300	2.56418300	2.28662700
H	-6.96292800	3.44069100	-0.17725000
H	-5.95618200	3.35971000	2.95158500
H	-6.98534000	4.53709600	1.97362600
H	-7.84694600	1.73780700	3.00858900
H	-8.87897400	2.86730000	1.99387300
C	-8.17686700	2.88686500	-0.66375100
H	-8.77037100	1.97617600	-0.47003500
H	-8.77968400	3.71910200	-0.26056500
C	-7.92801500	3.06298800	-2.14820600
H	-8.87652900	3.05618800	-2.70488700
H	-7.42283400	4.01219400	-2.37650400
H	-7.29144000	2.26491600	-2.55060800

$Ir(C_2H_6)$ (C_2H_4)@Al_8-NU-1000
Electronic Energy: -7191.8174964
Enthalpy: -7190.692828
Free Energy: -7190.912907

C	1.68444900	3.94340000	-3.15512000
C	0.64900600	-4.90821400	2.22466300
C	2.37166400	3.70494700	2.55373300
C	0.00185800	-4.64437500	-3.17737000
C	-5.46151900	-3.56982600	3.03745400
C	-4.20580100	5.17837300	-2.39073300
C	-6.09808200	-3.34301000	-2.42691000
C	-3.54710400	4.91457600	3.31258500
C	1.27405400	2.82442400	2.03808100
C	0.75414800	3.00361800	-2.46954200
C	-3.54119800	3.93047000	-1.89898000
C	-5.03724000	-2.44265700	-1.88260600
C	-4.54348900	-2.62143500	2.33676700
C	-0.02842900	-3.67126800	1.74594000
C	-3.03319600	3.71324300	2.58682700
C	-0.52889300	-3.45025000	-2.44888500
H	-1.88192100	-1.87178400	2.78190700
H	1.51133000	1.36084800	-0.23400700
H	-3.65954400	1.61105400	-3.99088000
H	-2.57307600	0.45547300	-3.98434600
H	-2.89398200	0.97228200	4.58104700
H	-6.33419700	0.29771200	-1.20468900
H	-5.96891300	0.13832000	2.18203700
H	-2.56957300	-1.61944600	-2.86887700
H	-4.20064800	2.62893500	0.43505800
H	-0.50092700	0.65916000	-4.56290700
H	-1.06508100	-0.02998300	3.98013400
H	0.40743600	0.55815300	4.02113500
H	2.26896200	-1.61210800	1.88089800
O	-1.74793700	1.26180600	-1.40703900
O	-2.55473900	4.06702400	-1.12099100
O	-2.21984000	3.91771600	1.63709600
O	0.11377100	3.45729800	-1.47387900
O	0.64968400	1.82483800	-2.90275700
O	1.81900400	-0.50684400	-2.37246000
O	-0.04927500	-2.32938700	-2.75450700
O	0.54486600	-2.56740800	2.00179400
O	-1.42410800	-3.63524000	-1.56720800
O	-1.10939700	-3.77650700	1.10866500
O	-4.11535600	-3.00358100	-1.22466100
O	-3.77446000	-3.12754100	1.46612700
O	-4.57151600	-1.40017400	2.64646000
O	-5.11183800	-1.19767400	-2.09578200
O	-3.44782800	-0.57714400	0.17705800
O	-2.38372400	-1.10013400	-2.08001200

O	-1.02917000	0.04836400	-4.03629600
O	-3.53849300	0.68180900	-3.75192800
O	-0.09044800	-0.23199700	3.76567800
O	-0.57905400	-1.22382600	-0.23998100
O	0.61613700	0.98507800	-0.24936100
O	1.23255300	1.62073300	2.40348200
O	2.23978800	-0.69701700	1.55787000
O	0.46352200	3.35412700	1.22081900
O	-5.78752900	1.06021600	-0.97504400
O	-5.47067700	0.93219000	1.94684500
O	-3.51300600	1.95438700	0.29996600
O	-4.02622500	2.81659000	-2.25379500
O	-3.45691800	2.57815800	2.93738100
O	-2.64944400	0.23844000	4.00681000
O	-1.85383000	-1.29397200	2.01271000
O	-1.39629300	1.13821600	1.45762000
Zr	-2.35609700	-2.31921400	-0.04916300
Zr	-0.32839800	-0.12318000	-2.08448900
Zr	-3.75490300	0.60213400	-1.47411800
Zr	-3.32851500	0.46893700	2.04357200
Zr	-1.27344700	2.64677200	0.05105000
Zr	0.10386400	-0.30157700	1.48229500
H	2.11827000	-1.26235100	-1.76597800
Al	5.66557100	-2.08949200	-1.67265800
Al	5.07574500	0.27698900	-2.90085700
Al	3.63515800	-0.73265500	0.18675300
Al	7.05399200	0.23887300	-0.17448300
Al	4.73555800	2.08613500	-0.99269700
Al	6.23216400	-2.55484400	0.95187500
Al	4.85735200	1.85564900	1.70111400
Al	5.75548600	-0.48874100	2.61582800
H	2.89006500	1.10087000	-2.22075100
H	4.92162700	-4.19243300	-0.46727600
H	9.14064700	1.27925000	0.20546100
H	5.58405200	-2.76771800	3.39987300
H	1.86902000	-2.50767400	-0.10738400
H	5.68713000	3.89393200	0.45952300
H	4.67204000	3.94675300	-2.75032900
H	8.01242800	-1.03985200	1.78971900
H	4.43615200	-1.96779900	4.12722300
H	5.07140500	3.30041000	3.65625100
H	7.30519200	-0.96631800	-3.01294700
H	3.57692300	-2.92892000	-2.18746200
H	6.60989600	1.34832700	-4.39426100
H	4.11898900	-2.24552300	-3.47167200
H	3.89530600	-0.41880800	-4.89358600
O	4.48549300	-0.78290400	-1.41895400
O	3.69827500	1.61041200	-2.38914200
O	5.62384200	-3.54083600	-0.54474300
O	8.77840900	0.41341700	0.01199500
O	6.91770700	-1.55015500	-0.44069100
O	6.17467000	1.13015200	-1.43865900
O	2.64189700	-2.17216800	-0.57919100

O	6.01105200	-3.84511100	2.18462900
O	5.40154600	3.46636600	-2.33918300
O	4.81461300	-1.49925800	1.33855300
O	3.77835600	1.15414500	0.32341200
O	4.98485700	3.23958900	0.39678800
O	6.27610600	0.79034800	1.35350500
O	7.28842400	-1.53763300	2.20413900
O	5.37774400	-1.92088800	3.92215700
O	4.24154300	0.59544300	2.97114900
O	5.62050100	2.84836800	3.01242900
O	6.62572700	0.60977500	4.00398300
O	6.37831700	-1.20823500	-3.11790900
O	5.71284400	1.49922000	-4.08613400
O	4.33111100	-2.98650300	-2.81955900
O	3.85095100	-0.67179600	-3.96596500
H	3.39657600	0.20547300	2.66930800
H	-4.86662300	-4.32117200	3.57265700
H	-6.11996000	-3.05985800	3.74751500
H	-6.05959300	-4.12140100	2.30101300
H	-5.63516800	-4.16139300	-2.99160700
H	-6.63680600	-3.81222500	-1.59301100
H	-6.80979900	-2.80839000	-3.06383600
H	-3.46740900	5.95851000	-2.60804100
H	-4.83558700	4.98880200	-3.26624400
H	-4.84611100	5.56676900	-1.58510100
H	-2.73437200	5.62297600	3.51314500
H	-4.26251600	5.43713500	2.66201600
H	-4.05656900	4.64526700	4.24347500
H	5.66312800	2.80232800	-3.07537600
H	6.78172700	-4.32008200	2.50517700
H	3.07992800	3.90759300	1.73539900
H	1.97770700	4.68205700	2.85938600
H	2.89352300	3.23287500	3.39474400
H	2.39022500	3.40813400	-3.79862600
H	1.10253000	4.64995400	-3.76391000
H	2.21700200	4.54792600	-2.40933900
H	1.05061600	-4.80215700	-2.88993200
H	-0.56817700	-5.55113900	-2.95255700
H	0.00398700	-4.45478200	-4.25751300
H	0.82758800	-4.84439400	3.30551100
H	0.06955900	-5.80788300	1.99714900
H	1.63912200	-4.98528100	1.75453900
H	7.58178500	0.61556000	3.87457300
H	6.31993000	1.55113200	3.76299900
H	2.44933500	-0.54876500	-3.16172200
Ir	-6.56358700	2.13358100	0.69635400
C	-6.71745500	3.53025400	2.23729800
C	-7.80936800	2.62579800	2.27974900
C	-8.00583900	3.32893200	-0.87552300
C	-8.77944300	4.58923500	-0.56779000
H	-6.86638300	4.56593300	1.90278500
H	-5.89319600	3.40237000	2.94833200
H	-8.81638200	2.94353400	1.97750000

H	-7.81809700	1.83066100	3.03665000
H	-8.53041800	2.42236100	-0.53825700
H	-7.79454100	3.18768600	-1.94532500
H	-8.96873200	4.70262000	0.50844900
H	-9.75704100	4.58529100	-1.06895800
H	-8.24745200	5.49125500	-0.90174700
H	-6.93188200	3.47603300	-0.46951600

Catalytic Dimerization Mechanism (Figure 4)

TS1@Al_8-NU-1000

Electronic Energy: -7191.7561133
Enthalpy: -7190.637128
Free Energy: -7190.852746

C	1.68444600	3.94340500	-3.15511700
C	0.64900300	-4.90821400	2.22466700
C	2.37165800	3.70495200	2.55373700
C	0.00184800	-4.64437300	-3.17738100
C	-5.46152000	-3.56981800	3.03746300
C	-4.20580200	5.17836900	-2.39074400
C	-6.09811400	-3.34297900	-2.42689700
C	-3.54715000	4.91456600	3.31257000
C	1.27404700	2.82442600	2.03808500
C	0.75415500	3.00363900	-2.46956500
C	-3.54109900	3.93049500	-1.89882300
C	-5.03720900	-2.44261100	-1.88241600
C	-4.54347600	-2.62148200	2.33667600
C	-0.02841200	-3.67131200	1.74597200
C	-3.03325900	3.71320700	2.58661400
C	-0.52888900	-3.45025300	-2.44893800
H	-1.90107800	-1.88795900	2.76651200
H	1.49054900	1.36807000	-0.23540900
H	-3.65220400	1.60919300	-3.99089300
H	-2.57730500	0.44642000	-3.97929800
H	-2.87723900	0.97841900	4.58101400
H	-5.96177100	2.06855000	-1.41243100
H	-5.47041800	1.92444900	2.51834100
H	-2.59304300	-1.63610200	-2.84825300
H	-4.22210100	2.57932700	0.40659800
H	-0.50737300	0.65043600	-4.56626200
H	-1.06802300	-0.03748100	3.97814800
H	0.40567100	0.54889400	4.01828000
H	2.26350000	-1.60938200	1.87338700
O	-1.76453200	1.25346800	-1.41448300
O	-2.55384200	4.05643600	-1.12449100
O	-2.21787800	3.90590300	1.64176800
O	0.11317300	3.45541500	-1.47294200
O	0.64532800	1.82565100	-2.90464700
O	1.81231400	-0.50248900	-2.36333200
O	-0.04666100	-2.32944100	-2.74932000

O	0.54422200	-2.56695500	2.00049500
O	-1.42385700	-3.63736100	-1.56635700
O	-1.10983100	-3.77732000	1.10821400
O	-4.12828800	-3.00945800	-1.20391600
O	-3.78970800	-3.13149400	1.45259800
O	-4.54574500	-1.41085700	2.67066000
O	-5.08469900	-1.20718200	-2.12461100
O	-3.52614200	-0.58751900	0.18686100
O	-2.38714100	-1.11206700	-2.06764000
O	-1.03304600	0.03797100	-4.03895800
O	-3.54003700	0.68043700	-3.74737700
O	-0.09288700	-0.24132400	3.76396200
O	-0.59641700	-1.21953400	-0.23784000
O	0.59634000	0.99003800	-0.24849800
O	1.22954600	1.62114600	2.40579500
O	2.23232200	-0.69439400	1.55022700
O	0.46225600	3.35192700	1.22015600
O	-5.78488800	1.18493700	-1.07298500
O	-5.42680900	1.06862500	2.07651200
O	-3.50207000	1.95167800	0.29839400
O	-4.04064300	2.82159800	-2.25688300
O	-3.47550100	2.58548800	2.94590400
O	-2.64195900	0.24286800	4.00563900
O	-1.86286600	-1.30409400	2.00249200
O	-1.40903600	1.12929200	1.46167700
Zr	-2.36873900	-2.32294400	-0.05099900
Zr	-0.33942700	-0.12721500	-2.08767700
Zr	-3.78358700	0.59356600	-1.47087100
Zr	-3.35014300	0.45593800	2.05047600
Zr	-1.27297000	2.62816400	0.04726300
Zr	0.09459500	-0.30569700	1.48398000
H	2.11125200	-1.26192200	-1.76156100
Al	5.65868400	-2.08623100	-1.67713700
Al	5.06798400	0.28147600	-2.90309500
Al	3.63059400	-0.73031800	0.18390000
Al	7.04892900	0.24042700	-0.17760300
Al	4.73126800	2.08946900	-0.99303900
Al	6.22568500	-2.55388800	0.94719300
Al	4.85406800	1.85649700	1.70011500
Al	5.75092300	-0.48903600	2.61313500
H	2.88464900	1.10522000	-2.21801200
H	4.91314800	-4.18851000	-0.47209900
H	9.13677200	1.27920300	0.20153200
H	5.57878100	-2.76845800	3.39544800
H	1.87231200	-2.51628500	-0.10626600
H	5.68536100	3.89514600	0.45991600
H	4.66721600	3.95181600	-2.74910000
H	8.00721700	-1.04078300	1.78564900
H	4.43169100	-1.96861900	4.12425600
H	5.07007900	3.30027000	3.65622300
H	7.29698800	-0.96091000	-3.01870600
H	3.57082000	-2.92903900	-2.19316900
H	6.59952300	1.35279700	-4.39966800

H	4.11130300	-2.24013600	-3.47528100
H	3.87961700	-0.41096600	-4.89292400
O	4.47913800	-0.77927000	-1.42166200
O	3.69205600	1.61521900	-2.38852600
O	5.61660200	-3.53828900	-0.54984300
O	8.77343600	0.41379600	0.00826200
O	6.91110400	-1.54828500	-0.44487800
O	6.16934700	1.13305400	-1.44065500
O	2.64119300	-2.17573800	-0.58082600
O	6.00370500	-3.84483700	2.17922300
O	5.39656100	3.47023400	-2.33908300
O	4.80879200	-1.49785700	1.33596700
O	3.77423300	1.15680300	0.32257900
O	4.98221900	3.24173300	0.39713000
O	6.27193300	0.79059500	1.35151500
O	7.28305900	-1.53848100	2.19989000
O	5.37316500	-1.92194600	3.91865300
O	4.23706600	0.59575100	2.96940300
O	5.61830400	2.84747700	3.01221200
O	6.62166300	0.60787300	4.00193900
O	6.37005100	-1.20318800	-3.12213600
O	5.70385800	1.50448200	-4.08794600
O	4.32558100	-2.98206800	-2.82496900
O	3.83976100	-0.66584600	-3.96561100
H	3.39176600	0.20749600	2.66672500
H	-4.86227600	-4.25795200	3.64899300
H	-6.17453300	-3.05677200	3.69145800
H	-5.99186700	-4.19581900	2.30849500
H	-5.63543500	-4.11767500	-3.05148300
H	-6.59052400	-3.87069300	-1.59927300
H	-6.84509900	-2.79721300	-3.01241200
H	-5.00190000	5.45023500	-1.68247300
H	-3.50348400	6.01759200	-2.42976100
H	-4.67791700	5.02493900	-3.36718500
H	-2.80414300	5.71917800	3.32685400
H	-4.42664000	5.29922700	2.77593300
H	-3.86423300	4.66613400	4.33098300
H	5.65698500	2.80674400	-3.07616800
H	6.77375500	-4.32173700	2.49841400
H	3.07995500	3.90842000	1.73566700
H	1.97729800	4.68174100	2.85990300
H	2.89330700	3.23245600	3.39459800
H	2.39005800	3.40798300	-3.79858500
H	1.10195400	4.64936000	-3.76405800
H	2.21693500	4.54842700	-2.40969500
H	1.01131700	-4.86689900	-2.80342700
H	-0.62584400	-5.52850400	-3.02790000
H	0.10669200	-4.42300200	-4.24578400
H	0.83481100	-4.84176000	3.30410800
H	0.06625000	-5.80710500	2.00275900
H	1.63592400	-4.98881700	1.74832900
H	7.57778200	0.61281100	3.87290900
H	6.31677000	1.54972800	3.76154800

H	2.44071100	-0.54352700	-3.15436100
Ir	-7.16436500	0.93184200	0.71055500
C	-7.81467400	-0.63232100	-0.49383100
C	-8.21394000	0.68116600	2.45225600
C	-7.05507900	-1.33102600	0.53684700
H	-8.88987200	-0.84147600	-0.53344900
H	-7.34731200	-0.49807900	-1.47399900
C	-7.74378600	-0.69127500	2.27784800
H	-7.74532000	1.24573000	3.26824600
H	-9.29753900	0.83922400	2.41069000
H	-7.41381200	-2.31372800	0.85086900
H	-5.96365700	-1.36131600	0.40481600
H	-6.88450600	-0.99535300	2.88317200
H	-8.54133300	-1.43826900	2.24380700
H	-8.49005800	1.38184700	-0.00200800
H	-7.17019400	2.54121500	0.59080500

Ir(C_4H_8) H_2@Al_8-NU-1000

Electronic Energy: -7191.7981736

Enthalpy: -7190.676452

Free Energy: -7190.894958

C	1.68445400	3.94340300	-3.15511000
C	0.64900700	-4.90821400	2.22466200
C	2.37166400	3.70494700	2.55373300
C	0.00185300	-4.64437900	-3.17736800
C	-5.46149600	-3.56986200	3.03743500
C	-4.20578100	5.17838500	-2.39073000
C	-6.09806700	-3.34303300	-2.42690200
C	-3.54711500	4.91460000	3.31253800
C	1.27403400	2.82441500	2.03809400
C	0.75415700	3.00361600	-2.46956800
C	-3.54111400	3.93052500	-1.89911800
C	-5.03730900	-2.44266800	-1.88269600
C	-4.54348900	-2.62149900	2.33699700
C	-0.02843500	-3.67126400	1.74592900
C	-3.03324000	3.71326100	2.58696800
C	-0.52889400	-3.45021500	-2.44896000
H	-1.88443900	-1.88093100	2.77988800
H	1.50323700	1.36185400	-0.23617400
H	-3.65123900	1.62190200	-3.95678100
H	-2.59070900	0.44667600	-3.97603200
H	-2.84217900	1.03769100	4.54074900
H	-6.41882400	0.84411400	-1.62943800
H	-5.87032500	0.82179800	2.84090200
H	-2.58009000	-1.62719500	-2.85883700
H	-4.20085600	2.64740300	0.39749500
H	-0.51822500	0.66065900	-4.56110600
H	-1.06626900	-0.03642300	3.97830000
H	0.40407100	0.55505300	4.02025800
H	2.26807000	-1.61027800	1.87733400

O	-1.76033600	1.25588400	-1.40024100
O	-2.56607100	4.06153300	-1.10370900
O	-2.23181100	3.91519800	1.62635400
O	0.11168200	3.45710800	-1.47419900
O	0.64607600	1.82529300	-2.90294100
O	1.81253300	-0.50617000	-2.36900800
O	-0.05146100	-2.32872900	-2.75493600
O	0.54653100	-2.56767800	1.99812200
O	-1.42178700	-3.63779300	-1.56512500
O	-1.11122700	-3.77804900	1.11164600
O	-4.11926200	-3.00450700	-1.21739000
O	-3.79241300	-3.12567500	1.44530100
O	-4.52744000	-1.41381100	2.68604800
O	-5.09607500	-1.20167500	-2.11664300
O	-3.45772700	-0.57951100	0.18462600
O	-2.38462300	-1.10631100	-2.07343900
O	-1.04218000	0.04801800	-4.03234400
O	-3.55279700	0.68360300	-3.74144300
O	-0.09266000	-0.23580000	3.76440700
O	-0.58481600	-1.22493500	-0.23887300
O	0.60747400	0.98729300	-0.24970000
O	1.22987900	1.62110000	2.40463400
O	2.23673000	-0.69535000	1.55403100
O	0.46224200	3.35354600	1.22087600
O	-5.79469900	1.08786000	-0.93584900
O	-5.46819600	0.97114100	1.97559300
O	-3.55078200	1.94011400	0.30564300
O	-4.01412600	2.81704300	-2.26914600
O	-3.44322200	2.57861100	2.95281100
O	-2.65695200	0.25377800	4.01164900
O	-1.85002500	-1.30028700	2.01319600
O	-1.40561500	1.13533000	1.45443900
Zr	-2.36343000	-2.33061400	-0.04786500
Zr	-0.33618200	-0.12571100	-2.08372100
Zr	-3.76820000	0.58708700	-1.46143000
Zr	-3.33069000	0.45519000	2.04433100
Zr	-1.27511400	2.64272300	0.04914400
Zr	0.10072500	-0.30510100	1.47922200
H	2.11201100	-1.26301300	-1.76424100
Al	5.66081600	-2.08872700	-1.67744200
Al	5.06816800	0.27685600	-2.90657900
Al	3.63289700	-0.73139000	0.18331400
Al	7.05037300	0.24124500	-0.18225300
Al	4.73057800	2.08717800	-0.99886700
Al	6.23059000	-2.55206000	0.94699100
Al	4.85523000	1.85846700	1.69479000
Al	5.75514700	-0.48507800	2.61022900
H	2.88388600	1.10080300	-2.22327800
H	4.91972100	-4.19155600	-0.46982100
H	9.13758100	1.28190100	0.19530000
H	5.58598200	-2.76359900	3.39611100
H	1.87017900	-2.51186800	-0.10615600
H	5.68234900	3.89643600	0.45106000

H	4.66555200	3.94766100	-2.75750500
H	8.01128200	-1.03570800	1.78162700
H	4.43894200	-1.96388100	4.12521400
H	5.07173000	3.30499600	3.64872000
H	7.29772400	-0.96580300	-3.02218400
H	3.57176400	-2.92933000	-2.18743100
H	6.59885400	1.34704000	-4.40483400
H	4.11084400	-2.24672300	-3.47335000
H	3.88184200	-0.42034500	-4.89573700
O	4.48084200	-0.78198300	-1.42295000
O	3.69159700	1.61049400	-2.39347600
O	5.62112500	-3.53920400	-0.54823700
O	8.77481000	0.41600900	0.00312700
O	6.91388200	-1.54792100	-0.44704900
O	6.16934200	1.13144500	-1.44591600
O	2.64044700	-2.17357800	-0.58017100
O	6.01113800	-3.84133500	2.18106300
O	5.39482400	3.46660500	-2.34674400
O	4.81275800	-1.49686200	1.33509100
O	3.77457600	1.15567000	0.31898400
O	4.98023000	3.24177400	0.38964800
O	6.27350300	0.79321500	1.34622800
O	7.28789000	-1.53346600	2.19719100
O	5.38003800	-1.91641400	3.91810600
O	4.24078200	0.59894100	2.96641300
O	5.61970800	2.85217500	3.00451700
O	6.62625800	0.61471800	3.99659900
O	6.37064300	-1.20805800	-3.12440300
O	5.70304800	1.49842500	-4.09337300
O	4.32475200	-2.98697700	-2.82111200
O	3.84069300	-0.67289100	-3.96784100
H	3.39572400	0.20869000	2.66551400
H	-4.86263400	-4.27725300	3.62632800
H	-6.15632600	-3.05142700	3.70541700
H	-6.01656800	-4.16969700	2.30584000
H	-5.63445000	-4.16131600	-2.99129500
H	-6.63813800	-3.81131700	-1.59347900
H	-6.80860300	-2.80769800	-3.06444400
H	-3.48925300	6.00188500	-2.48200500
H	-4.72786200	5.01188700	-3.33876400
H	-4.95712900	5.48249400	-1.64783900
H	-2.73455300	5.62234200	3.51559800
H	-4.26010700	5.44115000	2.66262900
H	-4.05770300	4.64325600	4.24179000
H	5.65554000	2.80233300	-3.08293800
H	6.78197800	-4.31675900	2.50054800
H	3.07978000	3.90829600	1.73542300
H	1.97732100	4.68182700	2.85961100
H	2.89353700	3.23256200	3.39452800
H	2.38849400	3.40825000	-3.80053700
H	1.10173400	4.65125400	-3.76157900
H	2.21872100	4.54642800	-2.40932200
H	1.04568900	-4.81132100	-2.87714000

H	-0.57689800	-5.54805800	-2.96271400
H	0.01880000	-4.45020200	-4.25648500
H	0.83245200	-4.84246500	3.30458000
H	0.06717100	-5.80736900	2.00138300
H	1.63698100	-4.98790100	1.75044800
H	7.58230500	0.62010900	3.86706700
H	6.32051300	1.55594900	3.75506900
H	2.44108700	-0.54910800	-3.15984900
Ir	-6.80839200	2.01548200	0.74307600
C	-8.15714700	2.13541900	2.35019400
H	-7.30374900	3.26017900	-0.06657200
C	-8.56000500	1.75668900	-0.36398000
H	-6.68409000	3.33442100	1.54235400
C	-9.44494700	1.47044300	1.89214800
H	-7.71066800	1.62592800	3.22408800
H	-8.37566800	3.16267900	2.68445900
C	-9.77270300	1.99070500	0.50626000
H	-8.62545100	2.24123500	-1.35008900
H	-8.41982000	0.66859800	-0.53864800
H	-9.31746000	0.37400100	1.84454100
H	-10.26487100	1.65047200	2.60892800
H	-9.99603500	3.07073900	0.55451000
H	-10.66907900	1.51115600	0.07628800

TS2@Al_8-NU-1000

Electronic Energy: -7191.7869599

Enthalpy: -7190.666440

Free Energy: -7190.883512

C	1.68444600	3.94340500	-3.15511700
C	0.64900300	-4.90821400	2.22466700
C	2.37165800	3.70495200	2.55373700
C	0.00184800	-4.64437300	-3.17738100
C	-5.46152000	-3.56981800	3.03746300
C	-4.20580200	5.17836900	-2.39074400
C	-6.09811400	-3.34297900	-2.42689700
C	-3.54715000	4.91456600	3.31257000
C	1.27404700	2.82442600	2.03808500
C	0.75415500	3.00363900	-2.46956500
C	-3.54109900	3.93049500	-1.89882300
C	-5.03720900	-2.44261100	-1.88241600
C	-4.54347600	-2.62148200	2.33667600
C	-0.02841200	-3.67131200	1.74597200
C	-3.03325900	3.71320700	2.58661400
C	-0.52888900	-3.45025300	-2.44893800
H	-1.87750500	-1.87514400	2.77931900
H	1.50459000	1.36439500	-0.23683600
H	-3.67633200	1.60773600	-3.98707400
H	-2.58666200	0.45591800	-3.98018800
H	-2.88773000	0.96946800	4.59143100
H	-6.33365400	0.33588500	-1.37634500

H	-5.85757400	0.14444400	2.36901300
H	-2.57459000	-1.62226100	-2.86352300
H	-4.14834100	2.66676300	0.40517100
H	-0.51162900	0.66170500	-4.56471700
H	-1.06721000	-0.02983500	3.98192500
H	0.40784400	0.55580000	4.02300800
H	2.26015800	-1.61119800	1.87448700
O	-1.75465600	1.26351500	-1.40986200
O	-2.56122400	4.06782200	-1.11169400
O	-2.23536900	3.92199000	1.62264500
O	0.11441000	3.45801400	-1.47378500
O	0.64719000	1.82575200	-2.90424800
O	1.81289100	-0.50472200	-2.36787300
O	-0.05262000	-2.32865400	-2.75763000
O	0.54511500	-2.56768800	2.00137100
O	-1.42265000	-3.63485000	-1.56557800
O	-1.11097100	-3.77617400	1.11079300
O	-4.11628700	-3.00266700	-1.22387000
O	-3.78417900	-3.12389500	1.45630600
O	-4.55555500	-1.40916400	2.67232500
O	-5.11076500	-1.19972100	-2.10394000
O	-3.45533200	-0.57412100	0.18129400
O	-2.38904000	-1.09959700	-2.07688100
O	-1.03838000	0.05011400	-4.03761600
O	-3.55208400	0.67907900	-3.74782600
O	-0.09120400	-0.23296100	3.76613600
O	-0.57997400	-1.22164700	-0.24078200
O	0.60825800	0.99157600	-0.25054900
O	1.23349000	1.62067400	2.40237600
O	2.23518200	-0.69569000	1.55205800
O	0.46278900	3.35561700	1.22235500
O	-5.80889300	1.06920300	-1.03418700
O	-5.43081500	0.94214600	2.03368100
O	-3.52546100	1.94510100	0.30080900
O	-4.02510100	2.81819800	-2.25369700
O	-3.44298400	2.58118700	2.94904200
O	-2.64231800	0.23712600	4.01585300
O	-1.85497900	-1.29452200	2.01220400
O	-1.39715900	1.14321200	1.45822800
Zr	-2.35669000	-2.31340900	-0.04808400
Zr	-0.33766200	-0.12036500	-2.08612600
Zr	-3.77322000	0.60019100	-1.46826000
Zr	-3.34427700	0.46959000	2.05706400
Zr	-1.26898600	2.63824200	0.05035200
Zr	0.09709100	-0.29747200	1.48358000
H	2.11034500	-1.26278500	-1.76403000
Al	5.65802000	-2.09418800	-1.67491200
Al	5.06992300	0.27201600	-2.90476000
Al	3.62991500	-0.73469800	0.18429900
Al	7.05012900	0.23330800	-0.17880600
Al	4.73418300	2.08238400	-0.99692700
Al	6.22631500	-2.55878100	0.94919900
Al	4.85570400	1.85311500	1.69659700

Al	5.75155300	-0.49157700	2.61200000
H	2.88679100	1.09953100	-2.22289800
H	4.91160300	-4.19405200	-0.46763600
H	9.13691800	1.27203300	0.20180200
H	5.57820700	-2.76970700	3.39718600
H	1.86596200	-2.51196100	-0.10916700
H	5.68827200	3.89026900	0.45381800
H	4.66946800	3.94001500	-2.75644600
H	8.00776000	-1.04444600	1.78563900
H	4.42887800	-1.96844200	4.11980200
H	5.06838100	3.29461400	3.65292700
H	7.29804100	-0.97391700	-3.01629300
H	3.56745400	-2.92981000	-2.18348900
H	6.60596400	1.33954500	-4.39814600
H	4.10776700	-2.24976400	-3.47057700
H	3.88617100	-0.42425100	-4.89511700
O	4.48093400	-0.78503700	-1.42094400
O	3.69545400	1.60805700	-2.39267700
O	5.61622700	-3.54515100	-0.54619200
O	8.77499700	0.40610400	0.00810100
O	6.91248600	-1.55576600	-0.44427400
O	6.17256300	1.12552500	-1.44338200
O	2.63899200	-2.17695700	-0.58113200
O	6.00570500	-3.84841500	2.18295600
O	5.40045800	3.46193600	-2.34519700
O	4.81010000	-1.50168400	1.33570600
O	3.77653800	1.15260500	0.31984100
O	4.98525500	3.23670100	0.39177200
O	6.27397100	0.78669100	1.34956100
O	7.28399200	-1.54187400	2.20095600
O	5.37153800	-1.92279700	3.91916500
O	4.23873000	0.59391100	2.96730200
O	5.61909300	2.84586000	3.00815200
O	6.62368600	0.60679400	3.99960600
O	6.37104800	-1.21526500	-3.12149500
O	5.70890500	1.49236200	-4.09099200
O	4.31996600	-2.99017900	-2.81796700
O	3.84289500	-0.67597200	-3.96713300
H	3.39327100	0.20496700	2.66508600
H	-4.86357600	-4.27029300	3.63552900
H	-6.16321500	-3.05263200	3.69956300
H	-6.00751600	-4.17942800	2.30684100
H	-5.63500200	-4.13990800	-3.02178300
H	-6.61350700	-3.84225500	-1.59587800
H	-6.82767200	-2.80327700	-3.03892200
H	-3.46408100	5.94844700	-2.63246700
H	-4.85334900	4.98448100	-3.25184000
H	-4.82632200	5.58841600	-1.58111500
H	-2.72394600	5.59400300	3.56516400
H	-4.21387000	5.47834500	2.64510400
H	-4.10252300	4.64011600	4.21483100
H	5.66146900	2.79671300	-3.08033100
H	6.77744700	-4.32078900	2.50477800

H	3.08240000	3.90368600	1.73649000
H	1.97873700	4.68380000	2.85505100
H	2.89100700	3.23468100	3.39730600
H	2.38686100	3.40893300	-3.80296400
H	1.10202900	4.65363000	-3.75912200
H	2.22113400	4.54393800	-2.40902100
H	1.05331200	-4.79729500	-2.89744100
H	-0.56323100	-5.55268000	-2.94627100
H	-0.00475400	-4.45770600	-4.25805500
H	0.82233300	-4.84631200	3.30652700
H	0.07195700	-5.80840300	1.99299800
H	1.64151400	-4.98283500	1.75924000
H	7.57935600	0.61213400	3.86727900
H	6.31791200	1.54808800	3.75810200
H	2.43989700	-0.54961100	-3.15898300
Ir	-6.92357600	1.95606500	0.67181600
C	-8.16713500	2.48295500	2.24022000
C	-8.53865900	2.62470900	-0.45974000
H	-7.86140800	0.57985000	0.94518300
C	-8.83227300	1.40237500	1.52199400
H	-7.77625500	2.27272700	3.24298100
H	-8.62959300	3.47340500	2.15752400
C	-9.61808700	1.84968100	0.29970000
H	-8.68532000	3.71498100	-0.41671900
H	-8.44685800	2.33627000	-1.51831000
H	-9.17031300	0.50951500	2.07440000
H	-10.51533200	2.42396600	0.58589000
H	-9.97240700	0.97673200	-0.26852700
H	-5.93603200	3.35513800	0.86930500
H	-6.13202200	3.33774400	-0.00318800

Ir(butane) H@Al_8-NU-1000

Electronic Energy: -7191.8182806

Enthalpy: -7190.692855

Free Energy: -7190.912025

C	1.68444400	3.94340200	-3.15512400
C	0.64900600	-4.90821500	2.22466000
C	2.37166400	3.70494300	2.55373900
C	0.00185900	-4.64437600	-3.17736700
C	-5.46154800	-3.56981600	3.03742900
C	-4.20581200	5.17836300	-2.39074400
C	-6.09809700	-3.34300200	-2.42689500
C	-3.54708600	4.91457200	3.31260500
C	1.27405300	2.82442400	2.03808100
C	0.75415000	3.00363900	-2.46956000
C	-3.54120500	3.93043200	-1.89896900
C	-5.03718800	-2.44268600	-1.88246900
C	-4.54354100	-2.62138500	2.33664000
C	-0.02841400	-3.67126600	1.74592500
C	-3.03318400	3.71322200	2.58683000

C	-0.52887500	-3.45023500	-2.44887700
H	-1.89473200	-1.87436600	2.76788800
H	1.50376000	1.36142600	-0.23718900
H	-3.73923500	1.55392700	-4.09809900
H	-2.59539600	0.45190100	-4.03581000
H	-2.86123400	0.91442300	4.66868300
H	-6.41024700	0.40151900	-2.00526000
H	-5.83906400	0.15095900	2.95418400
H	-2.60456000	-1.61382900	-2.84228600
H	-4.04266900	2.87796500	0.38938900
H	-0.50579000	0.65936800	-4.56852400
H	-1.02568100	-0.05309100	4.01304500
H	0.45055200	0.53126800	4.02878600
H	2.25167300	-1.60474700	1.86854800
O	-1.76772200	1.28111700	-1.39505900
O	-2.59696400	4.06089800	-1.06183000
O	-2.27771900	3.91557900	1.58594700
O	0.11589300	3.46183200	-1.47230900
O	0.64095700	1.82693400	-2.90126400
O	1.79562500	-0.50009000	-2.36265400
O	-0.05962900	-2.32529000	-2.76109200
O	0.54698400	-2.56571600	1.99548900
O	-1.42701600	-3.62418200	-1.56440600
O	-1.11688100	-3.76584100	1.11577200
O	-4.12578900	-2.98879500	-1.19460300
O	-3.79450900	-3.10816500	1.43685600
O	-4.51169700	-1.42723900	2.72223200
O	-5.09012400	-1.21230300	-2.14591800
O	-3.55515000	-0.52244200	0.20396200
O	-2.40746600	-1.07753700	-2.06700200
O	-1.04111300	0.05965900	-4.03641700
O	-3.56896300	0.64430900	-3.81837800
O	-0.05744900	-0.24897300	3.76346500
O	-0.61229500	-1.20017100	-0.23711900
O	0.60280300	0.99802500	-0.24908000
O	1.22706300	1.62156100	2.40092200
O	2.22474600	-0.68985100	1.54355700
O	0.46393100	3.35851900	1.22082600
O	-5.92051100	1.13092600	-1.60309800
O	-5.44767600	0.92043400	2.52043900
O	-3.73001900	1.96716400	0.32736500
O	-3.95890600	2.81803600	-2.31962200
O	-3.38170800	2.57614300	2.99331500
O	-2.59451100	0.21079800	4.06656500
O	-1.86278200	-1.27780800	2.01274700
O	-1.41432100	1.15997800	1.45386400
Zr	-2.38402100	-2.29398400	-0.04486300
Zr	-0.34934100	-0.11111300	-2.08738400
Zr	-3.79893900	0.62209500	-1.54380200
Zr	-3.32660100	0.47075800	2.13260400
Zr	-1.25397800	2.64538500	0.04458500
Zr	0.09396600	-0.28977700	1.48268800
H	2.09212400	-1.26153500	-1.76105600

Al	5.63961600	-2.09510100	-1.69101100
Al	5.05120700	0.27322200	-2.91789300
Al	3.62279300	-0.73186700	0.17450500
Al	7.04034700	0.23091800	-0.19752800
Al	4.72552000	2.08527500	-1.00880100
Al	6.21447400	-2.55985000	0.93267200
Al	4.85269300	1.85469900	1.68445800
Al	5.74958700	-0.49152700	2.59788200
H	2.87499800	1.10071500	-2.22334200
H	4.89861100	-4.19859400	-0.48220700
H	9.13355400	1.26241000	0.17907900
H	5.57686600	-2.76993600	3.38410800
H	1.86203500	-2.51781300	-0.10429400
H	5.68079500	3.89169700	0.44183300
H	4.66932600	3.95111100	-2.76591500
H	8.00256600	-1.04855500	1.76304100
H	4.43559700	-1.96772500	4.12046500
H	5.08082000	3.30497700	3.63711400
H	7.27485000	-0.97825900	-3.04584800
H	3.54635600	-2.93170300	-2.19224900
H	6.57625500	1.33817400	-4.42747600
H	4.08084600	-2.24859300	-3.48014400
H	3.84743500	-0.41922800	-4.90037400
O	4.46417500	-0.78400000	-1.43358800
O	3.67996500	1.61228500	-2.39974000
O	5.59867400	-3.54491900	-0.56141100
O	8.76499400	0.39888600	-0.01261300
O	6.89606200	-1.55724300	-0.46340400
O	6.15872300	1.12373500	-1.45906900
O	2.62544400	-2.17395000	-0.58522300
O	5.99258500	-3.84768700	2.16726700
O	5.39345400	3.46088900	-2.35708800
O	4.80019100	-1.50017400	1.32502300
O	3.76569200	1.15582400	0.31015400
O	4.97675500	3.23899900	0.37994400
O	6.26590100	0.78559900	1.33155200
O	7.27746800	-1.54336000	2.17931600
O	5.37513800	-1.92168900	3.90626500
O	4.23706200	0.59636900	2.95699300
O	5.62238700	2.84602500	2.99193900
O	6.62487100	0.60601300	3.98216500
O	6.34580000	-1.21588700	-3.14051100
O	5.68462400	1.49320700	-4.10604200
O	4.29624700	-2.98959800	-2.82970100
O	3.81239100	-0.67125700	-3.97203900
H	3.39221400	0.20617700	2.65649400
H	-4.91544100	-4.02423900	3.87585400
H	-6.33308400	-3.05321600	3.45337500
H	-5.77592400	-4.38230800	2.37389800
H	-5.67415400	-4.31337700	-2.70681100
H	-6.83881500	-3.53363800	-1.63726200
H	-6.61752000	-2.88881900	-3.27678200
H	-3.48681900	5.78652800	-2.95594900

H	-5.07190200	4.95359700	-3.02054900
H	-4.51637800	5.79041300	-1.53412500
H	-2.70879700	5.52664700	3.67004400
H	-4.11124700	5.54819800	2.61437800
H	-4.18995200	4.63531600	4.15286600
H	5.64827800	2.79640100	-3.09526100
H	6.76002100	-4.33178600	2.48186500
H	3.07686100	3.91092000	1.73353700
H	1.97624300	4.68033100	2.86270400
H	2.89672000	3.23150900	3.39191500
H	2.37926600	3.41047500	-3.81209500
H	1.10065100	4.66200300	-3.74767500
H	2.22943000	4.53438300	-2.40758000
H	1.08481500	-4.72076000	-3.01234000
H	-0.48323500	-5.57164700	-2.85770600
H	-0.13449400	-4.50577200	-4.25722700
H	0.80857600	-4.85032700	3.30885300
H	0.07716800	-5.80899400	1.98294200
H	1.64706300	-4.97614900	1.77063400
H	7.58141200	0.60776300	3.85619000
H	6.32271400	1.54842800	3.74173300
H	2.42229800	-0.54532900	-3.15646100
Ir	-5.78060900	0.81884700	0.46840600
C	-7.05420600	2.40233800	0.66403100
C	-6.30112000	3.71748200	0.65472400
H	-7.58820000	2.25267800	1.61600800
H	-7.78538300	2.36426600	-0.16021200
H	-7.02794800	-0.13811600	0.53045800
H	-5.73717900	3.79740800	-0.29310700
C	-7.17449300	4.96332600	0.79640600
H	-6.53708700	5.85750200	0.68127500
H	-7.88546900	5.00246800	-0.04719100
C	-7.92755800	5.04576200	2.10917600
H	-8.48280600	5.98934900	2.20195700
H	-8.65646400	4.23023600	2.21804300
H	-7.24413900	4.98044300	2.97020900
H	-5.56257600	3.71549000	1.48029100

TS3@Al_8-NU-1000

Electronic Energy: -7191.8132798

Enthalpy: -7190.691359

Free Energy: -7190.909096

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600

C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.89084700	-1.87497700	2.77593500
H	1.49708900	1.36588000	-0.23400600
H	-3.61524700	1.63548600	-3.94211700
H	-2.57931100	0.44269800	-3.97767400
H	-2.89292300	0.98146000	4.58974300
H	-6.30517500	1.45374600	-1.86430100
H	-5.89874200	0.12999500	2.27931200
H	-2.58278000	-1.62734100	-2.86083400
H	-4.23242600	2.62101000	0.38519700
H	-0.50823600	0.65400000	-4.56252800
H	-1.08261100	-0.02673200	3.98134700
H	0.39416500	0.55612300	4.02729000
H	2.25186400	-1.60857500	1.87869000
O	-1.76207000	1.25269000	-1.41031500
O	-2.56397200	4.05775000	-1.10922300
O	-2.22195000	3.91764400	1.63478600
O	0.10839500	3.45610600	-1.47647200
O	0.65001800	1.82402000	-2.90208900
O	1.82036900	-0.50606500	-2.36529600
O	-0.04412100	-2.32981200	-2.74842000
O	0.53943300	-2.56613400	2.00549600
O	-1.42376400	-3.63769100	-1.56762900
O	-1.10948900	-3.77779700	1.10734700
O	-4.12294900	-3.00644900	-1.20929200
O	-3.78049000	-3.11456100	1.45424500
O	-4.56473000	-1.40998200	2.67497600
O	-5.08356100	-1.20183300	-2.11796200
O	-3.47143800	-0.57866100	0.17490200
O	-2.37740200	-1.10923700	-2.07610400
O	-1.03176900	0.04138000	-4.03325700
O	-3.53813800	0.69166500	-3.74180600
O	-0.10653200	-0.23006200	3.76584200
O	-0.58764200	-1.22126600	-0.23870100
O	0.60191700	0.99034700	-0.24961600
O	1.22566100	1.62247400	2.40699500
O	2.22526600	-0.69336700	1.55545600
O	0.46485200	3.35418200	1.21809700
O	-5.85893200	1.18746100	-1.05066100
O	-5.44287200	0.91296400	1.94668100
O	-3.54645900	1.94731400	0.29802800
O	-4.02079500	2.81743900	-2.27080500
O	-3.45191100	2.58128000	2.94588800
O	-2.65679300	0.24444700	4.01637200
O	-1.86524300	-1.29289200	2.00985300
O	-1.41321800	1.14063500	1.44803000

Zr	-2.36171600	-2.32683200	-0.05044800
Zr	-0.32609500	-0.12913500	-2.08437700
Zr	-3.74679900	0.58128600	-1.45844800
Zr	-3.36183800	0.46771900	2.05835900
Zr	-1.27565200	2.64152100	0.05459500
Zr	0.08743900	-0.29742200	1.48558500
H	2.11851500	-1.26386500	-1.75984100
Al	5.65953100	-2.09182300	-1.66124100
Al	5.07835300	0.27729800	-2.88836900
Al	3.62700600	-0.73248200	0.19361000
Al	7.04932900	0.23115600	-0.15696100
Al	4.73767700	2.08549600	-0.97958100
Al	6.21592000	-2.56206300	0.96472900
Al	4.85232500	1.85110600	1.71398100
Al	5.74019300	-0.49664300	2.62955100
H	2.89292900	1.10501700	-2.21145700
H	4.90434300	-4.19271600	-0.45934900
H	9.13808000	1.26659200	0.22614300
H	5.55977200	-2.77594500	3.41063400
H	1.86297200	-2.50952200	-0.10539300
H	5.69298700	3.88788800	0.47673500
H	4.68417700	3.94976300	-2.73474000
H	7.99810700	-1.05375500	1.81004500
H	4.41156600	-1.97366500	4.13467900
H	5.06539300	3.29351000	3.67165500
H	7.30517900	-0.96948500	-2.99650600
H	3.57255400	-2.93209200	-2.18794600
H	6.61701400	1.34718600	-4.37838500
H	4.12014600	-2.24277800	-3.46679200
H	3.89691000	-0.41075400	-4.88374200
O	4.48109900	-0.78305600	-1.40990300
O	3.70185200	1.61351800	-2.37877700
O	5.60967800	-3.54425400	-0.53482000
O	8.77365200	0.40177700	0.03230800
O	6.90876000	-1.55730500	-0.42470000
O	6.17515800	1.12590700	-1.42256700
O	2.63701800	-2.17461900	-0.57569100
O	5.98645600	-3.85305100	2.19525300
O	5.41026200	3.46496100	-2.32278800
O	4.80055400	-1.50265000	1.34853700
O	3.77513600	1.15459400	0.33269900
O	4.98822900	3.23643900	0.41178400
O	6.26902200	0.78218900	1.36999700
O	7.27132700	-1.54981100	2.22151000
O	5.35404600	-1.92907400	3.93313700
O	4.22789200	0.59164600	2.98059400
O	5.61455300	2.83996100	3.02897800
O	6.60892300	0.59759700	4.02165600
O	6.37807800	-1.20965700	-3.10338300
O	5.72002600	1.49971500	-4.07086700
O	4.33031600	-2.98516400	-2.81585600
O	3.85281100	-0.66705900	-3.95700100
H	3.38290400	0.20489800	2.67474600

H	-5.33056900	-3.48290200	4.12360800
H	-6.50533400	-3.29747600	2.83049500
H	-5.29214200	-4.60330100	2.72220800
H	-6.81046500	-2.80565000	-3.06046000
H	-5.63371100	-4.15866100	-2.99450500
H	-6.63552300	-3.81366600	-1.59342300
H	-3.52076200	6.03221700	-2.37286900
H	-4.62622100	5.04053700	-3.39294400
H	-5.04550300	5.40880500	-1.71895200
H	-4.07912500	5.56702900	2.60700500
H	-4.21740000	4.64133800	4.13378000
H	-2.70960900	5.50894000	3.70084800
H	5.67127600	2.80130200	-3.05969900
H	6.75392100	-4.33247800	2.51684400
H	3.08116800	3.90705300	1.73643800
H	1.97702600	4.68214100	2.85818200
H	2.89202800	3.23348800	3.39600500
H	2.39739200	3.40670000	-3.78941800
H	1.10265700	4.64098500	-3.77429800
H	2.20818400	4.55728100	-2.41081600
H	1.00733200	-4.87248400	-2.79599800
H	-0.63063900	-5.52622200	-3.03473600
H	0.11584900	-4.42075700	-4.24433600
H	0.80541900	-4.85311600	3.30950800
H	0.07929300	-5.80924400	1.97890400
H	1.64887000	-4.97446100	1.77403700
H	7.56552100	0.60001600	3.89618400
H	6.30739300	1.54029200	3.78032900
H	2.45368100	-0.54489600	-3.15313900
Ir	-6.83474300	1.96089400	0.51625500
C	-6.60705400	3.63475800	1.64127100
H	-8.01912500	1.87987000	1.71637400
H	-7.82491300	2.69924600	-0.48164200
H	-5.67700100	3.59577300	2.22185600
H	-6.76911500	4.59466400	1.13212100
C	-7.77387200	3.00125200	2.25386700
H	-7.57201000	2.58011800	3.25352000
C	-9.11981500	3.69735700	2.16221800
H	-9.11131100	4.52710100	2.88901400
H	-9.20365200	4.16707200	1.16953400
C	-10.30439800	2.78965000	2.41541400
H	-10.24548900	2.30846600	3.40324400
H	-11.25466500	3.33773100	2.37647300
H	-10.35986800	1.98853700	1.66250700

Ir(1-butene) H_2@Al_8-NU-1000

Electronic Energy: -7191.8348741

Enthalpy: -7190.713697

Free Energy: -7190.933624

C	1.68444800	3.94339900	-3.15512300
C	0.64900600	-4.90821400	2.22466300

C	2.37166500	3.70494700	2.55373000
C	0.00186000	-4.64437500	-3.17736900
C	-5.46153100	-3.56981600	3.03745200
C	-4.20580800	5.17837300	-2.39072600
C	-6.09807600	-3.34301500	-2.42691400
C	-3.54710000	4.91457400	3.31259200
C	1.27406200	2.82442600	2.03808800
C	0.75414400	3.00361200	-2.46952700
C	-3.54123100	3.93045700	-1.89896300
C	-5.03725200	-2.44266700	-1.88262400
C	-4.54347700	-2.62141800	2.33672800
C	-0.02842200	-3.67126000	1.74594600
C	-3.03316500	3.71325500	2.58681700
C	-0.52889600	-3.45026100	-2.44886700
H	-1.88309700	-1.87720800	2.77945200
H	1.50561600	1.36230100	-0.23648600
H	-3.66962200	1.60522600	-3.99444900
H	-2.58039000	0.45224300	-3.98428600
H	-2.86353700	1.01671300	4.54987000
H	-6.37847900	0.37342200	-1.31121600
H	-5.94671200	0.55882700	2.67667200
H	-2.57248000	-1.62244800	-2.86896100
H	-4.15282200	2.69277900	0.41350600
H	-0.50879700	0.66175500	-4.56380700
H	-1.06958300	-0.03333900	3.97656300
H	0.40253900	0.55567600	4.02150500
H	2.26746800	-1.61065700	1.87578400
O	-1.75587500	1.26063500	-1.40594500
O	-2.55837500	4.06504300	-1.11612500
O	-2.23668300	3.91610200	1.62074700
O	0.11395000	3.45731100	-1.47329500
O	0.64683100	1.82543900	-2.90334400
O	1.81366300	-0.50636400	-2.37117400
O	-0.05310000	-2.32853500	-2.75744700
O	0.54665000	-2.56761900	1.99810000
O	-1.42104800	-3.63642800	-1.56435400
O	-1.11161500	-3.77699500	1.11203500
O	-4.11073100	-3.00344200	-1.23271600
O	-3.79610200	-3.12220300	1.44082400
O	-4.53209600	-1.41291000	2.68463400
O	-5.11330400	-1.19685100	-2.09489800
O	-3.44233300	-0.57239000	0.17583700
O	-2.38639000	-1.10115500	-2.08147000
O	-1.03626700	0.05076700	-4.03662900
O	-3.54634500	0.67739300	-3.75122400
O	-0.09492300	-0.23382300	3.76330000
O	-0.58066300	-1.22408000	-0.24183500
O	0.60921800	0.98908300	-0.25044600
O	1.23142100	1.62068100	2.40271500
O	2.23699700	-0.69551900	1.55289000
O	0.46163100	3.35466200	1.22231100
O	-5.79486300	1.06045300	-0.96475000
O	-5.46022600	0.92839500	1.93142200

O	-3.54385500	1.95077900	0.30114100
O	-4.02372500	2.81600600	-2.25694300
O	-3.44483300	2.57913400	2.94995400
O	-2.65676300	0.24734100	4.00766500
O	-1.85109800	-1.29880700	2.01091900
O	-1.40255300	1.13714400	1.45400000
Zr	-2.35916600	-2.32409400	-0.04910000
Zr	-0.33380200	-0.12387100	-2.08582700
Zr	-3.76341200	0.59609300	-1.47443800
Zr	-3.33513600	0.45789500	2.04185100
Zr	-1.27050800	2.64119000	0.04989200
Zr	0.10100300	-0.30327700	1.47965900
H	2.11332200	-1.26271600	-1.76557600
Al	5.66133800	-2.08909700	-1.67811600
Al	5.06992400	0.27692600	-2.90677900
Al	3.63310700	-0.73155200	0.18236600
Al	7.05106700	0.24015400	-0.18200200
Al	4.73204000	2.08704500	-0.99893700
Al	6.23031600	-2.55308800	0.94627900
Al	4.85564600	1.85760100	1.69471100
Al	5.75485300	-0.48635300	2.60984900
H	2.88564700	1.10105600	-2.22379600
H	4.91935000	-4.19201100	-0.47115800
H	9.13853300	1.28017500	0.19634000
H	5.58492400	-2.76503800	3.39510800
H	1.86866700	-2.50962800	-0.10873500
H	5.68354000	3.89573900	0.45191100
H	4.66852900	3.94780800	-2.75727100
H	8.01123000	-1.03740100	1.78181000
H	4.43781100	-1.96524000	4.12400000
H	5.07229900	3.30410900	3.64877000
H	7.29898600	-0.96656900	-3.02229700
H	3.57223100	-2.92889900	-2.18894000
H	6.60139300	1.34705700	-4.40424200
H	4.11192300	-2.24624800	-3.47459400
H	3.88383200	-0.41954200	-4.89648500
O	4.48153000	-0.78215400	-1.42380100
O	3.69324300	1.61088300	-2.39398800
O	5.62088800	-3.53977800	-0.54932600
O	8.77546200	0.41448100	0.00385700
O	6.91425200	-1.54888500	-0.44741800
O	6.17058100	1.13086000	-1.44575100
O	2.64015400	-2.17290700	-0.58193600
O	6.01030800	-3.84261400	2.17993800
O	5.39756400	3.46649700	-2.34640000
O	4.81269800	-1.49756200	1.33403400
O	3.77519800	1.15547800	0.31822400
O	4.98126800	3.24129500	0.38988300
O	6.27376600	0.79215500	1.34619800
O	7.28745500	-1.53495800	2.19693900
O	5.37898200	-1.91791200	3.91718000
O	4.24068800	0.59795300	2.96581600
O	5.62011700	2.85088600	3.00471800

O	6.62582400	0.61287400	3.99672600
O	6.37180000	-1.20834200	-3.12470700
O	5.70543800	1.49852300	-4.09324100
O	4.32527600	-2.98675000	-2.82250100
O	3.84232100	-0.67216400	-3.96862500
H	3.39556500	0.20787900	2.66482500
H	-4.86459000	-4.31940500	3.57323500
H	-6.11724200	-3.05827500	3.74873300
H	-6.06192300	-4.12262000	2.30409700
H	-5.63497700	-4.16434100	-2.98700800
H	-6.64023700	-3.80721000	-1.59242500
H	-6.80739000	-2.80933500	-3.06725700
H	-3.45973500	5.91698900	-2.70799900
H	-4.91111600	4.97522700	-3.20341400
H	-4.75459800	5.63431200	-1.55431100
H	-2.78982100	5.70496200	3.35829100
H	-4.40045700	5.31890600	2.74889600
H	-3.90215400	4.65992700	4.31654900
H	5.65816900	2.80217100	-3.08262900
H	6.78095000	-4.31831000	2.49949600
H	3.07978100	3.90795100	1.73532300
H	1.97748000	4.68190700	2.85948800
H	2.89361800	3.23258300	3.39448900
H	2.38725500	3.40863900	-3.80222100
H	1.10199500	4.65306000	-3.75975200
H	2.22034800	4.54459000	-2.40902700
H	1.05041600	-4.80266900	-2.88941900
H	-0.56851000	-5.55091700	-2.95260200
H	0.00448700	-4.45474700	-4.25747800
H	0.83231700	-4.84235000	3.30458900
H	0.06718800	-5.80740100	2.00143700
H	1.63698500	-4.98789000	1.75048900
H	7.58192900	0.61813600	3.86762700
H	6.32036400	1.55423900	3.75543100
H	2.44319500	-0.54859400	-3.16144800
Ir	-6.66001400	2.11555400	0.68914500
C	-8.21658800	2.66032800	-0.60052500
C	-7.21992800	3.66712300	-0.63081100
H	-9.17478600	2.86021300	-0.10710500
H	-8.27965200	1.93134600	-1.41745900
H	-6.49223600	3.60832700	-1.45598700
H	-6.72409200	3.28264300	1.73791300
C	-7.44176800	5.05399800	-0.09360500
H	-8.13326500	5.00820600	0.76447600
H	-7.69097600	2.30702700	1.85537400
C	-7.99154500	5.99964300	-1.14943000
H	-8.13530500	7.01422600	-0.75308700
H	-7.31841100	6.07773500	-2.01616300
H	-8.96300500	5.65069800	-1.52879100
H	-6.49479000	5.45436900	0.31135200

Table S4. XYZ Cartesian Coordinates of All Optimized Structures on the NU-1000 Support (All Energies Are in Hartree).

NU-1000

Electronic Energy: -3323.3052019
Enthalpy: -3322.672584
Free Energy: -3322.807208

C	4.31818800	2.42872700	3.42363400
C	-4.37565600	3.54230300	-2.15131200
C	4.30989200	3.54630100	-2.26423800
C	-4.34411200	2.52671000	3.32396300
C	-4.31378500	-2.56037200	-3.32528100
C	4.34707500	-3.50753900	2.28940900
C	-4.34435700	-3.58264100	2.15493800
C	4.35596000	-2.38179500	-3.42138300
Zr	-2.51866300	0.01125000	0.00601300
Zr	0.01514500	1.32927200	2.11852800
Zr	-0.01421000	-2.15596300	1.35369300
Zr	0.01878100	-1.33477500	-2.06591400
Zr	2.52488200	0.01423900	0.00796000
Zr	-0.01878500	2.16588200	-1.40333300
O	1.06001000	-0.32626600	1.42033500
O	3.59813600	-1.64141300	1.06465100
O	3.59902400	-1.04417100	-1.64445000
O	3.59010300	1.04313500	1.66745300
O	2.03901200	1.89690300	3.04070300
O	-0.04845000	3.62751300	2.02688000
O	-2.05044600	2.13667400	2.84219500
O	-2.09460200	3.04428100	-1.80966400
O	-3.60504500	1.06628800	1.63611800
O	-3.62924200	1.59498800	-1.05723400
O	-3.59580300	-1.65713600	1.03450000
O	-3.57929300	-1.12399500	-1.61999300
O	-2.01506500	-2.10540600	-2.89380300
O	-2.05192400	-3.05416500	1.86884800
O	-1.05789600	-1.46192300	-0.30873200
O	-1.38939300	-0.44822200	2.02631800
O	-0.03572400	0.52547600	4.05637000
O	0.05859400	-2.04865600	3.64303100
O	-0.05693400	2.10641000	-3.51760200
O	-1.06691600	1.40248400	0.29767300
O	1.38814300	2.01447300	0.42426300
O	2.04554000	2.89601400	-2.09251500
O	0.01991300	4.07540800	-0.53519200
O	3.59455100	1.63673600	-1.07507800
O	0.03893000	-4.08522400	0.53640000
O	-0.03583100	-3.64064600	-2.03712800
O	1.39441500	-2.04584300	-0.42886500
O	2.06104400	-2.87497900	2.13191600

O	2.05880400	-1.84570800	-3.06232000
O	0.07443900	-0.38287900	-4.13330900
O	-1.39177900	0.40580600	-2.02918800
O	1.05913700	0.28908100	-1.42631600
C	3.23220500	2.62024900	-1.79129200
C	3.23283600	1.72911200	2.66888900
C	3.25156500	-2.60448800	1.80674200
C	-3.24717500	-2.70013000	1.65262600
C	-3.22080000	-1.87957600	-2.55935500
C	-3.27905000	2.66315100	-1.64653900
C	3.25702800	-1.69512500	-2.66749900
C	-3.24639400	1.86377300	2.55112300
H	-1.94294700	0.57446400	-2.79961200
H	1.93208400	2.79567400	0.56297300
H	0.93813200	-2.36681100	3.88804400
H	0.03488900	-1.06464100	3.91231000
H	0.93819500	-0.57406800	-4.52092500
H	-0.03019500	-3.92940500	-1.06031100
H	-0.65973300	-4.65438200	0.87738500
H	-0.90672100	-3.88158600	-2.38089700
H	-1.94705400	-0.56990300	2.80092000
H	1.93339100	-2.83012400	-0.57033200
H	0.65663700	0.87466200	4.62795600
H	0.63304600	2.65725600	-3.90332900
H	-0.92000400	3.87351800	2.36453400
H	-0.66941600	4.65637500	-0.87405200
H	-0.04253900	3.90416400	1.04407000
H	0.04284800	0.64160700	-3.99104200
H	-3.95765200	3.16014200	4.12841600
H	-4.95849200	3.12928400	2.64201100
H	-5.01259200	1.76503800	3.74458300
H	-4.00240300	4.28790600	-2.86026500
H	-5.17230500	2.94505400	-2.61015300
H	-4.83193500	4.06678400	-1.30005700
H	4.57237300	3.35293600	2.88587100
H	3.99952900	2.70597200	4.43381700
H	5.22834300	1.81989500	3.45824600
H	5.24929400	3.01037100	-2.43886400
H	4.00397800	4.09399900	-3.16179800
H	4.50041400	4.28723100	-1.47499700
H	5.26928200	-2.94470600	2.46980900
H	4.05102500	-4.06429600	3.18481000
H	4.56417100	-4.24073800	1.50001300
H	5.27176400	-1.78122400	-3.40853300
H	4.58348900	-3.32763900	-2.91015400
H	4.06282900	-2.62061600	-4.44921100
H	-3.96623100	-4.38417700	2.79697000
H	-5.08835700	-2.98639900	2.69707500
H	-4.87175600	-4.02598600	1.29939500
H	-3.92839800	-3.16086700	-4.15528100
H	-4.89122600	-3.19967500	-2.64462800
H	-5.01640400	-1.81015900	-3.70900100

$Ir(CO)_2$@NU-1000
Electronic Energy: -3653.727525
Enthalpy: -3653.080961
Free Energy: -3653.228027

C	4.75049900	16.93540100	13.59150200
C	15.11750500	17.51770700	13.47070800
C	7.65139700	21.95139900	13.52460100
C	12.30939100	12.71058900	13.47590900
C	5.99458200	16.91131500	14.42099500
C	13.84205700	17.49262500	14.24868900
C	8.27870000	20.84290400	14.30839400
C	11.67340600	13.80127400	14.27539000
H	13.07780300	18.79401300	16.52233400
H	8.25382500	18.19993800	13.71936000
H	7.16510100	13.79209900	14.92594900
H	11.94767900	20.81373000	16.20017500
H	11.26789400	21.41315300	14.90403500
H	9.91169600	15.38827900	12.34812200
H	11.38376100	18.39266400	12.16705200
H	9.80236500	16.95380600	12.54054900
O	6.13070100	17.83383400	15.27309300
O	13.74928000	16.62858600	15.16626800
O	7.52238900	20.24235800	15.12835200
O	12.36149700	14.28179400	15.22006400
O	6.84919800	16.00969200	14.18721600
O	12.93642300	18.31218000	13.92996600
O	9.48892800	20.55530100	14.10305900
O	10.50605300	14.17308900	13.96829600
O	8.02027000	13.88653200	15.35920500
O	11.88428000	20.72492200	15.18888300
O	9.29816800	16.07626100	12.63994000
O	10.56216800	18.36559700	12.66894600
O	8.72218200	17.91772300	14.51074300
O	10.85072400	16.70727400	15.12325400
O	12.20169000	18.39656100	16.51823100
O	9.77366800	19.08830900	16.52166000
Zr	8.99533300	15.67477100	14.89108700
Zr	10.82775200	18.73748400	14.71221000
C	15.11098300	17.57701000	19.68442800
C	4.76731400	16.97131000	19.63402200
C	12.35368000	12.73390300	19.69492000
C	7.66550700	22.01628700	19.56352200
C	13.84592900	17.57877200	18.88996800
C	6.04699800	16.98756800	18.85832400
C	11.73966100	13.85285000	18.91946200
C	8.31079100	20.94298800	18.74286500
H	10.20973100	13.84535500	16.65458000
H	8.25529000	18.37746000	19.37241500
H	7.05155100	14.11578700	18.27852000

H	11.61863800	21.47680000	18.24981200
H	9.95456500	15.54819000	20.95854000
H	11.58545800	18.44377400	20.83907000
O	13.76662000	16.72531700	17.95782300
O	6.18735400	17.92125700	18.01882200
O	12.42898000	14.34687600	17.98716000
O	7.57522600	20.35499800	17.89446800
O	12.94701300	18.40771300	19.18917800
O	6.92359300	16.10729500	19.10866300
O	10.58659300	14.25383200	19.26108800
O	9.51437400	20.65374600	18.97603800
O	11.94234100	20.68688400	17.80399300
O	7.95379000	13.93289400	17.98297400
O	10.71343400	18.64017400	20.47520500
O	9.33382900	16.17605100	20.56928900
O	10.90612700	16.81696300	18.04268500
O	8.79083700	18.06165600	18.63145300
O	8.30663500	16.55071100	16.64122700
O	10.12248300	14.80351700	16.65619600
Zr	10.89011100	18.95231900	18.30086200
Zr	9.14946500	15.84814300	18.42603200
Zr	12.14725400	16.04583500	16.58016900
Zr	7.79020800	18.57001100	16.57461700
H	8.39768100	22.56729700	13.01251900
H	6.98855200	21.51349100	12.76570200
H	7.01988900	22.57058400	14.17194600
H	13.08194400	13.15337400	20.40315200
H	11.60537600	12.17180700	20.26264700
H	12.91335100	12.06543900	19.03111700
H	15.97102900	17.68676200	19.01197100
H	15.12849700	18.37346900	20.43479500
H	15.23261200	16.60361700	20.17776700
H	4.51902700	15.94956900	13.17480200
H	3.90117300	17.32363400	14.16388500
H	4.91245500	17.62248100	12.74896000
H	12.57751300	11.87854700	14.13943000
H	11.65307800	12.34285300	12.68104600
H	13.25187900	13.07105500	13.04368200
H	8.40522300	22.65930600	20.05144500
H	6.97314800	22.61125700	18.95736700
H	7.06561600	21.53498900	20.34928100
H	15.97863800	17.40442800	14.13951700
H	15.13660900	16.65424700	12.79126400
H	15.21416400	18.43163400	12.87650700
H	4.86140800	17.67981800	20.46959600
H	3.93058900	17.31253200	19.01522700
H	4.55860000	15.98503700	20.06229800
Ir	9.09922100	17.97969700	21.62396200
H	7.90261400	13.82531700	16.97380000
C	7.64266300	17.32120300	22.52989400
C	8.93907700	19.61054200	22.44944300
O	6.71520500	16.89289700	23.07044900
O	8.84552100	20.65016400	22.94487800

Catalytic Hydrogenation Mechanism on NU-1000 (Figure 3)

$Ir(C_2H_4)_2$@NU-1000
Electronic Energy: -3584.2779276
Enthalpy: -3583.539158
Free Energy: -3583.688069

C	4.75050000	16.93540000	13.59150000
C	15.11750000	17.51770000	13.47070000
C	7.65140000	21.95140000	13.52460000
C	12.30940000	12.71060000	13.47590000
C	5.99460000	16.91130000	14.42100100
C	13.84200000	17.49260000	14.24870000
C	8.27870000	20.84290000	14.30840000
C	11.67340000	13.80130000	14.27540000
H	13.07675000	18.79309700	16.52196500
H	8.25382900	18.20080900	13.72311400
H	7.16481600	13.79743300	14.92972700
H	11.94708600	20.81101300	16.20983000
H	11.26587200	21.41248800	14.91322900
H	9.91445000	15.38931400	12.36033000
H	11.38746800	18.39073600	12.17900300
H	9.80328100	16.95503600	12.54837200
O	6.12939000	17.83348600	15.27406500
O	13.75062400	16.62841500	15.16648700
O	7.52236200	20.24454300	15.13042000
O	12.36190300	14.28043900	15.22065600
O	6.84896000	16.00934600	14.18869900
O	12.93664100	18.31291400	13.93172700
O	9.48939400	20.55638300	14.10567400
O	10.50592700	14.17310200	13.96929800
O	8.02056800	13.88890800	15.36234900
O	11.88215000	20.72383200	15.19685300
O	9.29855100	16.07771300	12.64636300
O	10.56279800	18.36783100	12.67603200
O	8.72088500	17.91955600	14.51550800
O	10.85120200	16.70755600	15.12445600
O	12.20120200	18.39455700	16.51979300
O	9.76761200	19.08211600	16.53332100
Zr	8.99486900	15.67908400	14.89942900
Zr	10.82530800	18.73793600	14.72091000
C	15.11100000	17.57700000	19.68440000
C	4.76730000	16.97130000	19.63400000
C	12.35370000	12.73390000	19.69490000
C	7.66550000	22.01630000	19.56350000
C	13.84600000	17.57890000	18.89000000
C	6.04690000	16.98740000	18.85830000
C	11.73960000	13.85270000	18.91950000
C	8.31090000	20.94320000	18.74290000
H	10.21179300	13.84737700	16.65288200

H	8.29208000	18.35993900	19.44214800
H	7.05388600	14.12589900	18.27682900
H	11.61392400	21.47609400	18.24563800
O	13.76311100	16.71920300	17.96398200
O	6.18758500	17.92817900	18.02732000
O	12.43099900	14.35098000	17.99136700
O	7.56775500	20.34714600	17.90699300
O	12.95974900	18.42275000	19.17755200
O	6.91267500	16.09503100	19.09298500
O	10.58127000	14.23945500	19.25395300
O	9.51997100	20.67238300	18.95757400
O	11.94698400	20.68680500	17.80595000
O	7.95561000	13.92928000	17.98844000
O	10.91117200	16.81529500	18.04792000
O	8.80177300	18.05707900	18.67826200
O	8.30872000	16.55890800	16.65052600
O	10.12397100	14.80538000	16.65744600
Zr	10.89562500	18.94872800	18.31417800
Zr	9.15616100	15.84594400	18.43832700
Zr	12.14763100	16.04607500	16.58260400
Zr	7.78981400	18.57036700	16.58391200
H	8.39607200	22.55514900	12.99595500
H	6.96980300	21.51581300	12.78123100
H	7.03826100	22.58307600	14.17773800
H	13.07173900	13.15349900	20.41349700
H	11.60321200	12.16359300	20.25153100
H	12.92441700	12.07255100	19.03331300
H	15.96990300	17.69281700	19.01128500
H	15.12723000	18.37151600	20.43689300
H	15.23746600	16.60256000	20.17434400
H	4.52062400	15.95030700	13.17206300
H	3.90058300	17.32037600	14.16527100
H	4.91061500	17.62528800	12.75089700
H	12.56351900	11.87273200	14.13772100
H	11.65820800	12.35167400	12.67276200
H	13.25922600	13.06557700	13.05550700
H	8.40181700	22.62173500	20.10231500
H	7.03108100	22.65500200	18.93737200
H	6.99946300	21.54090500	20.29759600
H	15.97869400	17.42244800	14.14241200
H	15.14618500	16.64400900	12.80487300
H	15.20715900	18.42392700	12.86372700
H	4.76596700	17.82260300	20.32899200
H	3.91246100	17.11894800	18.96315900
H	4.64240900	16.04900700	20.21111400
H	7.90746600	13.82354300	16.97967700
H	11.64297800	18.61976800	20.83050000
H	9.84130200	15.41369800	20.95373700
O	10.75096400	18.70604400	20.47264100
O	9.30000900	16.11313100	20.56813300
Ir	9.28225300	17.88171100	21.75620200
C	7.40225600	17.28555200	22.44678900
H	6.76946500	18.09967300	22.81915500

H	6.93412100	16.65700500	21.67933500
C	8.41583200	16.73634200	23.26556900
H	8.69516000	15.68124800	23.14875300
H	8.58280700	17.12380400	24.27715200
C	9.87484500	19.28624600	23.17266700
H	9.66508800	18.99687400	24.20874500
H	10.91926600	19.57631800	23.00009100
C	8.85543500	19.83464300	22.36067100
H	9.12897200	20.51572200	21.54581500
H	7.84618100	19.98160000	22.76284300

$Ir(C_2H_4)_2H_2$@NU-1000

Electronic Energy: -3585.453032

Enthalpy: -3584.695028

Free Energy: -3584.844690

C	4.75050000	16.93540000	13.59150000
C	15.11750000	17.51770000	13.47070000
C	7.65140000	21.95140000	13.52460000
C	12.30940000	12.71060000	13.47590000
C	5.99460000	16.91130000	14.42100100
C	13.84200000	17.49260000	14.24870000
C	8.27870000	20.84290000	14.30840000
C	11.67340000	13.80130000	14.27540000
H	13.07755000	18.77678300	16.53355000
H	8.25377000	18.20078700	13.72626200
H	7.16469600	13.79761000	14.93125700
H	11.95199400	20.79566100	16.22341100
H	11.26874800	21.40858000	14.93299500
H	9.91292600	15.38804600	12.36577500
H	11.38766900	18.38838400	12.18487200
H	9.80158200	16.95409000	12.55179300
O	6.12854000	17.83275900	15.27546300
O	13.75119800	16.62793600	15.16692700
O	7.52371300	20.24714600	15.13415900
O	12.36122900	14.27824000	15.22301000
O	6.84866400	16.00899200	14.18939900
O	12.93590700	18.31213600	13.93229500
O	9.49016300	20.55691100	14.10786000
O	10.50663200	14.17435600	13.96938300
O	8.02047900	13.88882300	15.36389200
O	11.88425300	20.71649300	15.20981100
O	9.29680000	16.07687300	12.65035200
O	10.56231400	18.36508600	12.68074700
O	8.72031400	17.91979100	14.51898900
O	10.84882600	16.70716700	15.13398400
O	12.20055000	18.38171600	16.52277500
O	9.76715100	19.07417900	16.54021700
Zr	8.99270200	15.68067700	14.90412500
Zr	10.82396000	18.73555300	14.72598000
C	15.11100000	17.57700000	19.68440000

C	4.76730000	16.97130000	19.63400000
C	12.35370000	12.73390000	19.69490000
C	7.66550000	22.01630000	19.56350000
C	13.84600000	17.57890000	18.89000000
C	6.04690000	16.98740000	18.85830000
C	11.73960000	13.85270000	18.91950000
C	8.31090000	20.94320000	18.74290000
H	10.21148000	13.85257100	16.66205800
H	8.43621000	18.35577100	19.51298000
H	7.04687300	14.13687700	18.27051800
H	11.53071000	21.47118800	18.20183200
O	13.75304400	16.69817600	17.98192600
O	6.19447600	17.93963600	18.03985700
O	12.43726000	14.35520100	17.99876800
O	7.56019200	20.32865700	17.92634300
O	12.97365800	18.44104500	19.15672700
O	6.89621800	16.07919300	19.07091200
O	10.56658500	14.20891100	19.22746400
O	9.52821800	20.69961700	18.92746300
O	11.94020400	20.68590000	17.82294500
O	7.94785200	13.92381100	17.99048400
O	10.92850200	16.79969700	18.09115800
O	8.82494000	18.03582300	18.69395800
O	8.30709800	16.56223100	16.65546200
O	10.12299500	14.81049500	16.65972000
Zr	10.89542900	18.93693000	18.32314100
Zr	9.14754500	15.84067600	18.44739700
Zr	12.14868600	16.04286200	16.58827200
Zr	7.78640200	18.57001600	16.59407100
H	8.39357500	22.53926900	12.97503700
H	6.94634800	21.51920000	12.80153800
H	7.06204900	22.59881100	14.18445000
H	13.29238900	13.07400100	20.15267200
H	11.68246200	12.35015800	20.46959900
H	12.62703800	11.91890300	19.01233000
H	15.97824100	17.52945800	19.01457600
H	15.18780700	18.45377200	20.33559900
H	15.14776700	16.66855400	20.30227200
H	4.52358500	15.95154700	13.16758300
H	3.89955500	17.31486600	14.16745700
H	4.90784200	17.63006500	12.75431100
H	12.55223000	11.86809500	14.13614000
H	11.66234300	12.35905600	12.66616400
H	13.26502000	13.06106500	13.06509600
H	8.40525500	22.66926200	20.03799900
H	6.96680100	22.60474000	18.95767100
H	7.06888500	21.53977200	20.35454400
H	15.97869600	17.42509200	14.14278800
H	15.14741400	16.64254200	12.80687300
H	15.20614500	18.42277000	12.86182300
H	4.79665900	17.77610100	20.38206200
H	3.91722400	17.18970400	18.97716500
H	4.61289100	16.02128400	20.15611900

H	7.90531600	13.81863200	16.98169500
C	8.29064700	17.31300700	23.10295300
C	8.26562900	18.29247700	22.09803200
C	12.36008100	17.21916200	22.24902300
C	11.92182400	16.24322100	21.35034900
H	11.20044800	19.46811300	20.90894800
H	9.49419600	15.08766000	20.87221400
H	10.61589300	18.35361200	23.18914400
H	10.18145400	16.18608700	23.17556700
H	7.79352900	16.35546400	22.92763800
H	8.41032900	17.58664600	24.15322300
H	8.38262500	19.35460700	22.32707700
H	7.72986100	18.05893700	21.17274200
H	12.77509700	18.15559300	21.86602100
H	12.66210800	16.95443500	23.26438900
H	11.85406700	15.19571700	21.65769900
H	11.93981600	16.42409700	20.27088800
Ir	10.18524500	17.31898800	22.07723000
O	10.66266300	18.79653400	20.47586700
O	9.18023500	15.95683100	20.59210300

TS1@NU-1000

Electronic Energy: -3585.434354

Enthalpy: -3584.678941

Free Energy: -3584.826596

C	4.750487	16.935395	13.591518
C	15.117496	17.517693	13.470694
C	7.651401	21.951410	13.524613
C	12.309410	12.710614	13.475889
C	5.994651	16.911305	14.421007
C	13.842041	17.492630	14.248689
C	8.278695	20.842886	14.308396
C	11.673374	13.801191	14.275399
H	13.075911	18.792438	16.522149
H	8.251717	18.198950	13.724098
H	7.163850	13.798233	14.932746
H	11.945000	20.811900	16.206069
H	11.265630	21.410647	14.906788
H	9.914376	15.387800	12.360586
H	11.387382	18.385847	12.178059
H	9.802375	16.953700	12.547963
O	6.130448	17.834319	15.272751
O	13.751380	16.628600	15.166552
O	7.522902	20.245123	15.131225
O	12.361960	14.280581	15.220222
O	6.847849	16.007908	14.189180
O	12.936185	18.311635	13.930312
O	9.488455	20.555066	14.102315
O	10.505298	14.171963	13.969910
O	8.020217	13.888024	15.364501

O	11.882525	20.723216	15.191934
O	9.297844	16.075885	12.645958
O	10.562162	18.364651	12.674242
O	8.720467	17.917746	14.515468
O	10.850114	16.706879	15.126492
O	12.200729	18.393165	16.518620
O	9.767886	19.085319	16.526966
Zr	8.994884	15.677883	14.899169
Zr	10.825548	18.737676	14.719419
C	15.111037	17.577042	19.684341
C	4.767259	16.971156	19.633929
C	12.353679	12.733905	19.694924
C	7.665582	22.016380	19.563460
C	13.845798	17.578839	18.890101
C	6.047188	16.987856	18.858370
C	11.739665	13.852697	18.919408
C	8.310636	20.942900	18.742964
H	10.210931	13.848701	16.658868
H	8.394529	18.339524	19.477173
H	7.054294	14.131103	18.279634
H	11.616679	21.481116	18.240193
H	9.894593	15.391118	20.904916
H	11.636156	18.520012	20.749075
O	13.765120	16.719804	17.963030
O	6.180481	17.920550	18.019785
O	12.429398	14.349341	17.989608
O	7.566106	20.347975	17.906360
O	12.958492	18.421426	19.177197
O	6.917267	16.102562	19.105439
O	10.582950	14.242441	19.257182
O	9.517655	20.671894	18.959190
O	11.942837	20.691206	17.796748
O	7.955838	13.935005	17.991217
O	10.740264	18.737142	20.464477
O	9.272718	16.062558	20.599229
O	10.921607	16.809845	18.058178
O	8.811153	18.052583	18.653304
O	8.306864	16.555256	16.650445
O	10.123948	14.806774	16.659454
Zr	10.893063	18.952685	18.314240
Zr	9.159341	15.853821	18.436910
Zr	12.149092	16.046954	16.583322
Zr	7.792453	18.571856	16.586002
H	8.397029	22.561297	13.004348
H	6.979449	21.514728	12.773067
H	7.028899	22.576945	14.174714
H	12.970353	13.160278	20.498895
H	11.591949	12.099022	20.159630
H	13.019973	12.137816	19.062377
H	15.127233	18.372023	20.436339
H	15.236374	16.603117	20.175522
H	15.969780	17.691579	19.010836
H	4.516260	15.948467	13.178720

H	3.902207	17.328071	14.162470
H	4.913798	17.618308	12.745834
H	12.554997	11.869272	14.136599
H	11.661434	12.356983	12.667788
H	13.263636	13.062217	13.062812
H	8.404670	22.641660	20.075067
H	7.002319	22.634237	18.946917
H	7.030334	21.538967	20.323471
H	15.208002	18.424705	12.864974
H	15.978786	17.420458	14.141989
H	15.144934	16.645077	12.803384
H	4.730867	17.858210	20.281561
H	3.910889	17.056502	18.953719
H	4.664817	16.073532	20.253275
H	7.907274	13.828534	16.982537
Ir	9.411987	17.752073	21.896910
C	10.237396	19.027909	23.366775
H	10.156060	18.609465	24.373822
H	11.247542	19.343104	23.093262
C	9.129662	19.655127	22.752798
H	9.301878	20.428721	21.997616
H	8.179609	19.733428	23.293421
C	7.318835	17.296167	22.314502
H	6.638276	18.094661	22.629958
H	6.877257	16.606662	21.587109
C	8.240495	16.746598	23.280611
H	8.399536	15.663061	23.270365
H	8.254548	17.179177	24.288618
H	7.912546	18.194514	21.193888
H	10.827717	17.081310	22.378202

Ir(C_2H_5) (C_2H_4) H@NU-1000

Electronic Energy: -3585.459815

Enthalpy: -3584.700407

Free Energy: -3584.852553

C	4.750501	16.935400	13.591497
C	15.117501	17.517697	13.470702
C	7.651396	21.951389	13.524588
C	12.309406	12.710610	13.475892
C	5.994659	16.911302	14.421026
C	13.841964	17.492596	14.248723
C	8.278727	20.842856	14.308403
C	11.673419	13.801355	14.275414
H	13.076292	18.787661	16.531484
H	8.264960	18.203940	13.716995
H	7.168442	13.795007	14.918658
H	11.951418	20.811185	16.227936
H	11.275260	21.419554	14.929716
H	9.920264	15.398011	12.362089
H	11.391138	18.404888	12.192919

H	9.811963	16.963695	12.556309
O	6.127281	17.831772	15.276830
O	13.746983	16.627193	15.165479
O	7.517787	20.242631	15.126594
O	12.358287	14.280175	15.223630
O	6.851826	16.013409	14.186284
O	12.939270	18.319095	13.938659
O	9.490436	20.559644	14.115707
O	10.506617	14.175263	13.966624
O	8.022051	13.889034	15.354864
O	11.884144	20.724833	15.213660
O	9.305201	16.086668	12.649509
O	10.566645	18.377996	12.690053
O	8.722484	17.923304	14.515212
O	10.850131	16.710231	15.126751
O	12.198876	18.392955	16.533057
O	9.761768	19.079916	16.550084
Zr	8.997330	15.679472	14.899577
Zr	10.829946	18.741870	14.736866
C	15.111007	17.576993	19.684389
C	4.767307	16.971331	19.634012
C	12.353714	12.733864	19.694837
C	7.665482	22.016322	19.563458
C	13.846029	17.579108	18.890035
C	6.046836	16.987188	18.858391
C	11.739465	13.852444	18.919474
C	8.310987	20.943446	18.742858
H	10.216562	13.848210	16.652397
H	7.997184	18.441452	19.184139
H	7.049986	14.117095	18.264857
H	11.649721	21.476768	18.266006
H	9.792173	15.433642	21.072394
H	11.597592	18.480747	20.876600
O	13.755095	16.713371	17.969478
O	6.212612	17.952073	18.054972
O	12.434762	14.365168	18.001435
O	7.562596	20.322104	17.927890
O	12.964216	18.424107	19.179301
O	6.898902	16.077919	19.072606
O	10.571147	14.218941	19.237490
O	9.524789	20.687560	18.945255
O	11.958674	20.684171	17.814803
O	7.952218	13.918535	17.978559
O	10.751958	18.679727	20.463475
O	9.361298	16.115351	20.547836
O	10.879358	16.828623	18.045122
O	8.780407	18.059723	18.766869
O	8.305657	16.561352	16.652390
O	10.122143	14.805674	16.657259
Zr	10.904325	18.957784	18.353335
Zr	9.151684	15.829162	18.443606
Zr	12.141778	16.051670	16.590227
Zr	7.800193	18.567823	16.559151

H	8.393898	22.541870	12.978389
H	6.949387	21.518534	12.799026
H	7.058678	22.596282	14.183857
H	13.056725	13.153872	20.427992
H	11.599974	12.152407	20.235105
H	12.940750	12.083511	19.036585
H	15.978675	17.518555	19.016357
H	15.191038	18.458336	20.328356
H	15.143484	16.673802	20.309369
H	4.525862	15.952706	13.163832
H	3.898493	17.311162	14.168285
H	4.907281	17.633625	12.757192
H	12.560928	11.871512	14.137133
H	11.659060	12.353884	12.671136
H	13.260588	13.064673	13.057819
H	8.406004	22.688954	20.009128
H	6.942829	22.584321	18.965904
H	7.100375	21.547120	20.380419
H	15.978073	17.444145	14.146101
H	15.158516	16.632432	12.821153
H	15.198666	18.414934	12.849501
H	4.923085	17.541929	20.561044
H	3.959221	17.456172	19.076828
H	4.483374	15.954582	19.926830
Ir	8.879280	17.954249	21.433050
H	7.906478	13.814979	16.969570
C	8.855357	19.915200	22.155046
H	9.411277	20.028287	23.093763
H	9.175225	20.604116	21.368285
C	7.545753	19.377719	22.187901
H	6.799704	19.661236	21.432071
H	7.089753	19.106133	23.146557
C	9.441900	17.371958	23.316296
H	8.902923	17.962659	24.078110
H	9.118539	16.324911	23.448214
C	10.936993	17.500261	23.489779
H	11.492322	16.888829	22.760304
H	11.282428	18.538995	23.376840
H	7.555249	17.207722	21.840225
H	11.257269	17.163372	24.490481

TS2@NU-1000

Electronic Energy: -3585.44487

Enthalpy: -3584.686753

Free Energy: -3584.837529

C	4.750501	16.935400	13.591497
C	15.117501	17.517697	13.470702
C	7.651396	21.951389	13.524588
C	12.309406	12.710610	13.475892
C	5.994659	16.911302	14.421026

C	13.841964	17.492596	14.248723
C	8.278727	20.842856	14.308403
C	11.673419	13.801355	14.275414
H	13.075084	18.791662	16.525597
H	8.253803	18.202472	13.723262
H	7.164048	13.798825	14.924857
H	11.945343	20.809200	16.213715
H	11.263656	21.412093	14.918300
H	9.916930	15.390991	12.359583
H	11.388743	18.391245	12.179261
H	9.804065	16.956630	12.547332
O	6.129401	17.833406	15.273687
O	13.749691	16.627590	15.165437
O	7.522173	20.244261	15.129585
O	12.361248	14.279825	15.221317
O	6.848992	16.009570	14.186968
O	12.937432	18.314409	13.932918
O	9.489716	20.557119	14.105556
O	10.506442	14.173678	13.968021
O	8.019655	13.888172	15.358220
O	11.881873	20.724468	15.200260
O	9.299746	16.078762	12.644331
O	10.563528	18.368536	12.675375
O	8.721367	17.920147	14.514950
O	10.850758	16.707653	15.124588
O	12.199534	18.393164	16.522669
O	9.769829	19.084263	16.530721
Zr	8.994249	15.679467	14.897155
Zr	10.825514	18.738895	14.721021
C	15.111007	17.576993	19.684389
C	4.767307	16.971331	19.634012
C	12.353714	12.733864	19.694837
C	7.665482	22.016322	19.563458
C	13.846029	17.579108	18.890035
C	6.046836	16.987188	18.858391
C	11.739465	13.852444	18.919474
C	8.310987	20.943446	18.742858
H	10.209138	13.846915	16.651152
H	8.338849	18.354514	19.457198
H	7.048763	14.127174	18.273243
H	11.615230	21.472036	18.251269
H	9.957788	15.499972	20.891660
H	11.618869	18.453998	20.805068
O	13.768104	16.725430	17.958346
O	6.183475	17.924565	18.023216
O	12.431195	14.348284	17.990065
O	7.569829	20.355818	17.899792
O	12.950600	18.409978	19.189479
O	6.913976	16.097759	19.097460
O	10.583863	14.243998	19.257069
O	9.518156	20.665650	18.962441
O	11.944945	20.682638	17.809282
O	7.949984	13.929171	17.984238

O	10.736924	18.686356	20.487697
O	9.288122	16.112484	20.562976
O	10.913508	16.810751	18.052917
O	8.796375	18.059927	18.653989
O	8.304817	16.557068	16.646132
O	10.122030	14.804952	16.656821
Zr	10.889313	18.946161	18.315894
Zr	9.147530	15.847019	18.434119
Zr	12.145371	16.046617	16.583111
Zr	7.789034	18.571842	16.586134
H	8.396048	22.555525	12.996315
H	6.970175	21.515808	12.780862
H	7.037888	22.582760	14.177693
H	13.091314	13.150972	20.394808
H	11.607042	12.177309	20.270173
H	12.904010	12.059436	19.028971
H	15.970758	17.691010	19.012157
H	15.127471	18.371249	20.437223
H	15.235290	16.602263	20.174488
H	4.518503	15.949476	13.175084
H	3.901279	17.324045	14.163817
H	4.912383	17.621952	12.748494
H	12.565651	11.873522	14.137872
H	11.657457	12.350484	12.673894
H	13.258132	13.066440	13.053667
H	8.399163	22.606187	20.122781
H	7.053831	22.670963	18.930847
H	6.977022	21.543035	20.277566
H	15.978602	17.422154	14.142515
H	15.146204	16.644228	12.804582
H	15.207402	18.424166	12.864110
H	4.798993	17.782065	20.375749
H	3.915844	17.183911	18.977340
H	4.615250	16.024927	20.163759
Ir	9.224994	17.913129	21.717830
H	7.902196	13.824338	16.975304
C	9.733173	19.333894	23.144272
H	9.484147	19.054111	24.175797
H	10.781024	19.630249	23.010282
C	8.749187	19.868375	22.277859
H	9.056148	20.560850	21.486327
H	7.720150	20.006306	22.632547
C	8.039652	16.925491	23.295118
H	7.822855	17.690798	24.056361
H	7.072453	16.415496	23.119247
C	9.017990	15.884265	23.801804
H	9.217764	15.113257	23.045632
H	9.978905	16.324640	24.102325
H	7.716888	17.509299	22.089843
H	8.605793	15.362803	24.682239

Ir(C_2H_6) (C_2H_4)@NU-1000

Electronic Energy: -3585.453059
Enthalpy: -3584.691644
Free Energy: -3584.844042

C	4.750500	16.935400	13.591500
C	15.117500	17.517700	13.470700
C	7.651400	21.951400	13.524600
C	12.309400	12.710600	13.475900
C	5.994600	16.911300	14.421001
C	13.842000	17.492600	14.248700
C	8.278700	20.842900	14.308400
C	11.673400	13.801300	14.275400
H	13.076706	18.792427	16.521134
H	8.253187	18.200470	13.722360
H	7.163289	13.798763	14.927851
H	11.945391	20.809527	16.209811
H	11.263652	21.410552	14.913471
H	9.916202	15.390241	12.356571
H	11.387950	18.390524	12.178121
H	9.803874	16.955838	12.545952
O	6.129481	17.833010	15.274203
O	13.750940	16.628230	15.166197
O	7.522131	20.244048	15.129574
O	12.362090	14.280596	15.220013
O	6.848900	16.009487	14.187228
O	12.936630	18.312702	13.931375
O	9.489386	20.556627	14.104914
O	10.506034	14.172956	13.968485
O	8.019827	13.888173	15.359381
O	11.881910	20.723445	15.196630
O	9.299655	16.077842	12.643020
O	10.562812	18.367713	12.674373
O	8.720779	17.918554	14.514190
O	10.851256	16.706531	15.123484
O	12.201229	18.393812	16.519277
O	9.767458	19.083136	16.529811
Zr	8.995311	15.677725	14.895453
Zr	10.824839	18.737074	14.720080
C	15.111000	17.577000	19.684400
C	4.767300	16.971300	19.634000
C	12.353700	12.733900	19.694900
C	7.665500	22.016300	19.563500
C	13.846000	17.578900	18.890000
C	6.046900	16.987400	18.858300
C	11.739600	13.852700	18.919500
C	8.310900	20.943200	18.742900
H	10.209492	13.846456	16.653765
H	8.329694	18.316137	19.464693
H	7.054457	14.121167	18.278214
H	11.607190	21.477871	18.241160
O	13.764918	16.720306	17.962611
O	6.183707	17.924974	18.023166

O	12.429317	14.344946	17.986716
O	7.569772	20.355788	17.900019
O	12.956133	18.417822	19.181369
O	6.916152	16.097794	19.094151
O	10.585621	14.249887	19.259573
O	9.517065	20.667065	18.965796
O	11.944113	20.687446	17.806758
O	7.956053	13.929670	17.986087
O	10.914690	16.811474	18.047605
O	8.797136	18.055165	18.655701
O	8.308154	16.555393	16.646280
O	10.122978	14.804592	16.656192
Zr	10.892826	18.946233	18.312366
Zr	9.152261	15.849566	18.431461
Zr	12.147998	16.045142	16.582075
Zr	7.788641	18.570734	16.585605
H	8.396783	22.560530	13.003094
H	6.977879	21.514977	12.774335
H	7.030263	22.577698	14.175290
H	13.077291	13.153711	20.407759
H	11.604523	12.168441	20.258228
H	12.918096	12.068474	19.032035
H	15.970860	17.685426	19.011354
H	15.129469	18.374940	20.433228
H	15.232768	16.604646	20.179757
H	4.518984	15.949554	13.174696
H	3.901122	17.323365	14.164044
H	4.912035	17.622457	12.748839
H	12.569685	11.875273	14.138497
H	11.656044	12.347698	12.676307
H	13.256015	13.068054	13.050298
H	8.401264	22.611133	20.114713
H	7.046673	22.666370	18.933459
H	6.981184	21.544830	20.283400
H	15.978727	17.421431	14.142228
H	15.145612	16.644546	12.804133
H	15.207642	18.424318	12.864352
H	4.774782	17.813064	20.340512
H	3.913548	17.134346	18.965527
H	4.635774	16.043476	20.200723
H	7.905674	13.824467	16.977360
H	11.620012	18.538109	20.807470
H	9.952574	15.506729	20.944459
O	10.733000	18.706297	20.465466
O	9.319593	16.135752	20.576059
Ir	9.251466	17.839282	21.719791
C	7.372622	17.275374	22.416589
H	6.749658	18.106131	22.776148
H	6.874376	16.626352	21.686353
C	8.385869	16.731402	23.247722
H	8.636646	15.666000	23.164222
H	8.556224	17.137268	24.253235
C	9.934103	21.158579	22.539919

H	10.730580	21.197571	23.295926
H	10.404801	21.069153	21.552091
C	8.974771	20.017536	22.779117
H	8.227657	19.936317	21.977208
H	8.415630	20.089787	23.724919
H	9.406067	22.121906	22.574608
H	9.608700	19.066024	22.988920

Catalytic Dimerization Mechanism on NU-1000 (Figure 4)

TS1@NU-1000

Electronic Energy: -3585.3909954
Enthalpy: -3584.634922
Free Energy: -3584.783450

C	4.75049200	16.93539700	13.59151200
C	15.11751000	17.51771800	13.47071600
C	7.65140200	21.95140800	13.52461000
C	12.30938200	12.71057200	13.47592400
C	5.99449100	16.91130900	14.42098000
C	13.84214400	17.49265900	14.24865500
C	8.27865800	20.84295900	14.30837700
C	11.67338200	13.80117300	14.27536300
H	13.08275600	18.77099600	16.54096300
H	8.25315200	18.20255900	13.73612500
H	7.17119400	13.79284500	14.92152500
H	11.94911500	20.80419100	16.21482800
H	11.26857700	21.40551600	14.91810400
H	9.91055300	15.39259900	12.35865100
H	11.38614800	18.39061900	12.18312900
H	9.80127200	16.95814200	12.55136200
O	6.13120600	17.83319900	15.27433200
O	13.75006900	16.62651900	15.16519300
O	7.52380200	20.24213400	15.12997100
O	12.36351600	14.27987400	15.22036300
O	6.84852500	16.00855400	14.18946400
O	12.93715400	18.31381500	13.93310800
O	9.49088700	20.55863700	14.10841400
O	10.50910200	14.17810900	13.96521900
O	8.02797400	13.88183000	15.35266200
O	11.88818100	20.71929700	15.20081200
O	9.29651200	16.08060700	12.64942500
O	10.56278500	18.36592300	12.68219100
O	8.72461200	17.91804700	14.52472300
O	10.85083900	16.70978900	15.14165500
O	12.20436000	18.37913600	16.52757300
O	9.78015200	19.08158100	16.54006400
Zr	8.99804600	15.67457600	14.90181900
Zr	10.83072200	18.73691500	14.72682800
C	15.11094400	17.57700100	19.68449000
C	4.76733500	16.97128200	19.63405500

C	12.35365200	12.73393900	19.69499500
C	7.66552900	22.01626900	19.56356300
C	13.84574900	17.57841200	18.88997100
C	6.04720200	16.98792100	18.85824600
C	11.73991000	13.85325800	18.91938500
C	8.31062000	20.94262300	18.74285700
H	10.23478700	13.85192500	16.66586100
H	8.40159900	18.30096100	19.48001500
H	7.04615700	14.12764000	18.25496600
H	11.60118700	21.47507000	18.23887600
H	8.22534400	16.15039900	20.89246800
H	10.13867200	19.60699600	20.76761800
O	13.76864200	16.70879500	17.97053200
O	6.18794700	17.92015200	18.02169300
O	12.44897000	14.36061900	18.00385100
O	7.58110300	20.35790700	17.89380400
O	12.96354300	18.42592600	19.16581100
O	6.90875700	16.09365300	19.10596900
O	10.57104700	14.21647300	19.21979200
O	9.51682400	20.66681700	18.98372100
O	11.93617300	20.68378600	17.80489600
O	7.95086400	13.93104900	17.97774100
O	10.67043300	18.85033100	20.49691400
O	9.12681100	16.07751900	20.56280300
O	10.93917900	16.79846100	18.12041400
O	8.79797100	18.05695600	18.63928600
O	8.30989300	16.54657500	16.65467100
O	10.13771100	14.80883600	16.65315600
Zr	10.90354400	18.93954100	18.32960100
Zr	9.16013500	15.83866100	18.45140600
Zr	12.15143900	16.04009100	16.59286100
Zr	7.79972000	18.56212400	16.58518800
H	8.39596000	22.55283100	12.99320300
H	6.96609100	21.51681600	12.78410700
H	7.04192100	22.58547100	14.17894100
H	13.25245100	13.09821500	20.21110400
H	11.65853900	12.31287600	20.42813500
H	12.69346800	11.94716700	19.00961100
H	15.96395100	17.73641400	19.01178800
H	15.11940800	18.34986200	20.46013100
H	15.26843000	16.58873600	20.13715900
H	4.51753100	15.94871600	13.17751500
H	3.90173600	17.32616200	14.16307500
H	4.91283400	17.61975200	12.74682100
H	11.64125200	12.32075100	12.70156900
H	13.23236000	13.08487600	13.01388800
H	12.61247400	11.89339700	14.14257200
H	8.40387800	22.70445200	19.98856000
H	6.91997100	22.56622500	18.97882900
H	7.12801800	21.54183900	20.39734300
H	15.14006900	16.65073600	12.79591500
H	15.21210500	18.42911100	12.87220600
H	15.97850300	17.41055100	14.14078000

H	4.82343100	17.73443400	20.42321300
H	3.92246800	17.24621400	18.99273600
H	4.58642000	16.00244600	20.11143800
H	7.91218300	13.82273700	16.96950000
Ir	10.40407400	17.26050700	22.00857300
C	11.61810400	18.45846100	23.14201000
C	11.26868400	15.38071300	22.18795300
C	12.64811600	17.77596200	22.36200400
H	11.45553400	19.51504400	22.89464500
H	11.62446900	18.28436300	24.22405300
C	12.25414900	16.09939500	21.38713100
H	11.59513800	15.05274100	23.18168000
H	10.61210600	14.67012100	21.67680700
H	13.07217500	18.33158900	21.52054400
H	13.39763600	17.25528000	22.96419100
H	13.30706000	15.85599000	21.54495700
H	12.04888000	16.17012600	20.30874300
H	9.86492300	16.58845300	23.32321600
H	8.95828000	17.88492900	22.35882300

Ir(C_4H_8) H_2@NU-1000

Electronic Energy: -3585.4331284

Enthalpy: -3584.674415

Free Energy: -3584.825068

C	4.75049200	16.93539700	13.59151200
C	15.11751000	17.51771800	13.47071600
C	7.65140200	21.95140800	13.52461000
C	12.30938200	12.71057200	13.47592400
C	5.99449100	16.91130900	14.42098000
C	13.84214400	17.49265900	14.24865500
C	8.27865800	20.84295900	14.30837700
C	11.67338200	13.80117300	14.27536300
H	13.08219500	18.78643300	16.52814300
H	8.25368100	18.19934100	13.72746300
H	7.16766600	13.79845500	14.93894200
H	11.95055400	20.80540600	16.21036600
H	11.26553000	21.40958300	14.91871400
H	9.91176400	15.38807200	12.35921500
H	11.38628600	18.38905500	12.17623100
H	9.80196000	16.95380900	12.54755900
O	6.12962700	17.83252000	15.27594800
O	13.75254800	16.62823700	15.16626900
O	7.52347100	20.24418500	15.13146000
O	12.36454200	14.28020200	15.21887200
O	6.84909200	16.00913200	14.19041900
O	12.93612700	18.31137800	13.92992000
O	9.48991600	20.55689400	14.10659600
O	10.50696400	14.17477600	13.96847600
O	8.02563400	13.88918200	15.36735100
O	11.88446300	20.72178700	15.19901500

O	9.29728800	16.07684100	12.64734700
O	10.56265300	18.36593000	12.67493800
O	8.72265100	17.91828500	14.51879200
O	10.85424800	16.70801400	15.12980000
O	12.20486600	18.39208200	16.51617500
O	9.77294200	19.07941900	16.53520800
Zr	8.99943500	15.67826400	14.90146100
Zr	10.82799500	18.73365800	14.71945400
C	15.11094400	17.57700100	19.68449000
C	4.76733500	16.97128200	19.63405500
C	12.35365200	12.73393900	19.69499500
C	7.66552900	22.01626900	19.56356300
C	13.84574900	17.57841200	18.88997100
C	6.04720200	16.98792100	18.85824600
C	11.73991000	13.85325800	18.91938500
C	8.31062000	20.94262300	18.74285700
H	10.22294700	13.85041000	16.66004000
H	8.34139600	18.32943500	19.47178700
H	7.05277600	14.17068800	18.25943900
H	11.54101200	21.47606100	18.21505100
H	9.03567300	15.37014200	21.07913300
H	11.34749600	19.28258800	20.93811300
O	13.76105500	16.70752100	17.97090000
O	6.19767800	17.93512900	18.03537600
O	12.43989800	14.35775500	17.99796400
O	7.56812000	20.34300400	17.90907300
O	12.97043700	18.43971600	19.15167700
O	6.90399100	16.08577600	19.08429500
O	10.57188700	14.22349600	19.23098000
O	9.52274200	20.67855300	18.95108300
O	11.93709200	20.69209500	17.81960700
O	7.95422900	13.93969300	17.99498900
O	10.71497200	18.70250700	20.49574500
O	9.25605200	16.16716100	20.58340800
O	10.92209900	16.81304500	18.06120700
O	8.81924700	18.05347300	18.68036800
O	8.31677100	16.55871300	16.65597300
O	10.13248300	14.80805600	16.65324400
Zr	10.90032300	18.94059100	18.30775000
Zr	9.17196900	15.85142100	18.44133400
Zr	12.15908000	16.03971900	16.58693300
Zr	7.79102800	18.56887900	16.58851200
H	8.39594400	22.55273200	12.99306200
H	6.96632000	21.51648700	12.78407500
H	7.04172300	22.58545200	14.17874800
H	13.08624700	13.15087100	20.40008000
H	11.60457600	12.17530100	20.26491000
H	12.90794500	12.06260000	19.02919900
H	15.96751700	17.70881900	19.01109700
H	15.11967100	18.36400400	20.44484600
H	15.24630500	16.59877900	20.16393600
H	4.52351600	15.95121000	13.16847200
H	3.89960900	17.31553600	14.16711200

H	4.90808800	17.62932400	12.75376600
H	12.58903100	11.88346800	14.14077200
H	11.64941600	12.33519800	12.68755100
H	13.24559600	13.07579400	13.03400000
H	8.40481300	22.63918300	20.07724200
H	7.00503600	22.63546100	18.94538500
H	7.02741900	21.53970600	20.32112600
H	15.97878700	17.42263500	14.14232800
H	15.14596300	16.64368500	12.80532600
H	15.20726100	18.42358800	12.86318500
H	4.86385600	17.66996400	20.47745100
H	3.93269800	17.32563500	19.01937800
H	4.55029800	15.97995100	20.04588000
H	7.91977200	13.82511700	16.98678200
Ir	9.41814000	17.86129800	21.91242200
C	10.33836100	19.01466800	23.40968000
H	8.71053300	19.21379800	22.17629000
C	9.30261200	16.44567600	23.44856100
C	10.84537000	18.04173100	24.46066400
H	11.15617700	19.59715600	22.94687900
H	9.67806400	19.75601500	23.88814900
C	9.73041500	17.05981900	24.76156400
H	8.38570000	15.84132800	23.52852000
H	10.10200000	15.78052400	23.06105500
H	11.72180300	17.48634100	24.08115500
H	11.18898600	18.57303900	25.36534600
H	8.87989800	17.59090300	25.22358000
H	10.03575900	16.28269500	25.48363100
H	8.01707800	17.68199800	22.58458200

TS2@NU-1000

Electronic Energy: -3585.4218118

Enthalpy: -3584.663744

Free Energy: -3584.812201

C	4.75049900	16.93540100	13.59150200
C	15.11750500	17.51770700	13.47070800
C	7.65139700	21.95139900	13.52460100
C	12.30939100	12.71058900	13.47590900
C	5.99458200	16.91131500	14.42099500
C	13.84205700	17.49262500	14.24868900
C	8.27870000	20.84290400	14.30839400
C	11.67340600	13.80127400	14.27539000
H	13.07889900	18.78722000	16.52456100
H	8.26427800	18.19773900	13.71098800
H	7.16581600	13.79371100	14.93031200
H	11.95778700	20.81699300	16.20468300
H	11.27723100	21.41629200	14.90532200
H	9.91634600	15.38858800	12.36627400
H	11.38596300	18.39946400	12.18366100
H	9.80813300	16.95474500	12.55445900

O	6.12763400	17.83406000	15.27452100
O	13.74707300	16.63067200	15.16854800
O	7.51644800	20.24170700	15.12414200
O	12.35839500	14.28333600	15.22162600
O	6.85044600	16.01160100	14.18998700
O	12.93724300	18.31478700	13.93233200
O	9.48904700	20.55761000	14.11216500
O	10.50334400	14.17001000	13.97129700
O	8.02024700	13.88895300	15.36462300
O	11.88773000	20.72383500	15.19152900
O	9.30178600	16.07854800	12.65178100
O	10.56284900	18.37245800	12.68312300
O	8.72114500	17.92082800	14.51092200
O	10.84912700	16.70911300	15.12635600
O	12.20006100	18.39564000	16.52635500
O	9.76304800	19.08294500	16.53929300
Zr	8.99628900	15.67688000	14.90410500
Zr	10.83039700	18.73899400	14.72795700
C	15.11098300	17.57701000	19.68442800
C	4.76731400	16.97131000	19.63402200
C	12.35368000	12.73390300	19.69492000
C	7.66550700	22.01628700	19.56352200
C	13.84592900	17.57877200	18.88996800
C	6.04699800	16.98756800	18.85832400
C	11.73966100	13.85285000	18.91946200
C	8.31079100	20.94298800	18.74286500
H	10.21960600	13.85226100	16.65968000
H	7.95901100	18.47403000	19.11026300
H	7.06060000	14.10182600	18.28318000
H	11.66250400	21.48893000	18.24554700
H	9.94329000	15.60512000	21.05080300
H	11.57775900	18.45430000	20.88580200
O	13.75245100	16.70818900	17.97341700
O	6.21388300	17.95337400	18.05501400
O	12.42971900	14.35410900	17.99095300
O	7.56280000	20.32964600	17.91966800
O	12.97076100	18.43433900	19.16653000
O	6.89803000	16.07689400	19.06969400
O	10.58290600	14.24209500	19.25472100
O	9.52849900	20.69670100	18.93018600
O	11.96595800	20.69565200	17.79160200
O	7.96299900	13.91762600	17.98815500
O	10.76174500	18.71052900	20.44559200
O	9.32533700	16.15588500	20.56017400
O	10.87720900	16.83735100	18.05010000
O	8.76919100	18.07476400	18.75950800
O	8.30744200	16.56428900	16.65461400
O	10.12188500	14.80944100	16.66455400
Zr	10.91169400	18.97424800	18.33677700
Zr	9.14767900	15.83521000	18.45257700
Zr	12.13832400	16.05302300	16.59297700
Zr	7.80042100	18.57068100	16.54940900
H	8.39647100	22.55964700	13.00178700

H	6.97598000	21.51472400	12.77626900
H	7.03180100	22.57851300	14.17597100
H	13.06319800	13.15518200	20.42093300
H	11.60106100	12.15945300	20.24421200
H	12.93297400	12.07759100	19.03584200
H	15.96926600	17.70013800	19.01156100
H	15.12284100	18.36922600	20.43919900
H	15.24280400	16.60096900	20.16963300
H	4.52905700	15.95426900	13.15872600
H	3.89742500	17.30511900	14.17066800
H	4.90434300	17.63926200	12.76141200
H	11.67677200	12.38377500	12.64473100
H	13.28401100	13.04473100	13.09814500
H	12.51308100	11.85278200	14.12997000
H	8.34642800	22.41274000	20.32360100
H	7.33749500	22.83585900	18.90978800
H	6.75755700	21.62345000	20.03809100
H	15.97853200	17.42243200	14.14261000
H	15.14663300	16.64432700	12.80450500
H	15.20673800	18.42434200	12.86437500
H	4.94857200	17.46358600	20.60065900
H	3.97821700	17.52387300	19.11465000
H	4.44450700	15.94796600	19.85632300
H	7.91083300	13.81547700	16.97936800
Ir	8.80788200	18.07860000	21.28581300
C	9.33362100	17.72762300	23.23844400
H	8.90199100	19.62696900	21.48131400
C	8.68386600	18.72538600	24.18225400
H	9.01675200	16.69560700	23.47617900
H	10.43740500	17.75791500	23.29787500
H	8.68009100	18.36202900	25.22435700
H	9.26312400	19.66560900	24.18806300
C	7.28588300	19.01263200	23.67230400
C	7.40030400	19.47114300	22.22773200
H	6.76960800	19.77123300	24.28565900
H	6.68217000	18.09068800	23.72821100
H	7.64193000	20.54872400	22.22048500
H	6.46279500	19.38695200	21.65749700
H	7.43660900	17.38506400	21.63900500

Ir(butane) H@NU-1000

Electronic Energy: -3585.4551443

Enthalpy: -3584.692787

Free Energy: -3584.843815

C	4.750519	16.935392	13.591472
C	15.117502	17.517693	13.470703
C	7.651377	21.951377	13.524586
C	12.309406	12.710588	13.475922
C	5.994778	16.911268	14.421085
C	13.841976	17.492628	14.248713

C	8.278713	20.842908	14.308328
C	11.673207	13.801366	14.275433
H	13.069825	18.807684	16.518032
H	8.239497	18.172370	13.726451
H	7.109821	13.928582	14.150655
H	11.937345	20.804888	16.190273
H	11.251270	21.399262	14.893897
H	9.835352	15.376143	12.255594
H	11.395217	18.396908	12.153572
H	9.800337	16.944594	12.479265
O	6.132652	17.823505	15.284876
O	13.745236	16.628116	15.165007
O	7.530377	20.228429	15.126058
O	12.320324	14.258559	15.261157
O	6.857058	16.033278	14.155652
O	12.937401	18.313029	13.926311
O	9.490004	20.552988	14.095445
O	10.536936	14.208711	13.913433
O	7.969888	13.774451	14.561217
O	11.873100	20.715913	15.180041
O	9.265453	16.089285	12.573849
O	10.573036	18.360239	12.653936
O	8.728456	17.893073	14.506707
O	10.859923	16.692849	15.115128
O	12.199152	18.398473	16.506965
O	9.763439	19.049982	16.511623
Zr	9.009477	15.674659	14.830804
Zr	10.828297	18.726365	14.691992
C	15.111003	17.576990	19.684394
C	4.767326	16.971293	19.634043
C	12.353679	12.733877	19.694883
C	7.665481	22.016291	19.563497
C	13.845988	17.578955	18.890025
C	6.047137	16.987238	18.858214
C	11.739379	13.852803	18.919447
C	8.310929	20.943235	18.742956
H	10.479942	13.812526	16.623413
H	8.307262	18.325436	19.426789
H	7.182350	14.050203	19.149872
H	11.572822	21.452652	18.233234
H	10.185211	17.648541	20.652852
H	9.680009	15.577601	21.098390
H	11.595046	18.350937	20.814697
O	13.774663	16.731951	17.950854
O	6.185759	17.910665	17.998909
O	12.390415	14.316918	17.935866
O	7.579243	20.347998	17.896116
O	12.936612	18.397784	19.191351
O	6.920927	16.135012	19.143462
O	10.626319	14.280774	19.310828
O	9.517312	20.648253	18.972874
O	11.924732	20.668808	17.797552
O	8.027616	13.880318	18.715177

O	10.691492	18.522377	20.516912
O	9.348652	16.305658	20.561717
O	10.910746	16.793182	18.030898
O	8.798249	18.044257	18.648497
O	8.279445	16.456704	16.647763
O	10.000918	14.649946	16.645438
Zr	10.869662	18.926472	18.261154
Zr	9.117279	15.792606	18.550111
Zr	12.146838	16.058602	16.593551
Zr	7.777125	18.523412	16.590255
H	8.400677	22.637858	13.116582
H	7.105886	21.512205	12.677717
H	6.918398	22.493598	14.131663
H	12.708677	13.123358	20.659069
H	11.601115	11.969489	19.924138
H	13.203561	12.288873	19.167973
H	15.967105	17.722194	19.013600
H	15.116601	18.352772	20.456358
H	15.251320	16.592056	20.148457
H	4.465905	15.929444	13.264761
H	3.922926	17.416904	14.122305
H	4.955019	17.525760	12.687174
H	13.173471	12.282177	13.992855
H	11.576275	11.929147	13.240549
H	12.650587	13.121646	12.515450
H	8.403929	22.708318	19.981571
H	6.911758	22.557789	18.981841
H	7.142754	21.537976	20.403580
H	15.973489	17.294845	14.117249
H	15.082129	16.725591	12.709540
H	15.260287	18.474878	12.959117
H	4.897262	17.598716	20.527068
H	3.941605	17.393337	19.051824
H	4.519815	15.961299	19.977735
Ir	7.783272	13.890457	16.650608
H	6.238628	13.589924	16.638554
C	8.112955	11.878496	16.643654
C	9.590616	11.547460	16.623136
H	7.607929	11.451052	15.761990
H	7.635873	11.468739	17.549731
C	9.892481	10.052995	16.620718
H	10.058279	11.998002	15.725513
H	10.085175	12.000564	17.505044
C	11.374746	9.741999	16.598630
H	9.421903	9.589856	17.505024
H	9.395179	9.587892	15.752237
H	11.572953	8.661085	16.596485
H	11.863361	10.164430	15.707499
H	11.890020	10.165817	17.473869

TS3@NU-1000

Electronic Energy: -3585.4474166
Enthalpy: -3584.689874
Free Energy: -3584.840871

C	4.75048500	16.93541400	13.59152300
C	15.11751200	17.51775700	13.47072100
C	7.65142700	21.95149200	13.52470800
C	12.30937500	12.71061100	13.47586600
C	5.99466000	16.91122100	14.42101100
C	13.84189400	17.49238400	14.24873800
C	8.27868200	20.84268600	14.30829000
C	11.67348600	13.80135200	14.27549800
H	13.07606900	18.78559000	16.53297800
H	8.25469200	18.20112300	13.73027600
H	7.16987500	13.79772300	14.92863500
H	11.94676100	20.80931000	16.22410600
H	11.26958500	21.41245600	14.92425300
H	9.91695100	15.39895700	12.35092600
H	11.38999000	18.39572100	12.18989300
H	9.80840800	16.96475100	12.55058300
O	6.12987300	17.83003800	15.27771300
O	13.75140200	16.62554200	15.16478500
O	7.52109100	20.24272200	15.12884700
O	12.36277200	14.27891800	15.22082200
O	6.85027100	16.01020700	14.18676200
O	12.93758600	18.31520200	13.93725600
O	9.49057000	20.55848500	14.11114500
O	10.50900000	14.17826400	13.96410900
O	8.02798100	13.88773100	15.35698600
O	11.88283800	20.72188600	15.20944200
O	9.30282300	16.08581800	12.64405300
O	10.56475300	18.37027600	12.68582400
O	8.72221100	17.91794400	14.52171200
O	10.85234700	16.70747900	15.13350500
O	12.19967600	18.38887500	16.52920900
O	9.76637300	19.07415200	16.54270000
Zr	9.00090500	15.67770400	14.89246400
Zr	10.82684600	18.73878100	14.73337000
C	15.11098600	17.57679500	19.68442100
C	4.76735400	16.97131900	19.63408900
C	12.35373500	12.73385000	19.69480000
C	7.66593900	22.01501000	19.56485100
C	13.84602700	17.57935800	18.89005600
C	6.04658800	16.98718300	18.85817500
C	11.73948000	13.85272500	18.91972900
C	8.31077100	20.94474300	18.74122300
H	10.22163300	13.84799500	16.66238500
H	8.34460700	18.31551800	19.48335100
H	7.04548000	14.18055800	18.23846800
H	11.61479400	21.48284300	18.24817800
H	8.61031900	15.41634200	21.05649700
H	11.64616100	18.55701200	20.77485900

O	13.76478800	16.72027600	17.96323200
O	6.19744900	17.92949400	18.03228800
O	12.44387100	14.36285800	18.00282100
O	7.56726900	20.35303200	17.90226900
O	12.96555400	18.42830200	19.17373500
O	6.90489500	16.08524500	19.09148500
O	10.56884000	14.22215800	19.22196200
O	9.52017700	20.67818200	18.95198300
O	11.94659300	20.69100600	17.81249700
O	7.94742700	13.94095400	17.98359000
O	10.74359600	18.68183800	20.45808000
O	9.15982900	16.09255500	20.64159900
O	10.91917000	16.80426800	18.07127400
O	8.80790100	18.05082100	18.68042000
O	8.31438800	16.55027400	16.65460700
O	10.13159200	14.80561300	16.64815400
Zr	10.89976800	18.95285100	18.33887200
Zr	9.17400500	15.85225900	18.42129000
Zr	12.15692200	16.04157400	16.58696100
Zr	7.79418500	18.57270200	16.58836600
H	8.39448000	22.54417400	12.98153800
H	6.95281100	21.51864900	12.79581600
H	7.05538700	22.59416900	14.18313700
H	11.60463300	12.17393100	20.26327300
H	12.91046700	12.06490600	19.02869700
H	13.08343800	13.15181700	20.40209500
H	15.96951500	17.69434600	19.01107700
H	15.12621100	18.37035000	20.43790600
H	15.23820600	16.60188400	20.17320500
H	4.51966900	15.94959600	13.17430400
H	3.90101300	17.32246900	14.16452200
H	4.91142300	17.62298200	12.74916700
H	12.60519500	11.89024100	14.14190500
H	11.64382400	12.32555300	12.69693900
H	13.23657000	13.08226000	13.02025200
H	8.37780600	22.49795300	20.24213400
H	7.20452300	22.76862400	18.91335100
H	6.84548200	21.57650100	20.14884100
H	15.97824600	17.44667300	14.14619100
H	15.15940700	16.63097500	12.82331100
H	15.19788400	18.41358400	12.84729300
H	4.91377100	17.55728700	20.55330000
H	3.95574300	17.44132100	19.06937800
H	4.48969800	15.95648000	19.93980600
H	7.91873800	13.82286700	16.97548600
Ir	9.36966700	17.64729400	21.90751500
C	9.41183400	19.43873600	23.16799900
C	8.41292500	19.43905400	22.12357700
H	7.35656200	19.38033900	22.41820500
H	8.60636000	20.07781900	21.25348500
H	8.40438900	16.92334400	22.94119200
H	10.23701100	18.28078500	23.11450500
C	8.98990800	19.39371500	24.62130200

C	10.06096800	18.89597400	25.56838000
H	8.08558900	18.77096100	24.70735900
H	8.68057900	20.41500900	24.90359300
H	9.72912600	18.92785700	26.61437700
H	10.33536400	17.85354100	25.34516900
H	10.97854800	19.49951700	25.49833400
H	10.26908000	20.10535600	22.98068100

Ir(1-butene) H_2@NU-1000

Electronic Energy: -3585.4697721

Enthalpy: -3584.711930

Free Energy: -3584.863121

C	4.75050100	16.93540900	13.59149900
C	15.11750200	17.51769700	13.47070300
C	7.65139400	21.95139100	13.52459200
C	12.30939100	12.71058900	13.47590800
C	5.99466300	16.91129700	14.42100600
C	13.84201600	17.49260800	14.24870200
C	8.27876200	20.84286500	14.30841200
C	11.67336400	13.80128800	14.27541000
H	13.08100000	18.78868900	16.52400700
H	8.25428200	18.19832500	13.72194700
H	7.16329000	13.79991500	14.93520700
H	11.95130300	20.80565300	16.20507000
H	11.26838800	21.40886700	14.91083000
H	9.91288800	15.38535900	12.36162400
H	11.38396400	18.38876100	12.17318600
H	9.80153900	16.95126200	12.54722700
O	6.13060500	17.83445400	15.27311600
O	13.75253200	16.63072400	15.16875000
O	7.52202300	20.24325700	15.12908000
O	12.36339900	14.28213800	15.21836300
O	6.84845600	16.00834000	14.19050300
O	12.93507700	18.30927900	13.92706400
O	9.48944000	20.55648600	14.10575100
O	10.50442400	14.17065200	13.97156500
O	8.01984500	13.88940200	15.36666900
O	11.88578600	20.72038600	15.19258000
O	9.29722900	16.07413500	12.64727700
O	10.56058600	18.36557700	12.67233800
O	8.72164800	17.91829000	14.51459900
O	10.85254300	16.70570600	15.12362100
O	12.20475100	18.39181200	16.51414800
O	9.77291800	19.07952500	16.53020600
Zr	8.99650900	15.67799700	14.90159600
Zr	10.82792100	18.73385100	14.71682500
C	15.11103600	17.57704100	19.68434200
C	4.76730300	16.97133500	19.63400600
C	12.35368500	12.73386400	19.69486000
C	7.66547500	22.01627400	19.56351500

C	13.84611100	17.57916500	18.89001700
C	6.04687100	16.98735900	18.85830100
C	11.73942500	13.85253600	18.91949900
C	8.31090100	20.94318000	18.74292900
H	10.21417800	13.84736300	16.65477000
H	8.29727700	18.39047100	19.43910300
H	7.06049100	14.12034400	18.28208400
H	11.56366000	21.47549300	18.21618300
H	9.84275800	15.43755300	20.94763000
H	11.52479600	19.07508600	20.92541600
O	13.75135000	16.69801800	17.98196600
O	6.19464000	17.92365900	18.02411200
O	12.42602500	14.34157000	17.98363400
O	7.57088400	20.34759800	17.90220400
O	12.98030100	18.45189000	19.14283200
O	6.90222100	16.08420900	19.09077000
O	10.58486600	14.24693500	19.25980800
O	9.52601400	20.68720000	18.94110400
O	11.94331200	20.69053900	17.80692600
O	7.96218200	13.92627400	17.99186600
O	10.77031800	18.67736200	20.47761300
O	9.30171600	16.13793500	20.56260900
O	10.90975300	16.81742600	18.04517700
O	8.80755100	18.06246600	18.68664900
O	8.31307600	16.56128500	16.65330100
O	10.12465700	14.80521000	16.65889700
Zr	10.90266900	18.94383600	18.30878200
Zr	9.15668100	15.84635700	18.44120600
Zr	12.15108000	16.04353800	16.58497800
Zr	7.79497800	18.57172400	16.57996300
H	8.39785100	22.56830800	13.01388200
H	6.98976400	21.51394400	12.76434900
H	7.01870100	22.56947000	14.17186600
H	13.06922400	13.15463800	20.41527100
H	11.60306100	12.16270100	20.25051900
H	12.92632000	12.07376900	19.03383300
H	15.96838300	17.69594200	19.00947600
H	15.12618100	18.37229000	20.43594600
H	15.24082000	16.60322700	20.17424300
H	4.51855500	15.94938400	13.17538000
H	3.90154600	17.32416200	14.16412600
H	4.91209300	17.62196800	12.74845900
H	12.55892700	11.87103000	14.13737900
H	11.65984900	12.35415700	12.67030500
H	13.26157300	13.06365700	13.05937300
H	8.18805400	22.15816300	20.51607500
H	7.71413000	22.96780100	19.01440300
H	6.60530200	21.79735600	19.72969900
H	15.97888800	17.41376500	14.14077900
H	15.14118800	16.64885300	12.79830300
H	15.21047200	18.42746600	12.86949000
H	4.21106900	17.90537100	19.50927300
H	4.13554800	16.14564000	19.27599800

H	4.95331100	16.77528300	20.69767700
Ir	9.33026600	17.90805600	21.78315600
H	9.89165400	18.75516900	22.97470100
H	8.91087100	19.35606700	22.22736000
H	7.91211000	13.82166300	16.98286100
C	8.34482600	16.77543000	23.24646900
H	8.48375900	17.11615100	24.27849500
H	8.56639700	15.71219100	23.09484000
C	7.38639100	17.41431300	22.42099900
H	6.99961600	16.81685100	21.57954900
C	6.45343700	18.49717700	22.88617500
C	6.15627400	19.56322300	21.84741300
H	6.85401400	18.96322900	23.80242300
H	5.50929600	18.01158400	23.19674700
H	5.32443200	20.21460700	22.14996800
H	7.02955800	20.20847100	21.67814800
H	5.89297000	19.13047600	20.86886100

Table S5. XYZ Cartesian Coordinates of All Optimized Structures on the UiO-66 Site-1 Support (All Energies Are in Hartree).

UiO-66

Electronic Energy: -3551.824925
Enthalpy: -3551.186974
Free Energy: -3551.313139

O	13.74973200	11.56229600	23.34789400
Zr	13.69132500	13.51249200	24.56972500
C	10.48247900	13.51746100	23.85898200
C	9.43055900	13.62944900	22.79494800
O	10.09571800	13.47231800	25.05536000
O	11.69097900	13.47106800	23.47419500
O	15.71465300	13.45927200	23.54333200
O	13.60109600	15.43967800	23.47551300
Zr	13.71944200	10.93887800	27.06605300
Zr	11.12938000	13.40821600	27.03442300
O	15.04323000	14.94880200	25.66720100
O	12.30639600	12.00719200	25.61689900
O	12.58025400	14.50483200	25.99243100
O	14.73483900	12.47411500	26.01888400
C	13.49592700	16.64233700	23.85446400
C	13.29574100	17.68428400	22.79451300
O	13.51595600	17.03363200	25.05376600
C	16.90947300	13.43502200	23.95455100
O	17.26170600	13.52707400	25.16591300
Zr	13.56213400	16.00835500	27.05825000
Zr	16.15057600	13.56337000	27.10557500
H	11.76407200	11.40697500	25.09835300
H	15.59563300	15.51588100	25.12344000
H	11.57835100	15.40864200	28.99143900
O	12.16011900	14.87085400	28.44858300
O	15.49742400	17.12022800	27.13852600
O	11.55983400	16.99260800	26.94579500
O	13.55420800	17.06668700	29.02431700
Zr	13.59213800	13.48900000	29.56795900
O	14.62881900	14.57024900	28.11527400
H	15.64367300	11.59597500	29.06392600
O	15.07577000	12.11888400	28.49247200
O	11.72564700	9.89542600	27.21554100
O	15.76667300	9.97855900	27.01584600
O	13.69903200	9.91083500	29.05023100
O	12.60599300	12.42692400	28.08735800
O	17.15636000	13.67020400	29.11020500
O	17.13113300	15.57912800	27.18230000
O	17.28009300	11.63703800	27.07614000
O	10.04401300	13.33134600	28.98906200

O	10.10770300	11.43759200	27.03101400
O	10.01477300	15.36320700	26.95823400
C	10.36825400	16.57166100	26.87875800
C	9.29455800	17.59624600	26.66134400
C	13.61091100	16.68242900	30.22799500
C	13.76036900	17.74268300	31.27886000
O	13.58123100	15.48123500	30.61465900
C	16.94889000	10.42182000	26.99120900
C	18.05510100	9.41984000	26.83160200
C	13.57768500	10.30254300	30.24581800
C	13.40033200	9.24675300	31.29605400
O	13.57185100	11.50822400	30.62300700
C	16.70763100	16.76789400	27.23208400
C	10.52143200	10.24471200	27.15824800
C	9.48179700	9.17022800	27.28463300
C	16.74533900	13.71904700	30.30458500
C	17.77035700	13.95239300	31.37471400
O	15.54010200	13.60774500	30.66629800
C	10.41572100	13.28582000	30.19569400
C	9.35677700	13.06176900	31.23409300
O	11.60922000	13.38826000	30.59754200
H	9.57439600	18.56245200	27.09438300
H	9.17396300	17.74566100	25.57907700
H	8.33172400	17.25541100	27.05614600
H	9.23006600	9.05451600	28.34827800
H	8.55972100	9.44270100	26.75995700
H	9.86275700	8.20734700	26.92861200
H	18.96412900	9.75088100	27.34538300
H	17.75120800	8.42786300	27.18167800
H	18.30096200	9.33896700	25.76315800
C	17.72325600	17.85015900	27.45000700
H	17.38915400	18.80257300	27.02515000
H	17.84286500	17.99659100	28.53278900
H	18.70128800	17.56460800	27.04859400
H	13.72475000	9.60120300	32.27991100
H	12.33000600	9.00615800	31.36439500
H	13.92239200	8.32389600	31.02153100
H	14.83321700	17.92581800	31.43250900
H	13.30979000	18.68794700	30.95828500
H	13.34281100	17.41584000	32.23698200
H	13.74551600	17.37917200	21.84373700
H	12.21571400	17.79926200	22.62589300
H	13.68290800	18.65680900	23.11575400
H	9.76748300	13.18928000	21.85044800
H	8.48727000	13.17855900	23.12082400
H	9.23654300	14.69500700	22.60717600
H	18.74726000	13.55298100	31.08248800
H	17.88686700	15.03690400	31.51036500
H	17.44793900	13.53384100	32.33387900
H	9.64729500	13.49163200	32.19843600
H	8.38845600	13.45464200	30.90664000
H	9.24046600	11.97835800	31.37844000
C	18.00529500	13.28382000	22.93990900

H	18.87563300	13.88913400	23.21672700
H	18.33439200	12.23533000	22.93496500
H	17.66005700	13.53683000	21.93249100
O	13.73957500	9.82753900	25.26880200
H	14.45628500	9.18513500	25.23303000
H	12.93447300	11.41861900	22.85394100
H	13.79271200	10.80226700	24.03763700

$Ir(CO)_2$@UiO-66 site-1

Electronic Energy: -3882.2474418

Enthalpy: -3881.595930

Free Energy: -3881.736255

O	13.76084100	11.69318700	23.29750800
Zr	13.67797000	13.49212400	24.54554100
C	10.48247900	13.51746100	23.85898200
C	9.43055900	13.62944900	22.79494800
O	10.09578600	13.42032500	25.05938100
O	11.68608800	13.52950000	23.48347800
O	15.71646300	13.41993200	23.53164600
O	13.61801600	15.44232200	23.47433900
Zr	13.71025500	10.96996600	27.08918000
Zr	11.12419400	13.41713100	27.02682700
O	15.03732700	14.93617800	25.66198300
O	12.31644300	12.00387900	25.60987600
O	12.57466500	14.49961400	26.00032900
O	14.72853700	12.47378500	26.04450800
C	13.49592700	16.64233700	23.85446400
C	13.29574100	17.68428400	22.79451300
O	13.50528200	17.03130500	25.05584200
C	16.90947300	13.43502200	23.95455100
O	17.25513200	13.54202700	25.16246600
Zr	13.55639100	16.00199200	27.05149100
Zr	16.14163500	13.56840700	27.11141900
H	11.71014500	11.46455100	25.08304100
H	15.58530000	15.51708000	25.12854600
H	11.57759900	15.40768600	28.99464400
O	12.15888500	14.86885600	28.45242600
O	15.49730700	17.11657400	27.13316300
O	11.55912500	16.99092300	26.95447300
O	13.55644900	17.06233700	29.02419000
Zr	13.58980800	13.49638200	29.57889600
O	14.62709500	14.56906800	28.12282700
H	15.63673600	11.59439300	29.08272000
O	15.07372200	12.11581500	28.50530800
O	11.72922300	9.88359500	27.16146600
O	15.76129200	9.98370700	26.99539300
O	13.68975400	9.91465300	29.04694500
O	12.60202600	12.41910500	28.09881600
O	17.15453200	13.66738200	29.11031300
O	17.13057800	15.57800400	27.18372300
O	17.28064900	11.63457600	27.08632500

O	10.04500000	13.33980900	28.99020700
O	10.11984200	11.44017800	27.05671800
O	10.01386400	15.36223700	26.94886100
C	10.36825400	16.57166100	26.87875800
C	9.29455800	17.59624600	26.66134400
C	13.61091100	16.68242900	30.22799500
C	13.76036900	17.74268300	31.27886000
O	13.57843900	15.48114700	30.61850800
C	16.94889000	10.42182000	26.99120900
C	18.05510100	9.41984000	26.83160200
C	13.57768500	10.30254300	30.24581800
C	13.40033200	9.24675300	31.29605400
O	13.57718800	11.50653800	30.62568600
C	16.70763100	16.76789400	27.23208400
C	10.52143200	10.24471200	27.15824800
C	9.48179700	9.17022800	27.28463300
C	16.74533900	13.71904700	30.30458500
C	17.77035700	13.95239300	31.37471400
O	15.54000500	13.61049200	30.66818200
C	10.41572100	13.28582000	30.19569400
C	9.35677700	13.06176900	31.23409300
O	11.61038600	13.38302500	30.59896000
H	9.58207900	18.56808000	27.07589000
H	9.15817500	17.72698700	25.57856900
H	8.33659700	17.26270600	27.07392400
H	9.59626700	8.66978700	28.25518400
H	8.46832500	9.57318400	27.19996500
H	9.64567700	8.39959200	26.52024200
H	18.93416900	9.71312800	27.41605300
H	17.72994900	8.41062600	27.10409200
H	18.36628900	9.40676200	25.77740700
C	17.72325600	17.85015900	27.45000700
H	17.38801600	18.80287700	27.02692900
H	17.84517900	17.99498900	28.53271600
H	18.70045600	17.56511500	27.04629400
H	13.77895000	9.58316500	32.26685000
H	12.32425400	9.05445600	31.41058400
H	13.87107000	8.30419200	30.99753200
H	14.83339900	17.91419400	31.44406800
H	13.32278300	18.69200400	30.95262600
H	13.32963800	17.42103200	32.23289300
H	13.74557400	17.37875400	21.84408000
H	12.21576000	17.79938200	22.62593600
H	13.68225700	18.65716700	23.11574100
H	9.59743100	12.86823000	22.02187900
H	8.42233600	13.53089200	23.20786100
H	9.52653900	14.60220100	22.29481100
H	18.74915500	13.55963000	31.08004500
H	17.88057700	15.03686600	31.51567100
H	17.45059900	13.52791400	32.33212000
H	9.65371000	13.47737600	32.20261100
H	8.39253300	13.46916600	30.91242500
H	9.22733600	11.97816000	31.36499800

C	18.00529500	13.28382000	22.93990900
H	18.88135900	13.87894800	23.22034300
H	18.32762200	12.23297300	22.92683100
H	17.66497200	13.54872300	21.93365800
O	13.78415100	9.70525400	25.30133200
H	14.62676700	9.24169100	25.23441200
H	14.59592600	11.63405800	22.81958900
Ir	12.71589700	9.88915500	23.50785400
C	11.80730100	8.32486200	23.81944900
C	11.78441200	10.17942300	21.95296100
O	11.23500200	7.34640400	24.04459600
O	11.19722900	10.39217700	20.98056600

Catalytic Hydrogenation Mechanism on UiO-66 site-1 (Figure 3)

$Ir(C_2H_4)_2$@UiO-66 site-1

Electronic Energy: -3812.7981964

Enthalpy: -3812.054859

Free Energy: -3812.197856

O	13.75938400	11.74282200	23.25675500
Zr	13.68724200	13.48440500	24.54115800
C	10.48255300	13.51725800	23.85930100
C	9.43058100	13.62937000	22.79491800
O	10.08411100	13.39539200	25.05393100
O	11.68576300	13.55472500	23.49321200
O	15.72016900	13.44292800	23.52594400
O	13.62283500	15.44380400	23.47301300
Zr	13.71898500	10.96482600	27.08187000
Zr	11.12292100	13.40813900	27.01801100
O	15.03759000	14.93612500	25.66392500
O	12.33090600	11.97549400	25.58178600
O	12.57194700	14.48873200	26.00093500
O	14.73439100	12.47249100	26.04346000
C	13.49575800	16.64228000	23.85451700
C	13.29563300	17.68423000	22.79448000
O	13.50011200	17.02995200	25.05668600
C	16.90956700	13.43504600	23.95458600
O	17.25450600	13.53255500	25.16352700
Zr	13.55398400	15.99601300	27.05000700
Zr	16.14359400	13.56779300	27.11091000
H	11.74776600	11.42385200	25.04231200
H	15.58427000	15.51758000	25.12988300
H	11.57761000	15.40673600	28.99365300
O	12.15629500	14.86656100	28.45010900
O	15.49727700	17.11576100	27.13370600
O	11.55838300	16.99138900	26.95776200
O	13.55589900	17.06206000	29.02402700
Zr	13.58730500	13.49485400	29.57277700
O	14.62737500	14.56902900	28.12277500
H	15.63557800	11.59586700	29.08368800

O	15.07389100	12.11739100	28.50518800
O	11.72894200	9.89336800	27.18628300
O	15.76517000	9.97828500	27.01562900
O	13.69500100	9.91263500	29.04862500
O	12.59895600	12.41956000	28.08801800
O	17.15622400	13.66700300	29.11071800
O	17.13228400	15.57844900	27.18317100
O	17.27983700	11.63530400	27.07858000
O	10.04526800	13.33242800	28.98927300
O	10.10795400	11.43439100	27.03233600
O	10.01409600	15.36124300	26.94130500
C	10.36830300	16.57167600	26.87877000
C	9.29455300	17.59624100	26.66134200
C	13.61095900	16.68247600	30.22802100
C	13.76036800	17.74268300	31.27886100
O	13.57790100	15.48099400	30.61819800
C	16.94891500	10.42184500	26.99119200
C	18.05508300	9.41981700	26.83162000
C	13.57749300	10.30257100	30.24572400
C	13.40022700	9.24672200	31.29600600
O	13.57170700	11.50742700	30.62376100
C	16.70774000	16.76796900	27.23204400
C	10.52148800	10.24496100	27.15807500
C	9.48180800	9.17021100	27.28457700
C	16.74543500	13.71902000	30.30464000
C	17.77035600	13.95237900	31.37471800
O	15.53995000	13.61084700	30.66730800
C	10.41575500	13.28584000	30.19569800
C	9.35677400	13.06176900	31.23409000
O	11.60958500	13.38634100	30.59937300
H	9.57618200	18.56435300	27.08871700
H	9.16984700	17.73912100	25.57867300
H	8.33301400	17.25733900	27.06102600
H	8.79069300	9.41652900	28.10073400
H	8.87548900	9.13505900	26.36913000
H	9.93278400	8.18867600	27.45952400
H	18.94319800	9.72500200	27.39595100
H	17.73614000	8.41536800	27.12824700
H	18.34824200	9.38633800	25.77264600
C	17.72325600	17.85016200	27.44999500
H	17.38595600	18.80433400	27.03179600
H	17.84976200	17.99078000	28.53274200
H	18.69905400	17.56722500	27.04131400
H	13.72813500	9.60056300	32.27883200
H	12.32927600	9.00991400	31.36672000
H	13.91872700	8.32212300	31.02047900
H	14.83332400	17.91435500	31.44441600
H	13.32270900	18.69198100	30.95255800
H	13.32935800	17.42101800	32.23279700
H	13.76580100	17.38794600	21.85087900
H	12.21685000	17.78081500	22.60756100
H	13.66133500	18.66259800	23.12327500
H	9.87011000	13.79686900	21.80693800

H	8.82670400	12.71187200	22.77513700
H	8.73968900	14.44578400	23.04117600
H	18.74784800	13.55471500	31.08212500
H	17.88504900	15.03693100	31.51150100
H	17.44852800	13.53264900	32.33355000
H	9.64693100	13.49191900	32.19843000
H	8.38846900	13.45439800	30.90635600
H	9.24086300	11.97833600	31.37863400
C	18.00528100	13.28384700	22.93989000
H	18.88834800	13.86428000	23.22918900
H	18.31443500	12.22929100	22.91158300
H	17.66934000	13.56722200	21.93716900
O	13.78164400	9.65994300	25.35599800
H	14.57246300	9.10893500	25.37081000
H	14.52140500	11.77230600	22.66744600
Ir	12.90571700	9.80759500	23.42738100
C	11.56074200	10.35630200	21.92597300
H	10.62094800	9.79231700	21.92033900
H	11.43967500	11.44599800	21.95000600
C	12.72991400	9.80344100	21.35321900
H	13.48032100	10.46678600	20.90347800
H	12.70915900	8.80282600	20.90618600
C	12.75576300	7.73142400	23.44332600
H	12.73228600	7.27529500	22.44691400
H	13.51734600	7.29834200	24.10482400
C	11.58422100	8.29478100	24.00071200
H	11.47243700	8.32708600	25.09118400
H	10.63980300	8.27219800	23.44493800

Ir(C_2H_4)$_2H_2$@UiO-66 site-1

Electronic Energy: -3813.9749169

Enthalpy: -3813.212387

Free Energy: -3813.353849

Zr	13.68175000	13.48275600	24.53218000
C	10.48255300	13.51725800	23.85930100
C	9.43058100	13.62937000	22.79491800
O	10.08776300	13.39467500	25.05663600
O	11.68053700	13.58507100	23.49015700
O	15.72289600	13.47499400	23.52464900
O	13.62460400	15.44464100	23.47211900
Zr	13.72837900	10.96295900	27.07617900
Zr	11.12862400	13.41070800	27.01672300
O	15.03583500	14.92755100	25.66707600
O	12.33931600	11.99784700	25.58721100
O	12.57512900	14.49019700	26.00327000
O	14.75856500	12.43666800	26.01058800
C	13.49575800	16.64228000	23.85451700
C	13.29563300	17.68423000	22.79448000
O	13.50071900	17.02937100	25.05676600
C	16.90956700	13.43504600	23.95458600

O	17.25900200	13.53196700	25.16218200
Zr	13.55587800	15.99549200	27.04986200
Zr	16.14878400	13.56292300	27.10770200
H	11.85409100	11.38614200	25.02761300
H	15.58699400	15.49817800	25.12595500
H	11.57878500	15.40255000	28.99455400
O	12.15889900	14.86440300	28.45053300
O	15.49734900	17.11529300	27.13330800
O	11.55840300	16.99137700	26.95819400
O	13.55730100	17.06185100	29.02381600
Zr	13.59061300	13.49131800	29.57268900
O	14.62802200	14.56213400	28.11702300
H	15.64804700	11.59317900	29.06925600
O	15.08162800	12.12331700	28.50340800
O	11.72643000	9.88022900	27.18711700
O	15.76815200	9.98584300	27.04515000
O	13.68547400	9.91571000	29.04734800
O	12.60534000	12.41423300	28.08816300
O	17.15729900	13.66795500	29.11068700
O	17.13258100	15.57828300	27.18246400
O	17.28554400	11.63946700	27.05507900
O	10.04579700	13.33562800	28.98931200
O	10.11615700	11.43515700	27.05222100
O	10.01455000	15.36112900	26.94146300
C	10.36830300	16.57167600	26.87877000
C	9.29455300	17.59624100	26.66134200
C	13.61095900	16.68247600	30.22802100
C	13.76036800	17.74268300	31.27886100
O	13.57849600	15.48087500	30.61770900
C	16.94891500	10.42184500	26.99119200
C	18.05508300	9.41981700	26.83162000
C	13.57749300	10.30257100	30.24572400
C	13.40022700	9.24672200	31.29600600
O	13.57994900	11.50690900	30.62643000
C	16.70774000	16.76796900	27.23204400
C	10.52148800	10.24496100	27.15807500
C	9.48180800	9.17021100	27.28457700
C	16.74543500	13.71902000	30.30464000
C	17.77035600	13.95237900	31.37471800
O	15.54013600	13.61301000	30.66749900
C	10.41575500	13.28584000	30.19569800
C	9.35677400	13.06176900	31.23409000
O	11.61005900	13.38218300	30.59955800
H	9.57487600	18.56338900	27.09178300
H	9.17229700	17.74184500	25.57875900
H	8.33223300	17.25597100	27.05795400
H	9.19249600	9.09005500	28.34190600
H	8.57589400	9.42523000	26.72343700
H	9.86979100	8.19480800	26.97285900
H	18.91728300	9.69179900	27.45154200
H	17.71788500	8.40444700	27.06383000
H	18.39756800	9.44134500	25.78684200
C	17.72325600	17.85016200	27.44999500

H	17.38529800	18.80468600	27.03312100
H	17.85111500	17.98962600	28.53273200
H	18.69862200	17.56769000	27.03995700
H	13.78016100	9.58218000	32.26666800
H	12.32413800	9.05484000	31.41154700
H	13.87081300	8.30425800	30.99674800
H	14.83338200	17.91470100	31.44364000
H	13.32217000	18.69188100	30.95292900
H	13.33007400	17.42083500	32.23306100
H	13.76210200	17.38598100	21.84970600
H	12.21661900	17.78505600	22.61098300
H	13.66557700	18.66159300	23.12164200
H	9.76759300	13.16707000	21.86004400
H	8.47837200	13.19736800	23.12004900
H	9.26133300	14.69486800	22.58535900
H	18.74741000	13.55294300	31.08303100
H	17.88650200	15.03701800	31.50957200
H	17.44776500	13.53462500	32.33416800
H	9.64393100	13.49889800	32.19625300
H	8.38663000	13.44750000	30.90367300
H	9.24693000	11.97867400	31.38555800
C	18.00528100	13.28384700	22.93989000
H	18.66378700	14.16157200	22.97769000
H	18.63306400	12.42083300	23.19846600
H	17.61259100	13.16963600	21.92461800
C	12.39026200	9.55542300	21.78945400
C	11.83804200	9.59406100	23.08025000
C	15.90099600	8.75986900	23.87668800
C	16.00412400	10.15013700	23.76679900
H	12.90661400	8.95796800	25.60208000
H	14.42164800	12.06361800	22.51819700
H	13.87991400	8.00415400	23.18316600
H	14.58849700	9.53369500	21.77452900
H	12.43366500	10.47533300	21.20082700
H	12.39151000	8.63170200	21.20743300
H	11.39789900	8.69991500	23.53143600
H	11.44508700	10.55003400	23.44038400
H	15.72479600	8.31084900	24.85764400
H	16.33235200	8.10470200	23.11711500
H	16.49692700	10.60180900	22.90092700
H	15.90077600	10.79980200	24.64176600
Ir	13.98646700	9.57723300	23.23309300
O	13.63500000	9.56539900	25.43485800
O	13.74025400	11.81674900	23.15557200

TS1@UiO-66 site-1

Electronic Energy: -3813.950687

Enthalpy: -3813.190384

Free Energy: -3813.330997

O	13.734078	11.757208	23.228624

Zr	13.678360	13.477522	24.541266
C	10.482532	13.517328	23.859207
C	9.430581	13.629390	22.794920
O	10.081808	13.409082	25.054307
O	11.684617	13.542336	23.492057
O	15.720133	13.431610	23.527604
O	13.617376	15.443526	23.473701
Zr	13.700964	10.973235	27.083280
Zr	11.122321	13.409036	27.014611
O	15.036374	14.931886	25.663109
O	12.338679	12.009757	25.616443
O	12.570307	14.498448	26.000639
O	14.750566	12.459502	26.034747
C	13.495917	16.642293	23.854512
C	13.295622	17.684250	22.794502
O	13.505292	17.032603	25.056210
C	16.909550	13.434906	23.954667
O	17.257222	13.535623	25.162656
Zr	13.553255	15.996591	27.048051
Zr	16.139789	13.566616	27.110398
H	11.857767	11.407359	25.027620
H	15.582975	15.513102	25.128841
H	11.575895	15.405437	28.992688
O	12.157025	14.866502	28.450576
O	15.497567	17.116061	27.133423
O	11.558149	16.992536	26.956940
O	13.556112	17.061970	29.024437
Zr	13.586887	13.495833	29.576517
O	14.626864	14.567321	28.122678
H	15.630882	11.593324	29.083080
O	15.070679	12.115596	28.503948
O	11.726811	9.884559	27.170452
O	15.762271	9.982132	26.989523
O	13.689689	9.913651	29.047999
O	12.596016	12.417970	28.100889
O	17.155649	13.666513	29.110922
O	17.132127	15.578424	27.182875
O	17.283705	11.631925	27.095191
O	10.045193	13.335785	28.990172
O	10.115351	11.437476	27.044581
O	10.013114	15.362250	26.944145
C	10.368263	16.571680	26.878754
C	9.294558	17.596246	26.661341
C	13.610903	16.682464	30.228009
C	13.760404	17.742680	31.278859
O	13.578212	15.481341	30.619476
C	16.948888	10.421930	26.991048
C	18.055074	9.419797	26.831688
C	13.577646	10.302563	30.245734
C	13.400218	9.246746	31.296028
O	13.576409	11.506394	30.627109
C	16.707690	16.767947	27.232049
C	10.521462	10.244859	27.158152

C	9.481804	9.170218	27.284605
C	16.745381	13.719027	30.304616
C	17.770363	13.952374	31.374713
O	15.540293	13.610551	30.668509
C	10.415711	13.285825	30.195705
C	9.356779	13.061769	31.234095
O	11.609623	13.385442	30.601088
H	9.577009	18.565014	27.086756
H	9.167801	17.737503	25.578676
H	8.333575	17.258231	27.063199
H	8.489204	9.587328	27.480012
H	9.445286	8.598211	26.346649
H	9.762533	8.461474	28.072664
H	17.727484	8.408579	27.094245
H	18.376051	9.415365	25.780206
H	18.929709	9.707165	27.425800
C	17.723264	17.850155	27.449992
H	17.386833	18.803754	27.029697
H	17.848118	17.992729	28.532685
H	18.699638	17.566439	27.043171
H	13.788705	9.578721	32.264619
H	12.323531	9.063359	31.419254
H	13.861640	8.300926	30.993188
H	14.833383	17.912165	31.446583
H	13.325179	18.692805	30.951655
H	13.326957	17.422124	32.232109
H	13.752102	17.381376	21.846283
H	12.215927	17.793038	22.619920
H	13.675486	18.659299	23.117359
H	8.812090	12.721457	22.790780
H	8.752899	14.460065	23.029969
H	9.870657	13.776714	21.803921
H	18.748867	13.558254	31.080648
H	17.881926	15.036836	31.514850
H	17.450173	13.529038	32.332552
H	9.652958	13.478256	32.202547
H	8.392253	13.468497	30.912156
H	9.227933	11.978143	31.365581
C	18.005275	13.283925	22.939871
H	18.886576	13.868582	23.226147
H	18.318429	12.230386	22.915677
H	17.667943	13.561933	21.936037
O	13.759857	9.618101	25.361120
H	14.672969	9.305964	25.351955
H	14.606784	11.756446	22.820768
Ir	13.044599	9.668056	23.348873
C	11.694388	10.109230	21.772593
H	10.826469	9.444073	21.765188
H	11.460760	11.177237	21.780596
C	12.933804	9.682714	21.247057
H	13.621134	10.421321	20.822213
H	13.027364	8.678124	20.818948
C	13.859446	7.660147	23.226537

H	14.186928	7.270006	22.256989
H	14.539938	7.369526	24.035351
C	12.441998	7.698559	23.521712
H	12.129305	7.445574	24.540628
H	11.745650	7.354682	22.746456
H	14.571463	9.009141	22.995449
H	11.638418	10.281410	23.949510

Ir(C_2H_5) (C_2H_4) H@UiO-66 site-1

Electronic Energy: -3813.977509

Enthalpy: -3813.212808

Free Energy: -3813.357084

O	13.776581	11.755678	23.250496
Zr	13.694579	13.489603	24.544594
C	10.482506	13.517317	23.859331
C	9.430581	13.629344	22.794916
O	10.087602	13.399311	25.056268
O	11.684359	13.567244	23.491130
O	15.723308	13.481484	23.523510
O	13.622890	15.443700	23.473603
Zr	13.723382	10.972085	27.077446
Zr	11.124880	13.410236	27.017429
O	15.040757	14.937468	25.668909
O	12.345862	11.976015	25.574743
O	12.575174	14.489117	26.003766
O	14.739175	12.465696	26.037864
C	13.495725	16.642244	23.854588
C	13.295702	17.684195	22.794433
O	13.500723	17.029843	25.056532
C	16.909502	13.435107	23.954625
O	17.253017	13.514403	25.166585
Zr	13.556659	15.996379	27.051982
Zr	16.151401	13.564687	27.110233
H	11.790960	11.414958	25.020703
H	15.589318	15.511356	25.128633
H	11.578458	15.404797	28.995224
O	12.157625	14.865691	28.451122
O	15.497307	17.116143	27.135879
O	11.558435	16.991071	26.957241
O	13.555768	17.062280	29.024199
Zr	13.590861	13.495235	29.573430
O	14.628734	14.567009	28.121628
H	15.639276	11.591289	29.075457
O	15.076131	12.121531	28.506369
O	11.726968	9.889203	27.205935
O	15.764150	9.982428	27.032425
O	13.695171	9.915979	29.047073
O	12.606160	12.419581	28.083551
O	17.157150	13.668061	29.111179
O	17.133268	15.578773	27.182739

O	17.280829	11.637208	27.074153
O	10.045874	13.333533	28.989012
O	10.115115	11.437935	27.036786
O	10.014087	15.361198	26.942681
C	10.368272	16.571715	26.878764
C	9.294553	17.596241	26.661342
C	13.610976	16.682521	30.228016
C	13.760335	17.742681	31.278868
O	13.578802	15.481076	30.618194
C	16.948933	10.421798	26.991354
C	18.055094	9.419853	26.831469
C	13.577513	10.302571	30.245659
C	13.400271	9.246691	31.295983
O	13.571993	11.506914	30.625158
C	16.707724	16.767975	27.232066
C	10.521538	10.244951	27.158088
C	9.481796	9.170215	27.284511
C	16.745462	13.719060	30.304631
C	17.770348	13.952376	31.374726
O	15.540047	13.611972	30.667763
C	10.415742	13.285873	30.195697
C	9.356776	13.061768	31.234092
O	11.609995	13.384179	30.598899
H	9.575032	18.563354	27.091762
H	9.172349	17.742086	25.578791
H	8.332219	17.256130	27.058019
H	9.265909	9.020169	28.351943
H	8.544721	9.461565	26.797539
H	9.845678	8.216376	26.887131
H	18.974673	9.767583	27.314009
H	17.762602	8.436892	27.215358
H	18.271805	9.307740	25.759662
C	17.723254	17.850164	27.449996
H	17.384908	18.805141	27.034475
H	17.851951	17.988403	28.532796
H	18.698351	17.568376	27.038844
H	13.786336	9.580639	32.264788
H	12.323827	9.060604	31.417316
H	13.864992	8.301982	30.994860
H	14.833330	17.914639	31.443868
H	13.322254	18.691883	30.952855
H	13.329913	17.420824	32.233000
H	13.754282	17.382409	21.846938
H	12.216169	17.792171	22.618281
H	13.674095	18.659310	23.118623
H	9.830186	13.377343	21.807307
H	8.562158	13.004100	23.032964
H	9.074910	14.668847	22.762674
H	18.747206	13.552435	31.083109
H	17.887030	15.037001	31.509270
H	17.447624	13.535053	32.334308
H	9.646236	13.493784	32.197821
H	8.387925	13.452469	30.905712

H	9.242479	11.978431	31.380359
C	18.005282	13.283712	22.939911
H	18.924056	13.776137	23.276013
H	18.234070	12.214331	22.827265
H	17.698114	13.664278	21.960135
O	13.707948	9.648358	25.325833
H	13.994067	8.756247	25.552235
H	14.254891	11.964474	22.439101
Ir	13.159439	9.695457	23.307575
C	12.228503	9.990703	21.444098
H	11.430144	9.281086	21.205089
H	11.937195	11.044615	21.349554
C	13.578937	9.612510	21.268411
H	14.336711	10.365484	21.010112
H	13.831826	8.611189	20.907223
C	11.444132	8.568058	23.704591
H	11.262251	7.781836	22.956255
H	11.621388	8.060369	24.667566
C	10.243341	9.482756	23.805483
H	10.339334	10.258249	24.583685
H	10.020192	10.003719	22.862808
H	9.336527	8.912049	24.073467
H	13.452841	8.162905	23.263940

TS2@UiO-66 site-1

Electronic Energy: -3813.96748

Enthalpy: -3813.204687

Free Energy: -3813.348309

O	13.751465	11.740081	23.247558
Zr	13.684107	13.484025	24.538563
C	10.482642	13.517309	23.859166
C	9.430547	13.629355	22.794950
O	10.082814	13.395681	25.053433
O	11.686362	13.554500	23.494469
O	15.719196	13.429771	23.527798
O	13.622828	15.444140	23.472649
Zr	13.716444	10.963313	27.084311
Zr	11.124293	13.410448	27.020213
O	15.037047	14.934809	25.662130
O	12.322134	11.988196	25.594340
O	12.572293	14.492379	26.000252
O	14.734546	12.469899	26.040602
C	13.495711	16.642409	23.854447
C	13.295621	17.684240	22.794492
O	13.500607	17.030487	25.056546
C	16.909505	13.435325	23.954075
O	17.255235	13.539233	25.162312
Zr	13.554416	15.996739	27.049217
Zr	16.141552	13.567159	27.109636
H	11.741829	11.440558	25.047320

H	15.584739	15.516582	25.129458
H	11.577769	15.408140	28.993808
O	12.156619	14.867696	28.450734
O	15.497411	17.116037	27.132642
O	11.558219	16.991737	26.958254
O	13.556447	17.062070	29.024164
Zr	13.587802	13.495154	29.573575
O	14.627383	14.569047	28.122456
H	15.637265	11.596641	29.082985
O	15.073871	12.116567	28.504721
O	11.727964	9.891136	27.183647
O	15.764898	9.979413	27.010464
O	13.693619	9.911759	29.049121
O	12.599006	12.420414	28.092137
O	17.155597	13.666849	29.110676
O	17.131730	15.578302	27.183532
O	17.280481	11.635133	27.079903
O	10.044818	13.335343	28.989857
O	10.107267	11.435258	27.045361
O	10.014016	15.361336	26.941244
C	10.368382	16.571592	26.878789
C	9.294553	17.596243	26.661349
C	13.611018	16.682391	30.228043
C	13.760334	17.742698	31.278851
O	13.577773	15.481044	30.618585
C	16.948893	10.421711	26.991479
C	18.055097	9.419844	26.831552
C	13.577348	10.302584	30.245937
C	13.400251	9.246704	31.295992
O	13.572960	11.507130	30.624413
C	16.707781	16.767921	27.232066
C	10.521501	10.244881	27.158186
C	9.481790	9.170223	27.284535
C	16.745385	13.719009	30.304674
C	17.770359	13.952393	31.374712
O	15.539988	13.610563	30.667869
C	10.415812	13.285811	30.195702
C	9.356763	13.061788	31.234082
O	11.609615	13.385161	30.599819
H	9.576060	18.564231	27.089089
H	9.170113	17.739491	25.578693
H	8.332908	17.257223	27.060705
H	9.043995	9.218968	28.291352
H	8.658780	9.342440	26.580141
H	9.910188	8.173356	27.139281
H	18.941410	9.722204	27.400250
H	17.734657	8.414194	27.122405
H	18.352080	9.391145	25.773504
C	17.723240	17.850174	27.450007
H	17.386713	18.803737	27.029787
H	17.848082	17.992574	28.532717
H	18.699580	17.566433	27.043186
H	13.733581	9.598439	32.277790

H	12.328628	9.014358	31.371468
H	13.913867	8.320225	31.017707
H	14.833284	17.914353	31.444489
H	13.322762	18.692000	30.952423
H	13.329227	17.421185	32.232804
H	13.767584	17.388713	21.851538
H	12.217000	17.779057	22.605696
H	13.659322	18.663125	23.123959
H	9.869281	13.790938	21.805618
H	8.822009	12.714934	22.779983
H	8.744262	14.450414	23.038822
H	18.748337	13.556516	31.081325
H	17.883463	15.036910	31.513110
H	17.449370	13.530862	32.333048
H	9.646251	13.493524	32.197937
H	8.388112	13.452959	30.905648
H	9.242008	11.978442	31.380390
C	18.005352	13.283768	22.939979
H	18.886503	13.868441	23.226465
H	18.317886	12.230082	22.916730
H	17.668199	13.560758	21.935866
O	13.772606	9.662018	25.362795
H	14.623719	9.212163	25.314483
H	14.599951	11.691597	22.793246
Ir	12.848384	9.849127	23.455845
C	11.488005	10.438572	21.985667
H	10.502788	9.959522	22.051403
H	11.456433	11.533917	21.955657
C	12.584505	9.768188	21.390551
H	13.358119	10.354804	20.879024
H	12.468383	8.755569	20.986514
C	10.753399	7.290697	23.146743
H	10.389445	7.780188	22.232342
H	11.404414	6.462014	22.831621
C	11.454435	8.261366	24.075687
H	11.818553	7.767181	24.990123
H	10.748512	9.039127	24.413015
H	12.686889	8.258101	23.429476
H	9.878107	6.843503	23.640347

Ir(C_2H_6) (C_2H_4)@UiO-66 site-1

Electronic Energy: -3813.973599

Enthalpy: -3813.207319

Free Energy: -3813.352491

O	13.754634	11.718302	23.261198
Zr	13.680985	13.486351	24.545210
C	10.482553	13.517258	23.859301
C	9.430581	13.629370	22.794918
O	10.082032	13.403090	25.053792
O	11.687174	13.549196	23.495142

O	15.717506	13.419677	23.531020
O	13.622199	15.443693	23.473402
Zr	13.716851	10.968067	27.081096
Zr	11.121801	13.407948	27.017313
O	15.036845	14.936097	25.662706
O	12.324859	11.996808	25.598672
O	12.572723	14.494770	26.000465
O	14.741256	12.470996	26.040186
C	13.495758	16.642280	23.854517
C	13.295633	17.684230	22.794480
O	13.501181	17.030940	25.056475
C	16.909567	13.435046	23.954586
O	17.256792	13.545855	25.161676
Zr	13.554395	15.998526	27.050427
Zr	16.143542	13.568464	27.110495
H	11.797710	11.429158	25.014157
H	15.582875	15.517935	25.128419
H	11.576902	15.406842	28.992723
O	12.156465	14.867117	28.449674
O	15.497476	17.116317	27.132948
O	11.558232	16.992164	26.957974
O	13.556315	17.062669	29.024242
Zr	13.587214	13.495097	29.572771
O	14.627603	14.569481	28.122216
H	15.635888	11.596475	29.083689
O	15.074161	12.117330	28.504679
O	11.728428	9.891002	27.173992
O	15.764519	9.980273	27.007252
O	13.690878	9.912633	29.048130
O	12.597969	12.420410	28.091777
O	17.156355	13.666940	29.110829
O	17.132026	15.578617	27.183902
O	17.281325	11.635063	27.080504
O	10.044728	13.334517	28.989806
O	10.105760	11.434137	27.044903
O	10.014136	15.361558	26.941765
C	10.368303	16.571676	26.878770
C	9.294553	17.596241	26.661342
C	13.610959	16.682476	30.228021
C	13.760368	17.742683	31.278861
O	13.577617	15.481136	30.618116
C	16.948915	10.421845	26.991192
C	18.055083	9.419817	26.831620
C	13.577493	10.302571	30.245724
C	13.400227	9.246722	31.296006
O	13.574748	11.506976	30.624883
C	16.707740	16.767969	27.232044
C	10.521488	10.244961	27.158075
C	9.481808	9.170211	27.284577
C	16.745435	13.719020	30.304640
C	17.770356	13.952379	31.374718
O	15.540016	13.611062	30.667414
C	10.415755	13.285840	30.195698

C	9.356774	13.061769	31.234090
O	11.609661	13.385349	30.599729
H	9.575857	18.564168	27.089372
H	9.170337	17.739753	25.578698
H	8.332833	17.257058	27.060377
H	8.811249	9.402007	28.121972
H	8.851456	9.155815	26.384860
H	9.933451	8.184398	27.432037
H	18.940788	9.721280	27.401736
H	17.734121	8.413860	27.120883
H	18.353283	9.392308	25.773884
C	17.723256	17.850162	27.449995
H	17.386674	18.803925	27.030270
H	17.848425	17.992092	28.532731
H	18.699482	17.566565	27.042795
H	13.759945	9.589359	32.271810
H	12.325624	9.037705	31.393978
H	13.889358	8.310806	31.005829
H	14.833324	17.915666	31.443081
H	13.321284	18.691529	30.953124
H	13.330827	17.420529	32.233296
H	13.763335	17.386744	21.850031
H	12.216674	17.782776	22.609612
H	13.663745	18.661993	23.122397
H	9.869190	13.801732	21.807346
H	8.831747	12.708678	22.771578
H	8.736088	14.441615	23.044605
H	18.747891	13.554797	31.082131
H	17.884993	15.036932	31.511572
H	17.448592	13.532601	32.333563
H	9.647980	13.489544	32.199181
H	8.389157	13.457026	30.907414
H	9.238458	11.978323	31.376639
C	18.005281	13.283847	22.939890
H	18.884187	13.873248	23.223453
H	18.321757	12.231265	22.920853
H	17.666289	13.555204	21.934842
O	13.764196	9.665736	25.358790
H	14.620069	9.224400	25.308006
H	14.611786	11.648090	22.824669
Ir	12.870841	9.874531	23.431582
C	11.498083	10.416079	21.963622
H	10.547983	9.865492	22.001644
H	11.383837	11.505944	21.932842
C	12.643080	9.824489	21.369717
H	13.380657	10.464819	20.868773
H	12.589374	8.813687	20.945023
C	11.827898	6.986328	25.080604
H	12.509736	6.162489	24.827597
H	12.273954	7.559061	25.904243
C	11.546761	7.879510	23.896096
H	10.933124	8.747533	24.174543
H	11.021704	7.375895	23.069343

H	10.897589	6.534217	25.452358
H	12.564386	8.104656	23.378145

Catalytic Dimerization Mechanism on UiO-66 site-1 (Figure 4)

TS1@UiO-66 site-1

Electronic Energy: -3813.912206

Enthalpy: -3813.151149

Free Energy: -3813.290946

O	13.636015	11.810254	23.187611
Zr	13.692421	13.478003	24.531469
C	10.482600	13.517226	23.859328
C	9.430578	13.629355	22.794919
O	10.090717	13.427628	25.055970
O	11.683105	13.545282	23.479064
O	15.723190	13.478513	23.535302
O	13.611302	15.442866	23.474880
Zr	13.723538	10.962226	27.074128
Zr	11.131761	13.412927	27.020524
O	15.044228	14.928566	25.670531
O	12.315575	12.006506	25.614464
O	12.580170	14.492084	25.996473
O	14.768650	12.419587	25.990515
C	13.495702	16.642275	23.854484
C	13.295595	17.684231	22.794488
O	13.511208	17.031909	25.056393
C	16.909582	13.435097	23.954503
O	17.265671	13.518678	25.165680
Zr	13.558718	15.996291	27.045689
Zr	16.150881	13.562374	27.102786
H	11.860745	11.406462	25.017335
H	15.598105	15.492869	25.125587
H	11.579843	15.402000	28.990330
O	12.161876	14.863843	28.448288
O	15.497566	17.115480	27.135226
O	11.559181	16.990836	26.952957
O	13.557257	17.061014	29.023708
Zr	13.592825	13.491743	29.573610
O	14.628598	14.558102	28.112771
H	15.649486	11.592089	29.060413
O	15.081088	12.121649	28.495949
O	11.727271	9.878207	27.172962
O	15.767211	9.986108	27.032982
O	13.683412	9.915519	29.046817
O	12.609023	12.413325	28.091239
O	17.156707	13.667954	29.110428
O	17.133199	15.578156	27.183935
O	17.291289	11.635251	27.070388
O	10.046085	13.338815	28.989709

O	10.114951	11.435932	27.068184
O	10.014665	15.361689	26.947569
C	10.368338	16.571660	26.878783
C	9.294553	17.596241	26.661343
C	13.610984	16.682462	30.228036
C	13.760369	17.742684	31.278860
O	13.579674	15.480490	30.617641
C	16.948905	10.421831	26.991233
C	18.055078	9.419810	26.831629
C	13.577415	10.302575	30.245749
C	13.400196	9.246723	31.296001
O	13.583459	11.506857	30.626220
C	16.707774	16.767973	27.232036
C	10.521520	10.244989	27.158068
C	9.481807	9.170210	27.284555
C	16.745443	13.719011	30.304657
C	17.770357	13.952378	31.374717
O	15.540173	13.610945	30.667266
C	10.415777	13.285842	30.195700
C	9.356770	13.061770	31.234086
O	11.610687	13.380602	30.598963
H	9.573830	18.562378	27.094796
H	9.174990	17.745232	25.578942
H	8.331488	17.254928	27.055153
H	9.212875	9.072361	28.345779
H	8.566585	9.436613	26.744581
H	9.861889	8.199680	26.949260
H	18.854457	9.621392	27.555534
H	17.698607	8.390996	26.946377
H	18.510931	9.535783	25.838443
C	17.723256	17.850162	27.449994
H	17.385474	18.804640	27.032870
H	17.850497	17.989670	28.532793
H	18.698806	17.567743	27.040369
H	13.778049	9.582895	32.267203
H	12.324291	9.052689	31.409654
H	13.872659	8.305005	30.997341
H	14.833417	17.913907	31.444196
H	13.322983	18.692108	30.952550
H	13.329355	17.421232	32.232877
H	13.750046	17.379617	21.845898
H	12.215872	17.795656	22.621557
H	13.678288	18.658423	23.116394
H	9.785417	13.233494	21.837473
H	8.500089	13.137436	23.097906
H	9.203653	14.694303	22.644784
H	18.747859	13.554831	31.082043
H	17.884942	15.036965	31.511279
H	17.448619	13.532733	32.333630
H	9.644966	13.496852	32.196850
H	8.387259	13.449726	30.904457
H	9.244974	11.978624	31.383707
C	18.005287	13.283869	22.939894

H	18.737633	14.092701	23.058816
H	18.550214	12.348767	23.128188
H	17.617712	13.280787	21.916295
O	13.646424	9.575728	25.411510
H	12.827568	9.071751	25.476185
H	12.826173	11.837073	22.667813
Ir	14.231394	9.641045	23.279459
C	15.897953	10.454241	22.350313
C	14.750932	7.685047	23.604573
H	12.680196	9.473955	22.876728
C	16.392263	10.204729	23.700954
H	16.376109	9.883104	21.546031
H	15.642260	11.482381	22.077118
C	15.957113	8.323674	24.127037
H	14.089856	7.231143	24.353474
H	14.877335	7.044502	22.724387
H	17.437052	9.902979	23.799908
H	16.149526	10.963464	24.460116
H	16.034820	8.403293	25.215565
H	16.883622	7.993132	23.649715
H	14.134868	9.338869	21.740694

Ir(C_4H_8) H_2@UiO-66 site-1

Electronic Energy: -3813.963029

Enthalpy: -3813.200047

Free Energy: -3813.342317

O	13.635518	11.687321	23.255522
Zr	13.673069	13.490152	24.548819
C	10.482506	13.517317	23.859331
C	9.430581	13.629344	22.794916
O	10.089262	13.420272	25.055745
O	11.684955	13.565578	23.485771
O	15.715282	13.468540	23.542792
O	13.616216	15.442112	23.474916
Zr	13.716248	10.965271	27.088062
Zr	11.117905	13.402779	27.017069
O	15.035665	14.926813	25.670603
O	12.332518	12.000168	25.603412
O	12.578126	14.489687	26.000893
O	14.783386	12.407124	25.969367
C	13.495725	16.642244	23.854588
C	13.295702	17.684195	22.794433
O	13.506065	17.029644	25.056294
C	16.909502	13.435107	23.954625
O	17.264206	13.527704	25.164303
Zr	13.557788	15.999519	27.052081
Zr	16.153817	13.558492	27.100139
H	11.935994	11.368704	24.993247
H	15.588214	15.485200	25.118124
H	11.577884	15.406921	28.989784

O	12.158531	14.866996	28.447991
O	15.496953	17.115874	27.135587
O	11.559244	16.991261	26.953679
O	13.557906	17.062112	29.023865
Zr	13.590080	13.496343	29.573582
O	14.627099	14.557966	28.108717
H	15.645056	11.590570	29.047933
O	15.074384	12.129262	28.494368
O	11.727098	9.891935	27.214875
O	15.768848	9.983608	27.068346
O	13.694099	9.913631	29.048561
O	12.604724	12.426321	28.086798
O	17.156000	13.667518	29.110035
O	17.131498	15.577909	27.181930
O	17.287638	11.638149	27.067076
O	10.045172	13.333337	28.989350
O	10.110241	11.436598	27.044255
O	10.014600	15.361618	26.944911
C	10.368272	16.571715	26.878764
C	9.294553	17.596241	26.661342
C	13.610976	16.682521	30.228016
C	13.760335	17.742681	31.278868
O	13.579964	15.480970	30.616975
C	16.948933	10.421798	26.991354
C	18.055094	9.419853	26.831469
C	13.577513	10.302571	30.245659
C	13.400271	9.246691	31.295983
O	13.574577	11.507781	30.622242
C	16.707724	16.767975	27.232066
C	10.521538	10.244951	27.158088
C	9.481796	9.170215	27.284511
C	16.745462	13.719060	30.304631
C	17.770348	13.952376	31.374726
O	15.539611	13.612775	30.666766
C	10.415742	13.285873	30.195697
C	9.356776	13.061768	31.234092
O	11.610014	13.385486	30.598685
H	9.573725	18.562669	27.094219
H	9.174614	17.744479	25.578890
H	8.331608	17.254949	27.055434
H	9.192016	9.091998	28.341796
H	8.577397	9.423448	26.720448
H	9.873310	8.196581	26.972551
H	18.732407	9.480159	27.693471
H	17.670703	8.399456	26.739167
H	18.659148	9.672390	25.950012
C	17.723254	17.850164	27.449996
H	17.385673	18.804268	27.031907
H	17.849792	17.990561	28.532760
H	18.698912	17.567228	27.041076
H	13.736697	9.597813	32.276893
H	12.328275	9.016844	31.373939
H	13.911680	8.319480	31.016271

H	14.833438	17.915364	31.442272
H	13.321174	18.691559	30.953409
H	13.331372	17.420369	32.233480
H	13.752115	17.381267	21.846264
H	12.215978	17.793550	22.620303
H	13.676272	18.658680	23.117776
H	9.797866	13.263582	21.830442
H	8.512920	13.106102	23.084476
H	9.175619	14.691316	22.671415
H	18.747519	13.553629	31.082600
H	17.885874	15.036977	31.510327
H	17.447925	13.533777	32.333850
H	9.645534	13.494874	32.197545
H	8.387706	13.451265	30.904992
H	9.243461	11.978455	31.381388
C	18.005282	13.283712	22.939911
H	18.848199	13.938684	23.189965
H	18.383201	12.252502	22.983911
H	17.652875	13.479496	21.922401
O	13.691922	9.718742	25.342419
H	13.771641	8.775845	25.517959
H	13.574499	11.873130	22.311246
Ir	15.103303	10.236891	23.700853
C	15.979390	10.769028	21.854609
C	14.293036	8.714065	22.575522
C	15.262722	9.994023	20.755023
H	15.874735	11.858086	21.726618
H	17.058688	10.550615	21.807360
C	15.017811	8.586734	21.257858
H	14.241437	7.774575	23.147562
H	13.261005	9.085737	22.434486
H	14.284499	10.459432	20.528735
H	15.825091	10.009957	19.805423
H	15.981590	8.068021	21.404244
H	14.440298	7.969807	20.546249
H	15.890651	8.967358	24.246453
H	16.634896	9.912361	23.818451

TS2@UiO-66 site-1

Electronic Energy: -3813.942748

Enthalpy: -3813.178835

Free Energy: -3813.322311

O	13.770206	11.717955	23.299281
Zr	13.687277	13.489384	24.522002
C	10.482600	13.517226	23.859328
C	9.430578	13.629355	22.794919
O	10.098782	13.363649	25.058482
O	11.682058	13.597900	23.489805
O	15.720769	13.449671	23.525467
O	13.634047	15.446139	23.470342

Zr	13.721672	10.930705	27.079765
Zr	11.129861	13.430725	27.043807
O	15.034690	14.933315	25.661344
O	12.302598	11.916184	25.519297
O	12.570340	14.483266	26.002209
O	14.695604	12.472100	26.042107
C	13.495702	16.642275	23.854484
C	13.295595	17.684231	22.794488
O	13.493039	17.027064	25.057192
C	16.909582	13.435097	23.954503
O	17.251008	13.526338	25.165536
Zr	13.557780	15.996259	27.049231
Zr	16.133272	13.559817	27.104406
H	11.416106	11.631936	25.247280
H	15.588983	15.511492	25.131350
H	11.586103	15.419239	29.005896
O	12.156334	14.875004	28.457576
O	15.496753	17.117189	27.130791
O	11.558153	16.988867	26.957102
O	13.556836	17.062740	29.023590
Zr	13.590318	13.490237	29.568714
O	14.624912	14.568994	28.121654
H	15.640173	11.599010	29.077496
O	15.070877	12.113367	28.499743
O	11.725606	9.891778	27.215213
O	15.769136	9.976441	27.029051
O	13.700379	9.908074	29.051448
O	12.594477	12.421535	28.079262
O	17.152483	13.666367	29.109353
O	17.127917	15.577150	27.183263
O	17.276074	11.638604	27.065346
O	10.041616	13.338904	28.989787
O	10.115847	11.438054	27.010775
O	10.012056	15.361240	26.944430
C	10.368338	16.571660	26.878783
C	9.294553	17.596241	26.661343
C	13.610984	16.682462	30.228036
C	13.760369	17.742684	31.278860
O	13.578349	15.480580	30.617167
C	16.948905	10.421831	26.991233
C	18.055078	9.419810	26.831629
C	13.577415	10.302575	30.245749
C	13.400196	9.246723	31.296001
O	13.567866	11.508368	30.620360
C	16.707774	16.767973	27.232036
C	10.521520	10.244989	27.158068
C	9.481807	9.170210	27.284555
C	16.745443	13.719011	30.304657
C	17.770357	13.952378	31.374717
O	15.539365	13.608211	30.667517
C	10.415777	13.285842	30.195700
C	9.356770	13.061770	31.234086
O	11.609468	13.383460	30.595952

H	8.336073	17.262324	27.072409
H	9.581754	18.567528	27.077357
H	9.159698	17.728483	25.578554
H	8.635411	9.364386	26.615317
H	9.907755	8.180072	27.094322
H	9.084358	9.183968	28.309230
H	18.951839	9.735206	27.376334
H	17.740644	8.420499	27.149280
H	18.330838	9.368048	25.768704
C	17.723256	17.850162	27.449994
H	17.389969	18.801435	27.022098
H	17.841239	17.999213	28.532563
H	18.701623	17.562992	27.050671
H	13.698701	9.609366	32.284909
H	12.333922	8.984247	31.342241
H	13.945205	8.333612	31.033500
H	14.833373	17.916992	31.441243
H	13.319699	18.691063	30.953923
H	13.332805	17.419806	32.233910
H	13.657297	18.663400	23.125336
H	13.769859	17.389649	21.852509
H	12.217213	17.778300	22.603934
H	9.425627	14.656694	22.406629
H	9.681698	12.976411	21.949786
H	8.434247	13.389608	23.179002
H	18.749357	13.560819	31.079132
H	17.879578	15.036720	31.517399
H	17.451111	13.525960	32.331441
H	8.390223	13.461041	30.909332
H	9.235107	11.978259	31.373324
H	9.650595	13.485466	32.200095
C	18.005287	13.283869	22.939894
H	18.892447	13.855573	23.234000
H	18.306175	12.227201	22.903759
H	17.671050	13.576644	21.939417
O	13.784533	9.662904	25.384609
H	14.628571	9.245821	25.189666
H	14.469391	11.609002	22.649026
Ir	12.399885	10.170243	23.703497
C	12.907174	8.826757	22.231427
H	11.800738	8.916963	24.418664
H	11.555570	10.820181	22.547119
C	11.789029	7.813856	22.023537
H	13.100067	9.395184	21.303750
H	13.855233	8.337590	22.520782
C	10.433132	9.240349	23.510718
H	11.877591	7.301174	21.050117
H	11.858590	7.022500	22.791070
C	10.454153	8.521427	22.169497
H	10.101186	8.541787	24.299180
H	9.716886	10.076422	23.553601
H	9.606433	7.820650	22.080184
H	10.344839	9.256333	21.353575

Ir(butane) H@UiO-66 site-1
Electronic Energy: -3813.974263
Enthalpy: -3813.206749
Free Energy: -3813.348799

O	13.732868	12.109528	22.773527
Zr	13.680070	13.506141	24.471547
C	10.482523	13.517784	23.858835
C	9.430490	13.629310	22.795002
O	10.107326	13.333998	25.056363
O	11.674418	13.632132	23.489212
O	15.732198	13.501217	23.513716
O	13.646191	15.455211	23.453847
Zr	13.713693	10.896355	27.103899
Zr	11.121308	13.418118	27.027544
O	15.024064	14.910859	25.657962
O	12.368863	11.830260	25.436870
O	12.560893	14.465224	25.992722
O	14.717885	12.384365	25.956318
C	13.495782	16.642517	23.854139
C	13.295618	17.684294	22.794546
O	13.486478	17.014834	25.060053
C	16.909418	13.435235	23.954435
O	17.242025	13.504741	25.170474
Zr	13.550245	15.985873	27.043095
Zr	16.133240	13.547625	27.090768
H	11.554407	11.457154	25.077452
H	15.587787	15.477898	25.125170
H	11.585975	15.411695	28.998294
O	12.156097	14.866825	28.450297
O	15.494842	17.111432	27.129242
O	11.558796	16.986843	26.959025
O	13.558113	17.058203	29.021721
Zr	13.583637	13.487738	29.562886
O	14.617750	14.546291	28.100236
H	15.638538	11.591134	29.044077
O	15.060357	12.111747	28.480298
O	11.718712	9.890346	27.264783
O	15.778426	9.966371	27.076197
O	13.719586	9.894705	29.059796
O	12.587905	12.411361	28.064434
O	17.149387	13.662658	29.106647
O	17.125337	15.574133	27.178959
O	17.267017	11.642079	27.049455
O	10.043436	13.330743	28.988071
O	10.130615	11.436787	26.969920
O	10.012247	15.360101	26.939506
C	10.368268	16.571777	26.878667
C	9.294548	17.596240	26.661365

C	13.610926	16.682377	30.227973
C	13.760393	17.742683	31.278857
O	13.580214	15.478628	30.614371
C	16.948959	10.421519	26.991454
C	18.055153	9.419891	26.831644
C	13.577681	10.302249	30.246017
C	13.400169	9.246773	31.296047
O	13.557765	11.510438	30.609421
C	16.707610	16.767921	27.232087
C	10.521701	10.244740	27.158470
C	9.481787	9.170225	27.284525
C	16.745379	13.718948	30.304695
C	17.770372	13.952369	31.374705
O	15.537551	13.606292	30.663159
C	10.415790	13.285800	30.195654
C	9.356761	13.061774	31.234078
O	11.609971	13.387668	30.594689
H	9.579750	18.566540	27.081057
H	9.163647	17.731618	25.578471
H	8.335163	17.260183	27.068318
H	9.448440	8.832661	28.329297
H	8.487360	9.526118	26.997320
H	9.766759	8.298286	26.683105
H	19.025409	9.841802	27.111909
H	17.844910	8.512899	27.409258
H	18.106591	9.123475	25.773904
C	17.723270	17.850154	27.449965
H	17.387001	18.801987	27.025891
H	17.846015	17.995831	28.532413
H	18.699736	17.564289	27.045270
H	13.627157	9.627338	32.297003
H	12.349795	8.923637	31.284178
H	14.006814	8.363783	31.067524
H	14.833476	17.914099	31.443380
H	13.322449	18.691772	30.952523
H	13.329963	17.420711	32.232885
H	13.888208	17.452699	21.902890
H	12.239861	17.666278	22.489690
H	13.524327	18.688695	23.164881
H	9.714226	13.031337	21.920375
H	8.443368	13.329817	23.161082
H	9.380051	14.673566	22.457896
H	18.748449	13.558608	31.079267
H	17.881417	15.036616	31.516347
H	17.449648	13.527019	32.331325
H	9.651396	13.482530	32.201067
H	8.391088	13.463557	30.909943
H	9.232878	11.978070	31.369547
C	18.005285	13.283790	22.939904
H	18.977481	13.575720	23.349195
H	18.064133	12.225767	22.645950
H	17.777989	13.856318	22.033772
O	13.767316	9.186899	25.721812

H	14.592160	8.699156	25.833589
H	14.551033	12.227610	22.276151
Ir	13.972899	10.621271	24.218137
C	12.740877	9.459318	23.081016
C	11.285690	9.749605	23.384643
H	12.980229	8.403957	23.291980
H	12.966003	9.663041	22.021107
C	10.293471	8.922765	22.575142
H	11.090466	9.567345	24.459870
C	8.850041	9.243525	22.904808
H	10.481902	9.084452	21.499861
H	10.492689	7.850901	22.746337
H	8.143790	8.641652	22.316071
H	8.628268	9.060332	23.967354
H	8.617460	10.301883	22.711052
H	15.200354	9.927273	23.514589
H	11.076903	10.821096	23.195682

TS3@UiO-66 site-1

Electronic Energy: -3813.969741

Enthalpy: -3813.207279

Free Energy: -3813.350877

O	13.672351	11.748819	23.134707
Zr	13.693543	13.492320	24.561641
C	10.482600	13.517226	23.859328
C	9.430578	13.629355	22.794919
O	10.094376	13.408937	25.057042
O	11.685169	13.562579	23.484058
O	15.718625	13.470193	23.536091
O	13.621392	15.442081	23.476514
Zr	13.718659	10.947038	27.070088
Zr	11.125986	13.405603	27.020003
O	15.041538	14.941856	25.669397
O	12.334088	11.982096	25.581344
O	12.579323	14.494023	25.996619
O	14.742915	12.464437	26.021550
C	13.495702	16.642275	23.854484
C	13.295595	17.684231	22.794488
O	13.502714	17.031941	25.055673
C	16.909582	13.435097	23.954503
O	17.259197	13.518957	25.166838
Zr	13.558398	16.002500	27.053785
Zr	16.149945	13.564762	27.106559
H	11.804660	11.414526	25.009398
H	15.590041	15.509498	25.122515
H	11.578449	15.405806	28.991019
O	12.158318	14.867340	28.447022
O	15.497431	17.117931	27.136785
O	11.558783	16.992108	26.955600
O	13.555752	17.064441	29.024121

Zr	13.588996	13.490789	29.566156
O	14.628416	14.567467	28.116708
H	15.638861	11.595692	29.070248
O	15.073630	12.117243	28.495137
O	11.726932	9.893149	27.201736
O	15.767047	9.977245	27.017643
O	13.695715	9.910770	29.049742
O	12.601925	12.422342	28.079162
O	17.156875	13.667971	29.110512
O	17.132283	15.578920	27.182981
O	17.280580	11.635048	27.081186
O	10.044830	13.331820	28.988868
O	10.107631	11.434752	27.032435
O	10.015488	15.361234	26.943049
C	10.368338	16.571660	26.878783
C	9.294553	17.596241	26.661343
C	13.610984	16.682462	30.228036
C	13.760369	17.742684	31.278860
O	13.579301	15.480754	30.615377
C	16.948905	10.421831	26.991233
C	18.055078	9.419810	26.831629
C	13.577415	10.302575	30.245749
C	13.400196	9.246723	31.296001
O	13.571563	11.508254	30.622017
C	16.707774	16.767973	27.232036
C	10.521520	10.244989	27.158068
C	9.481807	9.170210	27.284555
C	16.745443	13.719011	30.304657
C	17.770357	13.952378	31.374717
O	15.539751	13.608957	30.665504
C	10.415777	13.285842	30.195700
C	9.356770	13.061770	31.234086
O	11.609848	13.386216	30.597636
H	9.577726	18.565401	27.085247
H	9.166655	17.735529	25.578592
H	8.333893	17.258827	27.064455
H	9.006655	9.251321	28.272045
H	8.684935	9.315088	26.544609
H	9.918961	8.171544	27.185876
H	18.948209	9.731073	27.384511
H	17.738971	8.418102	27.140383
H	18.337425	9.375698	25.770073
C	17.723256	17.850162	27.449994
H	17.387141	18.803800	27.029572
H	17.847129	17.992639	28.532810
H	18.699893	17.566380	27.043940
H	13.712977	9.604841	32.282217
H	12.331543	8.996481	31.354094
H	13.932734	8.328129	31.027090
H	14.833262	17.922861	31.435528
H	13.313101	18.688890	30.956525
H	13.339189	17.417273	32.235877
H	13.734764	17.374184	21.840535

H	12.215370	17.811089	22.636299
H	13.694738	18.653478	23.111482
H	9.400727	14.667535	22.436775
H	9.690464	13.005923	21.930743
H	8.439203	13.362466	23.173910
H	18.746422	13.550073	31.083695
H	17.889382	15.036933	31.507689
H	17.446625	13.536856	32.334732
H	9.647917	13.489683	32.199115
H	8.389016	13.456560	30.907298
H	9.239118	11.978227	31.376515
C	18.005287	13.283869	22.939894
H	18.887935	13.864297	23.230520
H	18.311820	12.228827	22.910738
H	17.667793	13.566411	21.937655
O	13.772182	9.679809	25.358851
H	14.613464	9.209474	25.362928
H	13.534206	12.081193	22.238832
Ir	13.066089	9.831720	23.220305
C	12.172086	7.840077	23.407025
C	11.317514	8.941044	23.790432
H	10.448767	9.167096	23.158212
H	11.140578	9.084046	24.863461
H	12.580041	9.926257	21.713249
H	13.477203	8.279967	23.032086
C	11.829683	7.002886	22.192728
C	12.999516	6.239452	21.609206
H	11.381246	7.656506	21.428026
H	11.032591	6.301059	22.493457
H	12.695703	5.608050	20.764020
H	13.777427	6.925440	21.240193
H	13.469145	5.581613	22.356124
H	12.562573	7.248937	24.250926

Ir(1-butene) H_2@UiO-66 site-1

Electronic Energy: -3813.992682

Enthalpy: -3813.230200

Free Energy: -3813.373302

Zr	13.694760	13.485742	24.545581
C	10.482553	13.517258	23.859301
C	9.430581	13.629370	22.794918
O	10.090094	13.408740	25.057331
O	11.685325	13.557498	23.487941
O	15.723906	13.495045	23.524967
O	13.619651	15.442717	23.475358
Zr	13.715783	10.958147	27.079837
Zr	11.128093	13.413920	27.019608
O	15.040665	14.938107	25.668707
O	12.327294	11.976951	25.577852
O	12.577398	14.491948	26.000127

O	14.729958	12.470912	26.040803
C	13.495758	16.642280	23.854517
C	13.295633	17.684230	22.794480
O	13.503814	17.031627	25.056045
C	16.909567	13.435046	23.954586
O	17.252660	13.499629	25.168752
Zr	13.557434	15.998738	27.051005
Zr	16.145971	13.564856	27.110095
H	11.723384	11.454504	25.032592
H	15.588759	15.510126	25.125952
H	11.578685	15.406555	28.994200
O	12.158221	14.867653	28.450300
O	15.497370	17.116870	27.136759
O	11.558735	16.991202	26.954874
O	13.555390	17.062914	29.024235
Zr	13.589194	13.493837	29.571578
O	14.628135	14.568114	28.122229
H	15.637782	11.595607	29.080151
O	15.073135	12.115246	28.502770
O	11.726196	9.884741	27.195371
O	15.763232	9.980713	26.997686
O	13.695818	9.912394	29.048638
O	12.601644	12.419220	28.085106
O	17.155922	13.668620	29.110715
O	17.132324	15.578489	27.181514
O	17.280650	11.633047	27.095626
O	10.045633	13.333751	28.989131
O	10.115488	11.436905	27.036841
O	10.014096	15.361702	26.945371
C	10.368303	16.571676	26.878770
C	9.294553	17.596241	26.661342
C	13.610959	16.682476	30.228021
C	13.760368	17.742683	31.278861
O	13.579081	15.480879	30.617544
C	16.948915	10.421845	26.991192
C	18.055083	9.419817	26.831620
C	13.577493	10.302571	30.245724
C	13.400227	9.246722	31.296006
O	13.571184	11.507137	30.623937
C	16.707740	16.767969	27.232044
C	10.521488	10.244961	27.158075
C	9.481808	9.170211	27.284577
C	16.745435	13.719020	30.304640
C	17.770356	13.952379	31.374718
O	15.539995	13.608641	30.667237
C	10.415755	13.285840	30.195698
C	9.356774	13.061769	31.234090
O	11.609945	13.385436	30.598743
H	9.575560	18.563722	27.090577
H	9.171346	17.740951	25.578757
H	8.332524	17.256603	27.059153
H	9.463514	8.822337	28.327057
H	8.482968	9.536189	27.025571

H	9.742101	8.297520	26.672496
H	18.939768	9.720144	27.403784
H	17.733090	8.413401	27.118108
H	18.354193	9.394541	25.774099
C	17.723256	17.850162	27.449995
H	17.386422	18.804028	27.030695
H	17.848392	17.991764	28.532779
H	18.699507	17.566927	27.042626
H	13.776934	9.583530	32.267519
H	12.324340	9.052649	31.409451
H	13.873321	8.305107	30.998263
H	14.833348	17.916795	31.441699
H	13.319897	18.691099	30.953767
H	13.332354	17.419948	32.233778
H	13.742458	17.377262	21.843070
H	12.215586	17.803287	22.629007
H	13.686427	18.655971	23.114168
H	9.771706	13.178376	21.856191
H	8.483560	13.183964	23.118147
H	9.248263	14.695136	22.596519
H	18.747542	13.553929	31.082187
H	17.885865	15.036925	31.510849
H	17.448317	13.533275	32.333742
H	9.649760	13.485842	32.200221
H	8.390089	13.460572	30.908970
H	9.235185	11.978207	31.372778
C	18.005281	13.283847	22.939890
H	18.917848	13.792934	23.268465
H	18.249102	12.216339	22.842801
H	17.692199	13.646958	21.955568
C	11.415421	8.469651	23.986138
C	12.531065	7.783745	23.445018
C	10.058140	8.528085	23.343013
C	9.300683	9.816426	23.606424
H	14.595452	9.190853	25.318270
H	14.144198	11.927745	22.378570
H	11.801262	10.281597	22.336698
H	12.924954	9.659268	21.831088
H	11.402899	8.577339	25.082111
H	12.447031	7.294681	22.468267
H	13.250700	7.308523	24.122321
H	9.467553	7.671895	23.720090
H	10.156442	8.357315	22.257395
H	9.807802	10.678741	23.147772
H	8.279799	9.785506	23.201220
H	9.216081	10.036085	24.681921
Ir	12.888956	9.848702	23.385677
O	13.759006	9.670229	25.344619
O	13.813371	11.722176	23.259190

Table S6. XYZ Cartesian Coordinates of Selected Optimized Al_8-NU-1000 Isomers at the M06-L Density Functional. See Figure S13 for the optimized geometries. Unscaled Carbonyl Frequencies Computed at the Same Level of Theory Are Also Given.

Al_8-NU-1000 (A)

Electronic Energy: -7260.082323

Enthalpy: -7259.074122

Free Energy: -7259.290807

ν_{CO} = 2073, 2154 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.87645000	-1.87228200	2.79172000
H	0	1.51458200	1.37231600	-0.22526500
H	0	-3.66956100	1.60361600	-3.99035500
H	0	-2.59014600	0.44457000	-3.97811600
H	0	-2.89304900	0.98670800	4.58222300
H	0	-5.72186000	0.96433800	0.77521900
H	0	-6.40439800	0.52075400	-1.23710900
H	0	-5.96584900	0.07869600	2.06495300
H	0	-2.56990600	-1.62614000	-2.85821900
H	0	-4.18651400	2.64934200	0.38844500
H	0	-0.51565300	0.65339000	-4.56454900
H	0	-1.07649800	-0.04609400	3.98818600
H	0	0.37905700	0.55701900	4.05987400
H	0	2.30032600	-1.61867600	1.89506400
O	0	-1.74834900	1.25846200	-1.39298900
O	0	-2.56925000	4.06760200	-1.09621500
O	0	-2.21145500	3.90900900	1.64570600
O	0	0.11804100	3.45602000	-1.46867400
O	0	0.64194700	1.82778500	-2.90581000
O	0	1.81559700	-0.50425200	-2.45176500
O	0	-0.05084000	-2.32771200	-2.74947600
O	0	0.54977200	-2.56558600	1.99335900
O	0	-1.42002000	-3.63936400	-1.56372700
O	0	-1.10984300	-3.77325300	1.10960000
O	0	-4.12322300	-3.00079300	-1.20660000
O	0	-3.76244300	-3.12706500	1.47905300
O	0	-4.57992900	-1.39434400	2.63661200
O	0	-5.10316900	-1.20222000	-2.11027400
O	0	-3.44332400	-0.57182300	0.19066000

O	0	-2.38518900	-1.10368100	-2.07103300
O	0	-1.04145500	0.04657100	-4.03104800
O	0	-3.55435900	0.67400700	-3.74895000
O	0	-0.10342700	-0.22939000	3.76817100
O	0	-0.58045500	-1.21881200	-0.23153800
O	0	0.63353200	0.96928400	-0.25035700
O	0	1.24816700	1.61543500	2.39649400
O	0	2.25819900	-0.70883400	1.55496300
O	0	0.46057500	3.34997900	1.22411900
O	0	-5.72372600	1.06976200	-0.83236000
O	0	-5.52667900	0.88866500	1.76954800
O	0	-3.52409100	1.95596200	0.30885300
O	0	-4.00023400	2.81595400	-2.27389700
O	0	-3.47649300	2.57702900	2.92590300
O	0	-2.67072100	0.24014400	4.01490200
O	0	-1.84518900	-1.29187800	2.02434800
O	0	-1.38769600	1.13810900	1.46357600
Zr	0	-2.35814700	-2.32003400	-0.05080700
Zr	0	-0.33514500	-0.12351000	-2.08453200
Zr	0	-3.79448200	0.59968000	-1.47498900
Zr	0	-3.28379800	0.47197700	2.04114100
Zr	0	-1.27928900	2.64812700	0.03662800
Zr	0	0.11457900	-0.30911200	1.48660500
H	0	2.13786900	-1.28022800	-1.89031000
Al	0	5.63454500	-1.96330300	-1.89404700
Al	0	5.05531400	0.48740700	-2.89469900
Al	0	3.62678500	-0.77495400	0.11125200
Al	0	7.02021000	0.17458000	-0.19674600
Al	0	4.69763000	2.14748500	-0.88396700
Al	0	6.11938600	-2.74535400	0.68216800
Al	0	4.92000800	1.75373100	1.76375000
Al	0	5.75141000	-0.75205000	2.55138700
H	0	2.85902200	1.16204300	-2.14176400
H	0	4.19311600	-3.40603400	-0.71353200
H	0	9.10887700	1.26147000	0.00558400
H	0	1.81046100	-2.45080600	-0.12000900
H	0	5.71598000	3.86117300	0.62412900
H	0	4.59005600	4.14020100	-2.46711600
H	0	7.98924000	-1.45588700	1.83405200
H	0	4.68798300	-2.58459900	3.82096800
H	0	5.17877300	3.19871200	3.75212300
H	0	6.37696800	1.33053000	3.80970500
H	0	7.32039700	-0.58713300	-2.97093100
H	0	3.96005100	-3.26859900	-3.17459400
H	0	2.45506400	-0.43911900	-3.22170000
H	0	6.54150100	1.73246000	-4.30136700
H	0	4.36009000	-1.91292100	-3.90682500
H	0	3.90992000	0.00354500	-4.95944500
O	0	4.41636900	-0.71941300	-1.53673900
O	0	3.63248700	1.73177800	-2.27822900
O	0	5.15788200	-3.38119400	-0.85332200
O	0	8.74178600	0.38830700	-0.13617900
O	0	6.85736700	-1.59832700	-0.57493400
O	0	6.12353600	1.20013300	-1.35852500
O	0	2.58958200	-2.16049000	-0.60995500
O	0	6.36912200	-4.32698300	1.35247800
O	0	5.31557900	3.61176200	-2.11230700
O	0	4.76670200	-1.63297500	1.25707500

O	0	3.81075600	1.11193900	0.39495600
O	0	5.01489200	3.20461900	0.57312100
O	0	6.26943900	0.61859300	1.39513100
O	0	7.16213200	-1.85251200	2.13562700
O	0	5.05275200	-1.71755900	4.03297800
O	0	4.13991400	0.45235900	2.96550600
O	0	5.65972600	2.62255400	3.15580000
O	0	6.58666200	0.35789900	4.01557800
O	0	6.42144000	-0.86946400	-3.17347600
O	0	5.64738800	1.84258500	-3.96704900
O	0	4.72618600	-2.74432800	-3.44003500
O	0	3.88951600	-0.39125200	-4.08115900
H	0	3.33413800	0.10433600	2.47711200
H	0	-4.86483600	-4.26158800	3.64649900
H	0	-6.17482400	-3.05254600	3.68672800
H	0	-5.99429200	-4.18778500	2.30429300
H	0	-5.63613700	-4.17042700	-2.97921200
H	0	-6.64729100	-3.79988400	-1.59300600
H	0	-6.80052500	-2.80930300	-3.07453800
H	0	-3.49978800	6.01405500	-2.43894600
H	0	-4.68849000	5.02073300	-3.36099000
H	0	-4.99374100	5.45388800	-1.67562600
H	0	-2.79337400	5.70832000	3.34715500
H	0	-4.41038200	5.31053300	2.75927800
H	0	-3.89017900	4.66148700	4.32109200
H	0	5.57337900	3.01320600	-2.92072700
H	0	6.95077300	-4.33748800	2.11558400
Ir	0	3.77155400	-0.32948300	4.92125500
C	0	3.52846300	-1.18210900	6.52360300
C	0	2.61556400	0.99067500	5.44009000
O	0	3.38144700	-1.72701700	7.53051300
O	0	1.84343600	1.81481700	5.70318500
H	0	7.54705700	0.27612400	4.04909500
H	0	2.42044200	3.40903300	-3.76391700
H	0	1.10233800	4.61647100	-3.80129400
H	0	2.17866000	4.58382300	-2.41349100
H	0	3.03193100	3.98052600	1.71933200
H	0	1.96396300	4.64342200	2.95034300
H	0	2.95232400	3.20304900	3.33750700
H	0	0.92085300	-4.97913100	-2.67428300
H	0	-0.70664500	-5.47908600	-3.15912000
H	0	0.26813300	-4.38474400	-4.20766500
H	0	0.95766000	-4.79474500	3.27087000
H	0	0.01515200	-5.79249000	2.10976200
H	0	1.57093200	-5.05684100	1.64432600

Al_8-NU-1000 (A_2)

Electronic Energy: -7260.087438

Enthalpy: -7259.078430

Free Energy: -7259.295944

ν_{CO} = 2080, 2155 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100

C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.86197200	-1.85928100	2.79863900
H	0	1.46966500	1.41908900	-0.24364000
H	0	-3.67614200	1.60448900	-3.98513200
H	0	-2.59831200	0.44533800	-3.97504800
H	0	-2.86555100	0.98689500	4.58820700
H	0	-5.72043800	0.96456200	0.79099100
H	0	-6.41266600	0.52253100	-1.22301700
H	0	-5.95895000	0.07498300	2.07806300
H	0	-2.57490900	-1.62912100	-2.85087200
H	0	-4.18963600	2.65028900	0.39684800
H	0	-0.52216600	0.66063100	-4.56295400
H	0	-1.02765600	-0.02521200	3.99316200
H	0	0.45078500	0.55103200	4.03743400
H	0	2.17284600	-1.73013500	1.70378800
O	0	-1.76129100	1.26276400	-1.39471400
O	0	-2.56913900	4.06773700	-1.09814600
O	0	-2.21963200	3.91139000	1.64045500
O	0	0.10543600	3.45633000	-1.47840700
O	0	0.65611400	1.82249400	-2.90034900
O	0	1.80342500	-0.48199500	-2.37704500
O	0	-0.04126200	-2.32956000	-2.74476600
O	0	0.54300000	-2.56971900	2.01643000
O	0	-1.42400700	-3.63696400	-1.56844100
O	0	-1.10250300	-3.77362000	1.10055300
O	0	-4.12194300	-2.99953900	-1.20684500
O	0	-3.76078800	-3.12490500	1.47871100
O	0	-4.57340600	-1.39606100	2.64483800
O	0	-5.10671200	-1.20150400	-2.10590500
O	0	-3.44127800	-0.56878000	0.19655700
O	0	-2.38902200	-1.10297000	-2.06650400
O	0	-1.04375800	0.04830300	-4.03170500
O	0	-3.56163100	0.67434300	-3.74502100
O	0	-0.05954300	-0.22599200	3.76562900
O	0	-0.57104000	-1.21702600	-0.22979100
O	0	0.59793300	1.00221700	-0.25404500
O	0	1.26366100	1.60022600	2.36280200
O	0	2.24982900	-0.79659600	1.44555800
O	0	0.44134800	3.34428700	1.23482300
O	0	-5.72973100	1.06935100	-0.81915600
O	0	-5.52203000	0.88666100	1.78400900
O	0	-3.52799300	1.95647000	0.31471100
O	0	-4.00523400	2.81574000	-2.26990300
O	0	-3.46906300	2.57531000	2.93190800
O	0	-2.63347500	0.24551900	4.01785900
O	0	-1.83360900	-1.28584000	2.02594600
O	0	-1.38890100	1.14205800	1.46594000

Zr	0	-2.35715500	-2.30981400	-0.04930600
Zr	0	-0.35029300	-0.11131200	-2.07878000
Zr	0	-3.80283900	0.60467500	-1.46954300
Zr	0	-3.27617200	0.47476600	2.05045900
Zr	0	-1.27944400	2.65523900	0.04097900
Zr	0	0.12555100	-0.28883100	1.48468200
H	0	2.13300300	-1.30371500	-1.90363600
Al	0	5.51035500	-2.06123500	-2.09136400
Al	0	5.04088100	0.48575500	-2.88271200
Al	0	3.62428400	-0.83192500	0.07219300
Al	0	6.89388300	-0.16867000	-0.16125200
Al	0	4.90112900	2.05676900	-0.72942800
Al	0	6.08275500	-2.90838400	0.45100100
Al	0	4.93126600	1.48273300	1.97132000
Al	0	5.83615600	-1.09094400	2.62745900
H	0	2.95662400	1.26434900	-1.98669300
H	0	4.10457000	-3.45341900	-0.87606000
H	0	9.22746500	0.66188000	-0.45566500
H	0	5.43919300	-3.56300400	2.85167300
H	0	1.81594200	-2.55665900	-0.22680200
H	0	5.93338300	3.61443600	0.98090500
H	0	4.92723900	4.14803200	-2.18059900
H	0	7.95333100	-2.38456300	2.22876000
H	0	4.14532600	-2.86015600	3.32235100
H	0	5.18042000	2.12818800	4.17481800
H	0	6.44839200	-0.58936200	4.86837000
H	0	7.20686800	-0.73854900	-3.15587200
H	0	3.62641800	-3.12553400	-3.28414900
H	0	2.42910900	-0.33343600	-3.14995400
H	0	6.55035600	1.68665700	-4.31978600
H	0	4.14054700	-1.81043400	-4.00562200
H	0	3.76469200	0.20254700	-4.92887800
O	0	4.38821500	-0.77875400	-1.60178700
O	0	3.76206500	1.78190000	-2.13275800
O	0	5.06891900	-3.52180400	-1.06291700
O	0	8.61982700	0.29735200	0.19125000
O	0	6.86339900	-1.83261100	-0.86198900
O	0	6.21477600	0.99085100	-1.31997600
O	0	2.63339200	-2.29050000	-0.66597900
O	0	5.99696500	-4.39430400	1.41312100
O	0	5.59997600	3.51208600	-1.90812200
O	0	4.90488000	-1.65914300	1.03237500
O	0	3.95956600	0.96967900	0.45156700
O	0	5.25723200	2.96329500	0.77491300
O	0	6.46157300	0.46499400	1.52646100
O	0	7.18324600	-2.08881700	1.73713000
O	0	5.10291400	-2.82517900	3.43849500
O	0	4.36342000	0.02113100	3.02880300
O	0	5.24706000	2.55857400	3.31830400
O	0	6.86229500	-0.68209000	4.00843500
O	0	6.28886300	-0.94870200	-3.35348800
O	0	5.71030500	1.85016100	-3.88447300
O	0	4.43733200	-2.69856800	-3.59214600
O	0	3.78024300	-0.24750100	-4.07776500
H	0	3.49161500	-0.25950900	2.69575300
H	0	-4.86695300	-4.22071700	3.69231500
H	0	-6.20698500	-3.04942900	3.64696200
H	0	-5.95351500	-4.22836800	2.31162800

H	0	-5.63782900	-4.18676000	-2.95509100
H	0	-6.66566300	-3.77586100	-1.59230800
H	0	-6.78560900	-2.81404700	-3.09415300
H	0	-3.49803900	6.01217500	-2.44558100
H	0	-4.69543300	5.01959400	-3.35731400
H	0	-4.98786700	5.45784200	-1.67074900
H	0	-2.78529600	5.69982200	3.36321600
H	0	-4.39600000	5.32424900	2.74721200
H	0	-3.90803800	4.65955700	4.31424400
H	0	5.77109300	2.96619200	-2.76756700
H	0	5.57035500	-5.16210300	1.02577100
Ir	0	8.39843600	1.22148400	2.09774800
C	0	8.02519400	1.82767800	3.79484600
C	0	10.09067600	1.86870800	2.26839500
O	0	7.86648800	2.19364000	4.87691800
O	0	11.17078200	2.28472800	2.34095500
H	0	3.15551300	3.76725800	1.78390000
H	0	2.00747800	4.72565000	2.71781500
H	0	2.84842600	3.30647300	3.45353600
H	0	2.48273900	3.40561800	-3.67716600
H	0	1.11849500	4.53381100	-3.89025300
H	0	2.10306900	4.65613300	-2.43483700
H	0	0.94204700	-4.95609500	-2.69890800
H	0	-0.69055200	-5.49135100	-3.13158200
H	0	0.23382700	-4.39217900	-4.21808400
H	0	0.92718000	-4.80695100	3.28081300
H	0	0.02742800	-5.79768900	2.08391600
H	0	1.58513300	-5.04317200	1.66352300

Al_8-NU-1000 (C)

Electronic Energy: -7260.067676

Enthalpy: -7259.059259

Free Energy: -7259.276594

ν_{CO} = 2073, 2146 cm^{-1}

C	-1	1.68441900	3.94341500	-3.15514000
C	-1	0.64899900	-4.90821600	2.22466600
C	-1	2.37165700	3.70494900	2.55374400
C	-1	0.00185000	-4.64437900	-3.17737000
C	-1	-5.46152400	-3.56982100	3.03745400
C	-1	-4.20580600	5.17837100	-2.39073300
C	-1	-6.09808400	-3.34300700	-2.42691100
C	-1	-3.54711000	4.91457400	3.31258500
C	-1	1.27407100	2.82442300	2.03809500
C	-1	0.75416700	3.00364000	-2.46953500
C	-1	-3.54118900	3.93046700	-1.89896000
C	-1	-5.03722900	-2.44266000	-1.88258700
C	-1	-4.54348500	-2.62142800	2.33674300
C	-1	-0.02842400	-3.67128600	1.74594600
C	-1	-3.03318900	3.71325000	2.58679300
C	-1	-0.52889700	-3.45027300	-2.44888800
H	0	-1.87278700	-1.86950600	2.79238800
H	0	1.52718600	1.33845600	-0.24026200
H	0	-3.66734000	1.60600300	-3.98638500
H	0	-2.59019500	0.44680300	-3.97561500
H	0	-2.87103000	0.98912200	4.58121200

H	0	-5.71665700	0.96363200	0.78363200
H	0	-6.40649300	0.52326400	-1.23042600
H	0	-5.95295100	0.06897600	2.06678400
H	0	-2.57407000	-1.62523600	-2.85757600
H	0	-4.18458600	2.64911200	0.39268800
H	0	-0.51466000	0.67160600	-4.55582200
H	0	-1.03399000	-0.03874300	3.98720300
H	0	0.42989200	0.55947900	4.00628700
H	0	2.30388900	-1.59327400	1.88649400
O	0	-1.75023400	1.25955400	-1.39211500
O	0	-2.57001100	4.06694800	-1.09562200
O	0	-2.20984400	3.90879900	1.64732100
O	0	0.11169300	3.45991400	-1.47582200
O	0	0.65305100	1.82139700	-2.89433800
O	0	1.81753900	-0.52279300	-2.38918400
O	0	-0.05507500	-2.32815100	-2.75733900
O	0	0.55304400	-2.56800500	1.99350700
O	0	-1.42223700	-3.63582300	-1.56482300
O	0	-1.11216600	-3.77293500	1.11418100
O	0	-4.12261700	-3.00134000	-1.20791400
O	0	-3.76584700	-3.12678100	1.47609300
O	0	-4.57287600	-1.39578600	2.64327200
O	0	-5.10457900	-1.20194800	-2.10743700
O	0	-3.44112500	-0.57129800	0.19265900
O	0	-2.38917600	-1.10157800	-2.07142100
O	0	-1.03364300	0.05133000	-4.03155600
O	0	-3.55350800	0.67570300	-3.74699500
O	0	-0.06526100	-0.23723000	3.76496700
O	0	-0.57922000	-1.22878800	-0.23685300
O	0	0.62740800	0.97234700	-0.25215600
O	0	1.23103000	1.62191600	2.40749700
O	0	2.24827800	-0.68447300	1.55054200
O	0	0.46856300	3.35161000	1.21562800
O	0	-5.72389000	1.07055000	-0.82694000
O	0	-5.52005400	0.88421800	1.77665400
O	0	-3.52238400	1.95584600	0.31152800
O	0	-4.00059500	2.81559600	-2.27352900
O	0	-3.47455600	2.57673400	2.92777200
O	0	-2.63981000	0.24563700	4.01369900
O	0	-1.84068000	-1.29188200	2.02329200
O	0	-1.38414200	1.13843600	1.46113600
Zr	0	-2.36035100	-2.32027500	-0.05144900
Zr	0	-0.34187700	-0.12304900	-2.08008600
Zr	0	-3.79641300	0.60174400	-1.47194200
Zr	0	-3.27419200	0.47283500	2.04367100
Zr	0	-1.27325200	2.64983800	0.03683800
Zr	0	0.11973300	-0.31323500	1.47462200
H	0	2.12238700	-1.27028500	-1.77224700
Al	0	5.71481300	-2.08041800	-1.66916800
Al	0	5.05133000	0.26574900	-2.86527400
Al	0	3.64806000	-0.72729200	0.17222100
Al	0	7.05717400	0.29995700	-0.24116100
Al	0	4.64726600	2.20456700	-1.05972100
Al	0	6.22911100	-2.50192600	0.97217700
Al	0	4.85190100	1.79734300	1.60192300
Al	0	5.83881400	-0.42136600	2.67348100
H	0	2.84592400	1.11606500	-2.31594400
H	0	4.98613600	-4.18416400	-0.44462600

H	0	9.08673000	1.50994300	-0.33996500
H	0	6.66451400	-4.29857800	2.52709900
H	0	1.88169900	-2.50210000	-0.10039400
H	0	5.62799900	3.93507000	0.48477000
H	0	4.60540200	3.72567300	-2.90959400
H	0	8.06998600	-1.08208600	1.98788700
H	0	4.31745500	-1.89155700	3.98040000
H	0	5.51487100	-2.70772000	3.40427700
H	0	5.17335400	3.15178400	3.71803700
H	0	6.23895500	1.97161500	3.50948900
H	0	6.58203600	0.37830600	4.83169800
H	0	7.31570300	-0.89571100	-3.03755700
H	0	3.63343600	-2.94245800	-2.20413300
H	0	2.42664800	-0.57838900	-3.18113400
H	0	6.02937800	1.29199100	-4.96530800
H	0	4.17943700	-2.26372700	-3.48176800
H	0	3.91553700	-0.48552900	-4.94951000
O	0	4.49036600	-0.80543900	-1.43632300
O	0	3.67331400	1.59849400	-2.46792400
O	0	5.66580000	-3.51041100	-0.53050000
O	0	8.75626500	0.61132200	-0.36343700
O	0	6.92890500	-1.49552700	-0.43465600
O	0	6.08293200	1.19040600	-1.47855800
O	0	2.64781000	-2.16350500	-0.58077400
O	0	5.91630100	-3.80118300	2.18763800
O	0	5.22621600	3.61654400	-2.17899900
O	0	4.83124300	-1.42214600	1.35159400
O	0	3.74696500	1.17462500	0.24442900
O	0	4.95966400	3.24371200	0.45515600
O	0	6.30651200	0.80989600	1.30885100
O	0	7.27984100	-1.57893000	2.23128800
O	0	5.28126700	-1.86992100	3.93183500
O	0	4.21491700	0.68723300	2.92043000
O	0	5.74449300	2.78993400	3.03147100
O	0	6.68000800	0.63067500	3.91045600
O	0	6.39661300	-1.17917900	-3.11071700
O	0	5.90248700	1.46161100	-4.02976900
O	0	4.39131900	-2.99904500	-2.83033900
O	0	3.89668100	-0.66611800	-4.00627800
H	0	3.37984100	0.27489700	2.62076000
Ir	0	7.07316900	3.02484000	-3.14496900
C	0	8.57726500	2.57025600	-4.07293800
C	0	7.91090500	4.51712400	-2.51358900
O	0	9.51244300	2.26899200	-4.68595000
O	0	8.41440200	5.48302100	-2.11868400
H	0	-4.86466800	-4.24937400	3.66006400
H	0	-6.18433800	-3.05168700	3.67548900
H	0	-5.98232700	-4.20023300	2.30649200
H	0	-5.63647400	-4.17475600	-2.97283600
H	0	-6.65199600	-3.79360500	-1.59266600
H	0	-6.79677100	-2.81053100	-3.07957300
H	0	-3.49788200	6.01201600	-2.44592400
H	0	-4.69532900	5.01907700	-3.35722600
H	0	-4.98778000	5.45832600	-1.67084300
H	0	-2.79124400	5.70610400	3.35190800
H	0	-4.40605500	5.31497800	2.75574400
H	0	-3.89636400	4.66064100	4.31874500
H	0	3.06271500	3.93169000	1.72807500

H	0	1.97383200	4.67099300	2.88845500
H	0	2.90907500	3.21867800	3.37782900
H	0	1.63435700	-4.99022700	1.74555400
H	0	0.83872000	-4.84005200	3.30327700
H	0	0.06456200	-5.80691500	2.00649000
H	0	1.05478500	-4.79416300	-2.90109700
H	0	-0.55996000	-5.55360800	-2.94243000
H	0	-0.01016200	-4.45977300	-4.25832300
H	0	2.28233900	3.43801600	-3.91928500
H	0	1.10802600	4.75912400	-3.61292800
H	0	2.34017500	4.41869200	-2.41342000

Al_8-NU-1000 (C_geminal)

Electronic Energy: -7260.079171

Enthalpy: -7259.069431

Free Energy: -7259.285969

ν_{CO} = 2084, 2154 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.86790100	-1.86450900	2.79622200
H	0	1.47861000	1.41189500	-0.22162600
H	0	-3.66658800	1.60512700	-3.98517600
H	0	-2.59039100	0.44414800	-3.97427100
H	0	-2.87296700	0.98925800	4.58521300
H	0	-5.71957200	0.96356200	0.78519800
H	0	-6.40748800	0.51941600	-1.22843200
H	0	-5.95727600	0.07135600	2.07053500
H	0	-2.57101500	-1.62835200	-2.85251100
H	0	-4.18858200	2.64988800	0.39290300
H	0	-0.51547600	0.65942200	-4.55842900
H	0	-1.03470400	-0.02841900	3.99362800
H	0	0.43425200	0.56565000	4.02170100
H	0	2.22824100	-1.68933400	1.74367900
O	0	-1.75627400	1.26040000	-1.39392500
O	0	-2.56992200	4.06756900	-1.09698000
O	0	-2.21540400	3.91041000	1.64383800
O	0	0.10707300	3.45849500	-1.47845700
O	0	0.65180200	1.82288000	-2.90021100
O	0	1.81557300	-0.49332400	-2.36938400
O	0	-0.04213100	-2.32981300	-2.74505400
O	0	0.54288200	-2.56964100	2.01501200

O	0	-1.42451600	-3.63779400	-1.56869100
O	0	-1.10513400	-3.77420000	1.10315000
O	0	-4.12298300	-3.00018800	-1.20623100
O	0	-3.76168100	-3.12592900	1.47889700
O	0	-4.57522400	-1.39588800	2.64337300
O	0	-5.10501900	-1.20198500	-2.10851400
O	0	-3.44254900	-0.57013300	0.19494300
O	0	-2.38639300	-1.10351700	-2.06699400
O	0	-1.03733500	0.04501800	-4.02972900
O	0	-3.55428600	0.67432400	-3.74660900
O	0	-0.06540400	-0.22541500	3.77017300
O	0	-0.57317800	-1.21813000	-0.23050800
O	0	0.60265500	1.00106400	-0.24816000
O	0	1.24405800	1.60868300	2.38324700
O	0	2.24223400	-0.75955500	1.46348600
O	0	0.45316700	3.34666000	1.22371400
O	0	-5.72705400	1.06918600	-0.82437900
O	0	-5.52354500	0.88562000	1.77883100
O	0	-3.52648200	1.95635900	0.31261500
O	0	-4.00323400	2.81580300	-2.27242000
O	0	-3.47296100	2.57632800	2.92995100
O	0	-2.64182600	0.24532800	4.01791400
O	0	-1.83780900	-1.28803900	2.02598900
O	0	-1.39053000	1.14093800	1.46632400
Zr	0	-2.35658500	-2.31190100	-0.04979500
Zr	0	-0.34185600	-0.11488500	-2.07716500
Zr	0	-3.79801200	0.60353500	-1.47122900
Zr	0	-3.27688800	0.47466600	2.04766500
Zr	0	-1.27558600	2.65211200	0.04080900
Zr	0	0.12291400	-0.29747200	1.48532200
H	0	2.16077600	-1.29741900	-1.86706400
Al	0	5.64078100	-1.86467900	-2.01599500
Al	0	5.03035700	0.62393100	-2.85476800
Al	0	3.63644300	-0.74771100	0.11326100
Al	0	7.08712700	0.22887900	-0.20662500
Al	0	4.75771200	2.17693100	-0.73308700
Al	0	6.12733100	-2.61407200	0.50344600
Al	0	4.98607400	1.61135800	1.93367500
Al	0	5.82416000	-0.88161900	2.54085900
H	0	2.87454100	1.24603400	-1.98682100
H	0	4.34825400	-3.45431900	-0.81842600
H	0	9.21360400	1.21709400	0.06942500
H	0	5.55509300	-3.66492600	2.53669600
H	0	1.94601300	-2.58332700	-0.19993600
H	0	5.82286400	3.79522000	0.90562700
H	0	4.57388100	4.24814500	-2.22156400
H	0	8.05059600	-1.61881800	1.69487000
H	0	4.40770000	-2.35704900	3.93566400
H	0	5.13707500	2.26359500	4.14650500
H	0	6.96624800	0.54024300	4.20935000
H	0	7.27794400	-0.46051200	-3.07020700
H	0	3.80686700	-3.02944200	-3.14509900
H	0	2.45047100	-0.34594600	-3.13288000
H	0	6.45515400	1.92879800	-4.27331200
H	0	4.27458600	-1.73785900	-3.92649100
H	0	3.81594100	0.20257400	-4.90295500
O	0	4.42890700	-0.67049200	-1.54224800
O	0	3.64161300	1.81998900	-2.12879000

O	0	5.31625700	-3.39786100	-0.97627200
O	0	8.81164100	0.39874100	-0.22409400
O	0	6.90091700	-1.53368600	-0.72253800
O	0	6.14908100	1.24068700	-1.34043200
O	0	2.72252000	-2.24823100	-0.66524400
O	0	5.73605100	-4.16769800	1.68684300
O	0	5.31290600	3.70031600	-1.93013300
O	0	4.79374300	-1.67108700	1.17968600
O	0	3.88328400	1.08121400	0.47815400
O	0	5.18127000	3.09786000	0.75344600
O	0	6.38383300	0.50677400	1.43071200
O	0	7.23437600	-2.09912000	1.88863400
O	0	5.35129700	-2.40634600	3.73100700
O	0	4.36592000	0.20325600	3.04966100
O	0	5.43067700	2.62642200	3.30760300
O	0	6.87961100	-0.40247600	4.02285400
O	0	6.37933400	-0.74402200	-3.27624800
O	0	5.57460900	2.01363000	-3.89857800
O	0	4.60737800	-2.60666400	-3.48676400
O	0	3.83167100	-0.22522600	-4.04006900
H	0	3.50123900	-0.09521900	2.71137600
H	0	-4.86622000	-4.23129600	3.68087500
H	0	-6.19903800	-3.05009600	3.65716100
H	0	-5.96400600	-4.21822500	2.30953400
H	0	-5.63708200	-4.18076000	-2.96406500
H	0	-6.65905600	-3.78478000	-1.59257000
H	0	-6.79110200	-2.81229500	-3.08708600
H	0	-3.49899900	6.01326100	-2.44135000
H	0	-4.69117400	5.02061700	-3.35966700
H	0	-4.99147100	5.45535100	-1.67369800
H	0	-2.78515900	5.69965600	3.36443200
H	0	-4.39544000	5.32492600	2.74683500
H	0	-3.90921500	4.65912000	4.31375200
H	0	5.53492300	3.15210000	-2.77455400
H	0	6.47522200	-4.74826700	1.91108600
Ir	0	6.49424700	-1.85532600	5.43924100
C	0	6.01373300	-3.27516900	6.49832700
C	0	7.54637000	-1.20849000	6.79275000
O	0	5.68973700	-4.17509800	7.15009400
O	0	8.20804700	-0.78677500	7.64065500
H	0	3.10909200	3.85311800	1.75180400
H	0	1.98443300	4.69820600	2.81064700
H	0	2.89933900	3.26511600	3.40570000
H	0	2.45722400	3.40992800	-3.71772600
H	0	1.10803300	4.57273300	-3.84903300
H	0	2.13364600	4.62483600	-2.42232300
H	0	0.95003200	-4.94613000	-2.70878300
H	0	-0.68454000	-5.49555200	-3.12074200
H	0	0.22156900	-4.39462600	-4.22132600
H	0	0.84292700	-4.83764000	3.30236300
H	0	0.06298300	-5.80717400	2.01098700
H	0	1.63072000	-4.99537600	1.73807000

Al_8-NU-1000 (geminal)

Electronic Energy: -7260.092324

Enthalpy: -7259.082441

Free Energy: -7259.297700

v_{CO} = 2084, 2155 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.89576700	-1.93768000	2.72114900
H	0	1.49721600	1.37111300	-0.23396700
H	0	-3.65623100	1.60395300	-4.00929000
H	0	-2.57410800	0.44433800	-3.97870300
H	0	-2.74861100	1.15928300	4.50892100
H	0	-5.73195300	0.95133300	0.76210200
H	0	-6.40931300	0.51310700	-1.24299700
H	0	-5.97383100	0.07736200	2.06597600
H	0	-2.56654800	-1.62411800	-2.85491800
H	0	-4.20463800	2.64705800	0.39386900
H	0	-0.50782600	0.64808300	-4.55343300
H	0	0.54120500	0.43454400	4.06001300
H	0	2.27960900	-1.62604400	1.84054300
O	0	-1.76333700	1.26312300	-1.39115800
O	0	-2.56974800	4.06522900	-1.09762700
O	0	-2.22856500	3.91247600	1.63570500
O	0	0.10998200	3.46390300	-1.47634400
O	0	0.64628500	1.82459200	-2.89513800
O	0	1.80926600	-0.49989200	-2.36335800
O	0	-0.05095900	-2.32800300	-2.74728800
O	0	0.54474300	-2.57009200	2.00681600
O	0	-1.42336500	-3.63788200	-1.56483900
O	0	-1.11584600	-3.77075500	1.11515100
O	0	-4.12108600	-2.99810500	-1.20975100
O	0	-3.77671400	-3.11442600	1.46371400
O	0	-4.55007100	-1.39872900	2.67734600
O	0	-5.10479300	-1.20164900	-2.11450500
O	0	-3.46707800	-0.56453700	0.18484800
O	0	-2.39005000	-1.09965100	-2.06706700
O	0	-1.03857300	0.04649700	-4.01896200
O	0	-3.54342400	0.67652600	-3.75903700
O	0	0.02513200	-0.30446200	3.71173200
O	0	-0.58174000	-1.21479000	-0.22446300
O	0	0.59922900	1.00225000	-0.23624300
O	0	1.24541800	1.61639300	2.38956100
O	0	2.25381200	-0.71597200	1.50321500
O	0	0.45111400	3.35660200	1.23380500
O	0	-5.73390800	1.06871700	-0.83803600
O	0	-5.52852200	0.87852900	1.75714700
O	0	-3.53944100	1.95718700	0.30699300

O	0	-4.00453600	2.81669000	-2.27560000
O	0	-3.45720400	2.56832900	2.93904300
O	0	-2.71699400	0.29446000	4.08058800
O	0	-1.85986700	-1.28962400	2.00351000
O	0	-1.40821200	1.14159200	1.46107300
Zr	0	-2.34454900	-2.31227100	-0.06214400
Zr	0	-0.33746300	-0.11988300	-2.06399400
Zr	0	-3.80294800	0.60956300	-1.49296900
Zr	0	-3.28430400	0.46661500	1.99459000
Zr	0	-1.26821800	2.64963600	0.03258400
Zr	0	0.12747800	-0.29316900	1.52657100
H	0	2.11327800	-1.27148800	-1.77823800
Al	0	5.66489000	-2.08367300	-1.73799700
Al	0	5.06242500	0.29573100	-2.93641500
Al	0	3.64770800	-0.74913200	0.14512800
Al	0	7.06187400	0.22926900	-0.22010800
Al	0	4.74316100	2.08610100	-1.00531700
Al	0	6.24637900	-2.57693100	0.87895900
Al	0	4.87288800	1.82322600	1.68398600
Al	0	5.77822100	-0.53028800	2.56922300
H	0	2.88925600	1.11238600	-2.22020900
H	0	4.92833300	-4.19760300	-0.54930100
H	0	9.15145400	1.26344500	0.16438400
H	0	5.61302500	-2.81823000	3.32953200
H	0	1.90022300	-2.54642800	-0.14707900
H	0	5.69685200	3.87950200	0.46617000
H	0	4.67310300	3.96887700	-2.74269900
H	0	8.03117000	-1.06982100	1.72385800
H	0	4.47579100	-2.02967000	4.08770500
H	0	5.08019400	3.23001800	3.66518700
H	0	7.29054600	-0.94165500	-3.08225000
H	0	3.57574400	-2.92691600	-2.24269000
H	0	6.58141200	1.37964000	-4.43746700
H	0	4.10036100	-2.22127200	-3.52267800
H	0	3.84726500	-0.37588400	-4.91926000
O	0	4.48562500	-0.77959300	-1.46342900
O	0	3.69212600	1.62661300	-2.39796600
O	0	5.63143500	-3.54671700	-0.62510400
O	0	8.78695200	0.40065700	-0.03812900
O	0	6.92264300	-1.55595800	-0.50695300
O	0	6.17663000	1.13308500	-1.47135800
O	0	2.66457700	-2.20073400	-0.62482300
O	0	6.03009800	-3.87982400	2.09855100
O	0	5.40166400	3.47852600	-2.34200900
O	0	4.83069900	-1.52489000	1.28602200
O	0	3.79207000	1.13846200	0.30277800
O	0	4.99578300	3.22461500	0.39588600
O	0	6.29195800	0.76470600	1.31873900
O	0	7.30918900	-1.57255500	2.13593600
O	0	5.41241100	-1.97651300	3.86218800
O	0	4.26292700	0.54855800	2.94391300
O	0	5.63202400	2.80468300	3.00561500
O	0	6.65201000	0.55542500	3.96513200
O	0	6.36324300	-1.18495200	-3.17970400
O	0	5.69013700	1.53050300	-4.11305800
O	0	4.32385200	-2.96985100	-2.88384400
O	0	3.82045600	-0.63932600	-3.99388000
H	0	3.41950400	0.16044800	2.63722600

H	0	-4.92931500	-3.99317700	3.90171900
H	0	-6.35348500	-3.06474400	3.42395000
H	0	-5.73831300	-4.40359700	2.38410500
H	0	-5.63533600	-4.15625600	-2.99949900
H	0	-6.63189500	-3.82005400	-1.59441300
H	0	-6.81281600	-2.80544400	-3.05763200
H	0	-3.50630800	6.02039300	-2.41558200
H	0	-4.66667300	5.02696400	-3.37262300
H	0	-5.01242300	5.43823400	-1.69074700
H	0	-2.79764800	5.71268800	3.33231300
H	0	-4.41927800	5.30157100	2.76699100
H	0	-3.87785100	4.66702800	4.32670800
H	0	5.65532200	2.82212400	-3.08777900
H	0	6.79948200	-4.36473200	2.40700300
H	0	3.08392200	3.89961400	1.73677400
H	0	1.98029600	4.68448100	2.85427100
H	0	2.89127200	3.23420600	3.39669000
H	0	2.38247700	3.41031200	-3.80850600
H	0	1.10087700	4.65961200	-3.75081100
H	0	2.22644900	4.53708700	-2.40751200
H	0	1.00352500	-4.87821100	-2.78951300
H	0	-0.63498400	-5.52411200	-3.04114800
H	0	0.12386300	-4.41785800	-4.24272900
H	0	0.75597600	-4.87320800	3.31690200
H	0	0.10414300	-5.81301000	1.93930000
H	0	1.66906800	-4.94862000	1.81929600
H	0	7.60788900	0.56320600	3.83442500
H	0	6.34468400	1.49859700	3.73509500
Ir	0	-1.42692400	-1.09574200	4.99275200
C	0	-2.78830300	-1.77285100	6.02513400
C	0	-0.23247800	-2.30571800	5.67908600
O	0	0.54205300	-3.06400400	6.08017000
O	0	-3.66062600	-2.19734700	6.65226000
H	0	2.43078300	-0.52776000	-3.16078100

Al_8-NU-1000 (opposite)

Electronic Energy: -7260.093549

Enthalpy: -7259.083675

Free Energy: -7259.298270

ν_{CO} = 2084, 2156 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900

C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.87657000	-1.87426300	2.78452900
H	0	1.51229300	1.35993900	-0.23621500
H	0	-3.67437500	1.60341300	-3.99756800
H	0	-2.57541300	0.45634400	-3.98240100
H	0	-2.88929200	0.97082400	4.59093200
H	0	-6.38323900	0.32828000	-1.14158300
H	0	-5.95820400	0.13682300	2.16421000
H	0	-2.57681500	-1.61911500	-2.86866400
H	0	-4.09241400	2.71168700	0.39080000
H	0	-0.50740700	0.65805400	-4.56833300
H	0	-1.04998100	-0.03153600	3.98457600
H	0	0.42330900	0.55156100	4.02088500
H	0	2.27910000	-1.61117900	1.87865200
O	0	-1.74636500	1.25637000	-1.41322500
O	0	-2.55063700	4.06169800	-1.12422600
O	0	-2.21552600	3.91171100	1.63921200
O	0	0.11524500	3.45657500	-1.47258300
O	0	0.64811900	1.82512200	-2.90296900
O	0	1.81961200	-0.50811600	-2.37852000
O	0	-0.05190100	-2.32886500	-2.75718600
O	0	0.54743900	-2.56778100	1.99780400
O	0	-1.42136100	-3.63473500	-1.56442500
O	0	-1.11119000	-3.77550900	1.11115300
O	0	-4.11040300	-3.00326200	-1.23143100
O	0	-3.77826300	-3.12474200	1.46089700
O	0	-4.56603600	-1.40078300	2.65081300
O	0	-5.11804000	-1.19351400	-2.07999200
O	0	-3.43567100	-0.56768300	0.17906700
O	0	-2.38579700	-1.10020700	-2.08066000
O	0	-1.03408000	0.04910400	-4.03791100
O	0	-3.54123500	0.67937600	-3.74511800
O	0	-0.07853100	-0.23631200	3.76567400
O	0	-0.57851800	-1.22390000	-0.24158100
O	0	0.61593300	0.98598300	-0.25118000
O	0	1.23352300	1.62027100	2.40159600
O	0	2.24417000	-0.69636300	1.55561200
O	0	0.46442400	3.35403400	1.21982600
O	0	-5.79482900	1.05123500	-0.88977500
O	0	-5.45367400	0.91940300	1.90817100
O	0	-3.49275600	1.95829200	0.29592100
O	0	-4.03582000	2.81321000	-2.23889900
O	0	-3.47358400	2.57980600	2.92725100
O	0	-2.63967000	0.24281800	4.01130900
O	0	-1.84946400	-1.29499100	2.01633500
O	0	-1.38872500	1.13630000	1.46146800
Zr	0	-2.35389300	-2.32014700	-0.04940500
Zr	0	-0.32497500	-0.12741700	-2.09038100
Zr	0	-3.74876700	0.60221800	-1.47105100
Zr	0	-3.31563200	0.46857100	2.05197700
Zr	0	-1.26073900	2.64076100	0.04848800
Zr	0	0.11044200	-0.30566800	1.48125000
H	0	2.12137400	-1.26166200	-1.76985600
Al	0	5.67140000	-2.08099500	-1.68105300
Al	0	5.07493900	0.28483700	-2.90748700
Al	0	3.64083200	-0.72808700	0.18103200
Al	0	7.05606000	0.25057800	-0.18350500
Al	0	4.73217700	2.09346000	-0.99909900

Al	0	6.24072100	-2.54536000	0.94344600
Al	0	4.85760500	1.86269200	1.69486100
Al	0	5.76237600	-0.48014500	2.60860600
H	0	2.88773500	1.10349800	-2.22493100
H	0	4.93628900	-4.18915600	-0.47630400
H	0	9.14307100	1.29370500	0.19346600
H	0	5.59716200	-2.75990500	3.39273600
H	0	1.87545300	-2.50586700	-0.10878300
H	0	5.67921100	3.90315600	0.45302800
H	0	4.66848000	3.95844800	-2.75489800
H	0	8.01951600	-1.02720100	1.77943100
H	0	4.45132400	-1.96261000	4.12748000
H	0	5.07652900	3.31430500	3.64674700
H	0	7.30611000	-0.95412400	-3.02659800
H	0	3.58453800	-2.92620600	-2.19624700
H	0	6.60128400	1.36010400	-4.40788200
H	0	4.12425900	-2.24047200	-3.47968600
H	0	3.88965900	-0.41123900	-4.89821500
O	0	4.48697500	-0.77804800	-1.42625100
O	0	3.69434200	1.61494700	-2.39411300
O	0	5.63349600	-3.53221500	-0.55326500
O	0	8.77977500	0.42802500	0.00143500
O	0	6.92173900	-1.53844100	-0.44967500
O	0	6.17174500	1.13911000	-1.44626800
O	0	2.64511500	-2.16694200	-0.58327100
O	0	6.02210500	-3.83577500	2.17611400
O	0	5.39568800	3.47379000	-2.34478700
O	0	4.82062900	-1.49293900	1.33241900
O	0	3.77678200	1.15857800	0.31786500
O	0	4.97858300	3.24692400	0.39055000
O	0	6.27675100	0.79963500	1.34455000
O	0	7.29605300	-1.52576300	2.19387100
O	0	5.39110500	-1.91306000	3.91521900
O	0	4.24593100	0.60113000	2.96551500
O	0	5.62190900	2.85639500	3.00399600
O	0	6.63070500	0.62010400	3.99554700
O	0	6.37903500	-1.19718700	-3.12693900
O	0	5.70606300	1.50883300	-4.09348500
O	0	4.33864500	-2.98115100	-2.82813900
O	0	3.84892100	-0.66603300	-3.97085700
H	0	3.40188000	0.20880700	2.66502500
H	0	-4.86622700	-4.32223500	3.57070000
H	0	-6.11797400	-3.06004300	3.74938500
H	0	-6.06115600	-4.12025600	2.30149100
H	0	-5.63613800	-4.17103500	-2.97781000
H	0	-6.64627200	-3.79791600	-1.59118200
H	0	-6.80233300	-2.81094100	-3.07411700
H	0	-3.46983300	5.96675600	-2.58386000
H	0	-4.81842200	4.99196600	-3.27877800
H	0	-4.87011200	5.54944700	-1.59716100
H	0	-2.74850700	5.64822000	3.47133800
H	0	-4.30352800	5.40416100	2.68238400
H	0	-4.02113600	4.64611700	4.26208500
H	0	5.65661900	2.81128000	-3.08267000
H	0	6.79225300	-4.31352100	2.49381500
H	0	3.07713800	3.91049900	1.73375800
H	0	1.97732100	4.68088600	2.86263800
H	0	2.89609800	3.23135700	3.39224000

H	0	2.38722000	3.40867700	-3.80218000
H	0	1.10203500	4.65332800	-3.75948100
H	0	2.22008000	4.54445300	-2.40876400
H	0	1.05144300	-4.80035600	-2.89201800
H	0	-0.56652100	-5.55158900	-2.95041600
H	0	0.00129700	-4.45566000	-4.25762900
H	0	0.83636400	-4.84064400	3.30373300
H	0	0.06558400	-5.80718700	2.00481700
H	0	1.63505800	-4.98961700	1.74683700
H	0	7.58729100	0.62669800	3.87020400
H	0	6.32432000	1.56133200	3.75513600
Ir	0	-6.47740100	2.26836100	0.68251400
C	0	-6.95522700	3.30052500	2.12353100
C	0	-7.30436000	3.42479000	-0.48129700
O	0	-7.22530300	3.94696600	3.04189300
O	0	-7.80708800	4.14799800	-1.22932100
H	0	2.45378100	-0.54668700	-3.16646600

Table S7. XYZ Cartesian Coordinates of Selected Optimized Al_8-NU-1000 Isomers at the M06 Density Functional.

Al_8-NU-1000 (A)

Electronic Energy: -7257.804163
Enthalpy: -7256.796085
Free Energy: -7257.012297
ν_{CO} = 2089, 2176 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.87038300	-1.84782700	2.78006700
H	0	1.53492700	1.31652300	-0.24214300
H	0	-3.70112100	1.63489600	-3.93159500
H	0	-2.62112800	0.47118800	-3.98482600
H	0	-2.93219100	0.97259000	4.57752900
H	0	-5.73207900	0.94817400	0.81297200
H	0	-6.39009600	0.53253900	-1.25951800
H	0	-5.90413700	0.03767500	2.10065200
H	0	-2.56688100	-1.60274000	-2.84582200
H	0	-4.17803100	2.62401500	0.39120200
H	0	-0.50963300	0.63260200	-4.56893500
H	0	-1.04833100	-0.03360100	3.99786200
H	0	0.38878100	0.61415600	4.00564600
H	0	2.26227400	-1.66184900	1.83923600
O	0	-1.73849000	1.26623700	-1.38798800
O	0	-2.57263000	4.06403300	-1.09612800
O	0	-2.21466800	3.90749600	1.64567300
O	0	0.11616400	3.45034500	-1.47017000
O	0	0.64722800	1.82908600	-2.90279000
O	0	1.78826600	-0.52416900	-2.50724700
O	0	-0.06141700	-2.32888800	-2.75632500
O	0	0.54050800	-2.56807200	2.00921700
O	0	-1.41418500	-3.63544600	-1.56039700
O	0	-1.10244800	-3.76883500	1.10201800
O	0	-4.12405500	-2.99661700	-1.20512100
O	0	-3.75744700	-3.12171300	1.48431600

O	0	-4.58232300	-1.39645500	2.63400300
O	0	-5.09614900	-1.20581900	-2.11479600
O	0	-3.43782700	-0.57687900	0.19050900
O	0	-2.37913600	-1.09123900	-2.05141800
O	0	-1.05175100	0.06169300	-4.01280900
O	0	-3.57557700	0.69506700	-3.73119100
O	0	-0.08321700	-0.19509300	3.75467600
O	0	-0.58085500	-1.22525800	-0.22876200
O	0	0.64275700	0.93618700	-0.26257400
O	0	1.26433100	1.61064200	2.37809200
O	0	2.24834300	-0.75771800	1.47868900
O	0	0.45387300	3.34392200	1.23201000
O	0	-5.70212600	1.05343600	-0.83054300
O	0	-5.51079500	0.86981300	1.79502000
O	0	-3.50460400	1.94126200	0.30784700
O	0	-3.99907800	2.81842200	-2.27300700
O	0	-3.47572300	2.57785400	2.91859900
O	0	-2.67523400	0.24980100	3.99419700
O	0	-1.83641800	-1.27477400	2.00651300
O	0	-1.37498700	1.14048700	1.44834300
Zr	0	-2.35495300	-2.31842000	-0.05081600
Zr	0	-0.34193900	-0.12223400	-2.08525400
Zr	0	-3.78546700	0.59299700	-1.46071500
Zr	0	-3.26287800	0.47442900	2.03108000
Zr	0	-1.28282400	2.65032700	0.03461100
Zr	0	0.11819700	-0.31024800	1.47030300
H	0	2.12391400	-1.30838500	-1.96484100
Al	0	5.64545200	-1.97828700	-1.99260900
Al	0	5.03285800	0.48495700	-2.93304400
Al	0	3.62730100	-0.84164200	0.04604800
Al	0	7.02672800	0.14789000	-0.25920400
Al	0	4.67713100	2.12802000	-0.89742000
Al	0	6.12784400	-2.81154000	0.56846300
Al	0	4.92962800	1.66227500	1.73786200
Al	0	5.76585200	-0.85623300	2.48738700
H	0	2.81469400	1.17910700	-2.18886300
H	0	4.22400200	-3.48029900	-0.85554200
H	0	9.10663200	1.28751500	-0.18240500
H	0	1.80723600	-2.50574500	-0.22442900
H	0	5.68610600	3.81976100	0.65433300
H	0	4.53810500	4.13658200	-2.45914000
H	0	8.02025600	-1.63364500	1.82122200
H	0	4.69199300	-2.66764200	3.73747300
H	0	5.16026100	3.07540500	3.74847900
H	0	6.43530200	1.20846500	3.77933300
H	0	7.32396200	-0.57392200	-3.06057800
H	0	3.98583600	-3.30209900	-3.30884400
H	0	2.41608400	-0.43966400	-3.28304600
H	0	6.49432300	1.74373000	-4.36399700
H	0	4.34277500	-1.90662800	-4.00366500
H	0	3.89270300	0.05929000	-5.00536100
O	0	4.42662100	-0.75616800	-1.60004600
O	0	3.61464800	1.71728100	-2.28687300

O	0	5.18733800	-3.41987800	-0.98860000
O	0	8.73531500	0.40728800	-0.24400500
O	0	6.85313000	-1.62419200	-0.65495400
O	0	6.09501800	1.18336000	-1.38223500
O	0	2.58900300	-2.20057400	-0.69895900
O	0	6.39986900	-4.41089300	1.17369200
O	0	5.27285100	3.61643600	-2.10855200
O	0	4.77792600	-1.71707200	1.17774600
O	0	3.82652500	1.04967100	0.35773500
O	0	5.00327800	3.14524700	0.58262500
O	0	6.27384100	0.52511100	1.35271800
O	0	7.14979100	-1.97401000	2.05651000
O	0	5.04854200	-1.79900400	3.96000700
O	0	4.13028700	0.36235000	2.91877600
O	0	5.64898100	2.51318600	3.14486700
O	0	6.67853900	0.24066000	3.93721600
O	0	6.41907100	-0.85279000	-3.24065000
O	0	5.62225100	1.86069100	-3.97810100
O	0	4.72780400	-2.73349400	-3.55126100
O	0	3.87048200	-0.36634200	-4.14152900
H	0	3.31680500	0.04278400	2.42939900
H	0	-4.85814800	-4.24899400	3.65926900
H	0	-6.18410900	-3.04482900	3.67454800
H	0	-5.97960800	-4.19872500	2.29898900
H	0	-5.62732600	-4.15757900	-2.99655100
H	0	-6.63080800	-3.81624400	-1.58788900
H	0	-6.80963100	-2.79959600	-3.06077700
H	0	-3.49365500	6.01266700	-2.43526400
H	0	-4.68605800	5.01441300	-3.36420200
H	0	-4.99567500	5.44868200	-1.67140900
H	0	-2.78371300	5.70273000	3.35078700
H	0	-4.40598700	5.31267400	2.74847400
H	0	-3.89719100	4.65402700	4.31972300
H	0	5.55151700	3.04077700	-2.92146100
H	0	6.96126400	-4.46195800	1.94979100
Ir	0	3.75644800	-0.43783400	4.83419200
C	0	3.50716000	-1.30925800	6.43844700
C	0	2.58408800	0.87494000	5.35377400
O	0	3.35817300	-1.86094600	7.43329400
O	0	1.80775600	1.69090000	5.60287200
H	0	7.63982600	0.18397800	3.87889600
H	0	2.47312200	3.39282100	-3.68475600
H	0	1.11282800	4.54408100	-3.88155300
H	0	2.10548100	4.64887100	-2.42286900
H	0	3.09718100	3.86252500	1.73769900
H	0	1.98025500	4.69434600	2.82915300
H	0	2.87856900	3.24382200	3.41391300
H	0	0.97501600	-4.91292500	-2.73427600
H	0	-0.66953800	-5.50715100	-3.08197900
H	0	0.17779900	-4.39647100	-4.23298200
H	0	0.90212800	-4.80650100	3.29000200
H	0	0.03127800	-5.79919100	2.05927700
H	0	1.60245700	-5.02082800	1.68313300

Al_8-NU-1000 (A_2)

Electronic Energy: -7257.807618

Enthalpy: -7256.798692

Free Energy: -7257.014368

ν_{CO} = 2102, 2182 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.86362800	-1.83541900	2.79269800
H	0	1.46831000	1.39411100	-0.22891200
H	0	-3.68974100	1.63717600	-3.92653100
H	0	-2.61327500	0.47180800	-3.97982400
H	0	-2.91494600	0.97794500	4.58395200
H	0	-5.73208900	0.94899300	0.81914700
H	0	-6.39253300	0.53254200	-1.25530200
H	0	-5.90544100	0.03558900	2.10376600
H	0	-2.56383900	-1.60490300	-2.83891000
H	0	-4.18058700	2.62470800	0.39308800
H	0	-0.49472400	0.64311400	-4.55351600
H	0	-1.00237100	-0.00459300	4.01192000
H	0	0.47385700	0.58685400	3.99226300
H	0	2.12122800	-1.76149300	1.70050900
O	0	-1.74524900	1.26805300	-1.38968500
O	0	-2.57390400	4.06356800	-1.09575500
O	0	-2.21849200	3.90851700	1.64403300
O	0	0.10658600	3.44085400	-1.47406400
O	0	0.68295500	1.81887100	-2.89023000
O	0	1.79958500	-0.49588200	-2.39741700
O	0	-0.03923200	-2.33236500	-2.73977500
O	0	0.52788800	-2.57263400	2.04206000
O	0	-1.42548200	-3.63229200	-1.57256400
O	0	-1.09117300	-3.76924400	1.08684200
O	0	-4.12556400	-2.99498400	-1.20154800
O	0	-3.75461900	-3.12026400	1.48553500
O	0	-4.57964600	-1.39756500	2.63924800
O	0	-5.09506700	-1.20598400	-2.11647600

O	0	-3.43572200	-0.57474200	0.19526800
O	0	-2.37605000	-1.09140900	-2.04591500
O	0	-1.03430400	0.06186800	-4.00565800
O	0	-3.56744300	0.69589000	-3.72992400
O	0	-0.04573200	-0.19977500	3.76209000
O	0	-0.57318500	-1.22188200	-0.22048100
O	0	0.60077500	0.97055000	-0.24704800
O	0	1.26316600	1.60178500	2.36266800
O	0	2.21925500	-0.83310800	1.42735000
O	0	0.44162900	3.33858300	1.23565000
O	0	-5.70391800	1.05186300	-0.82553800
O	0	-5.51199500	0.86866000	1.80121200
O	0	-3.50823500	1.94069800	0.31125400
O	0	-4.00057400	2.81784700	-2.27267400
O	0	-3.47474000	2.57753300	2.92119400
O	0	-2.64873300	0.25903000	3.99988300
O	0	-1.83169600	-1.27024000	2.01325400
O	0	-1.38458000	1.14502900	1.45983100
Zr	0	-2.35514400	-2.30857500	-0.04996900
Zr	0	-0.34150200	-0.11163100	-2.07075300
Zr	0	-3.78700000	0.59620700	-1.45809000
Zr	0	-3.26240400	0.47796400	2.04171600
Zr	0	-1.28276800	2.65270900	0.04223900
Zr	0	0.11764700	-0.29246300	1.48087300
H	0	2.15450900	-1.30919300	-1.92468100
Al	0	5.57841500	-1.97487500	-2.06076600
Al	0	5.06170100	0.58307000	-2.77896200
Al	0	3.63412100	-0.86974300	0.11102000
Al	0	6.95461500	-0.10124200	-0.07304200
Al	0	4.89390000	2.08242300	-0.56002300
Al	0	6.08214200	-2.94067100	0.46713600
Al	0	4.91374000	1.36821200	2.10693000
Al	0	5.77823200	-1.26086100	2.69340200
H	0	2.95035400	1.33465500	-1.89441500
H	0	4.18265400	-3.46249000	-0.96393100
H	0	9.21898600	0.89215600	-0.27426800
H	0	5.34459900	-3.75360200	2.83422200
H	0	1.84880500	-2.59450400	-0.29782100
H	0	5.91238100	3.56869000	1.24208000
H	0	4.93036500	4.27877900	-1.91479100
H	0	7.83310700	-2.62277900	2.38164600
H	0	4.03579300	-3.05077800	3.24548200
H	0	5.04551500	1.94474200	4.33978800
H	0	6.28571600	-0.85185400	4.96785200
H	0	7.28114400	-0.58757200	-3.08632000
H	0	3.74859500	-3.06355100	-3.36125200
H	0	2.43680700	-0.28617400	-3.14123900
H	0	6.55260500	1.85261700	-4.18921200
H	0	4.22154700	-1.68900400	-4.00764700
H	0	3.83147300	0.39156100	-4.84710200
O	0	4.43140400	-0.73205500	-1.54904500
O	0	3.77212700	1.83788000	-1.97875300
O	0	5.15219700	-3.48824900	-1.12741700

O	0	8.65166100	0.39546900	0.32059200
O	0	6.86966300	-1.75912400	-0.75633300
O	0	6.22296000	1.06265700	-1.17625800
O	0	2.66685200	-2.29192900	-0.70963000
O	0	5.95199600	-4.49142000	1.31196600
O	0	5.57436800	3.59933600	-1.68019400
O	0	4.85834900	-1.76323200	1.08663800
O	0	3.97846200	0.92756300	0.55884300
O	0	5.26716800	2.90607500	0.98057100
O	0	6.46014300	0.35453100	1.65243400
O	0	7.14205400	-2.24316600	1.83343900
O	0	4.98449100	-3.03656200	3.42666000
O	0	4.33067100	-0.12255400	3.10097900
O	0	5.14566600	2.40031700	3.49956400
O	0	6.74646000	-0.93047900	4.13032600
O	0	6.36224100	-0.81234700	-3.26012800
O	0	5.73269700	1.99350900	-3.71015000
O	0	4.54177700	-2.57114900	-3.61270700
O	0	3.83829100	-0.10657600	-4.02303500
H	0	3.44607600	-0.36884900	2.77874100
H	0	-4.86030400	-4.21850700	3.69327000
H	0	-6.20785900	-3.04262800	3.64468400
H	0	-5.94932000	-4.22859100	2.30475400
H	0	-5.62774200	-4.16824000	-2.98115600
H	0	-6.64294300	-3.80114900	-1.58722200
H	0	-6.79988400	-2.80242400	-3.07390900
H	0	-3.49345000	6.01245900	-2.43511300
H	0	-4.68635600	5.01489200	-3.36413800
H	0	-4.99532100	5.44854200	-1.67098700
H	0	-2.77505600	5.69325200	3.36983700
H	0	-4.38942500	5.32800500	2.73477000
H	0	-3.91802800	4.65160600	4.31147700
H	0	5.76233400	3.10523800	-2.56139700
H	0	5.57780700	-5.24385100	0.84834100
Ir	0	8.35314100	1.10296800	2.29740500
C	0	7.91975900	1.54767400	4.04082000
C	0	10.03456500	1.76007300	2.58887500
O	0	7.71698600	1.82302200	5.13462500
O	0	11.09783100	2.17814900	2.73989100
H	0	3.12380200	3.80686500	1.75287800
H	0	1.98711500	4.71196300	2.76755500
H	0	2.89394400	3.27530200	3.41747300
H	0	2.70270300	3.52813800	-3.08197800
H	0	1.44187100	3.99098000	-4.22772700
H	0	1.63324200	4.94754900	-2.71629200
H	0	0.96888800	-4.92098600	-2.72583500
H	0	-0.67539800	-5.50385400	-3.09332600
H	0	0.18933500	-4.39383800	-4.23046400
H	0	0.84199300	-4.83123700	3.30486000
H	0	0.05841000	-5.80661400	2.00755600
H	0	1.63056900	-4.99086800	1.72937900

Al_8-NU-1000 (C)

Electronic Energy: -7257.819875

Enthalpy: -7256.809948

Free Energy: -7257.026005

ν_{CO} = 2094, 2168 cm^{-1}

C	-1	1.68441900	3.94341500	-3.15514000
C	-1	0.64899900	-4.90821600	2.22466600
C	-1	2.37165700	3.70494900	2.55374400
C	-1	0.00185000	-4.64437900	-3.17737000
C	-1	-5.46152400	-3.56982100	3.03745400
C	-1	-4.20580600	5.17837100	-2.39073300
C	-1	-6.09808400	-3.34300700	-2.42691100
C	-1	-3.54711000	4.91457400	3.31258500
C	-1	1.27407100	2.82442300	2.03809500
C	-1	0.75416700	3.00364000	-2.46953500
C	-1	-3.54118900	3.93046700	-1.89896000
C	-1	-5.03722900	-2.44266000	-1.88258700
C	-1	-4.54348500	-2.62142800	2.33674300
C	-1	-0.02842400	-3.67128600	1.74594600
C	-1	-3.03318900	3.71325000	2.58679300
C	-1	-0.52889700	-3.45027300	-2.44888800
H	0	-1.86130000	-1.84202700	2.78133100
H	0	1.54840400	1.29646400	-0.24963000
H	0	-3.70581800	1.63741600	-3.92760500
H	0	-2.62679800	0.47397400	-3.98439400
H	0	-2.90078400	0.97784500	4.57549500
H	0	-5.72568500	0.94752400	0.82388500
H	0	-6.39109800	0.53244500	-1.24921000
H	0	-5.89053100	0.03139000	2.10758500
H	0	-2.57150700	-1.60010800	-2.84592700
H	0	-4.17533300	2.62416200	0.39660400
H	0	-0.51519800	0.65200600	-4.56502300
H	0	-0.98990500	-0.01977400	3.99657200
H	0	0.46695600	0.60155100	3.93954100
H	0	2.24918900	-1.66781700	1.80154300
O	0	-1.74016700	1.26902000	-1.38750800
O	0	-2.57315600	4.06414700	-1.09609300
O	0	-2.21364400	3.90819600	1.64693600
O	0	0.11149400	3.45504800	-1.47625600
O	0	0.65269900	1.82501300	-2.89511400
O	0	1.78289200	-0.53060800	-2.46923300
O	0	-0.06863400	-2.32901000	-2.76705800
O	0	0.54542100	-2.57108500	2.00763600
O	0	-1.41482900	-3.63258900	-1.55990300
O	0	-1.10470900	-3.76896700	1.10703000
O	0	-4.12252100	-2.99716800	-1.20753000
O	0	-3.76191100	-3.12097800	1.47996800
O	0	-4.57325700	-1.39826000	2.64314900
O	0	-5.09904100	-1.20528300	-2.11050000
O	0	-3.43548100	-0.57601400	0.19320500

O	0	-2.38408800	-1.08779400	-2.05202300
O	0	-1.05132600	0.06888600	-4.01591700
O	0	-3.58038200	0.69699500	-3.72937000
O	0	-0.03212300	-0.20959100	3.74996700
O	0	-0.57821800	-1.23122700	-0.23624800
O	0	0.64346800	0.93970500	-0.26502300
O	0	1.24570200	1.61548200	2.39038200
O	0	2.24577300	-0.75474400	1.46880800
O	0	0.45999000	3.34385800	1.22394900
O	0	-5.70238500	1.05394400	-0.82218500
O	0	-5.50198400	0.86681200	1.80476700
O	0	-3.50183600	1.94173700	0.31135200
O	0	-4.00043600	2.81800900	-2.27160300
O	0	-3.47244700	2.57722600	2.92114400
O	0	-2.63526900	0.25757000	3.99297400
O	0	-1.82844700	-1.27415300	2.00406500
O	0	-1.36984800	1.14081100	1.44483000
Zr	0	-2.35604100	-2.31635600	-0.05220300
Zr	0	-0.34910100	-0.11747700	-2.08530000
Zr	0	-3.78725100	0.59628900	-1.45698700
Zr	0	-3.25021100	0.47572200	2.03469300
Zr	0	-1.27650200	2.65401700	0.03511400
Zr	0	0.12810700	-0.31196900	1.45645000
H	0	2.10179500	-1.28869700	-1.86939500
Al	0	5.73392400	-2.10509600	-1.78496600
Al	0	5.03040900	0.26939800	-2.89818600
Al	0	3.64531600	-0.78887800	0.09517600
Al	0	7.06144700	0.26210200	-0.28684500
Al	0	4.65105300	2.17154100	-1.03697000
Al	0	6.26122400	-2.62204600	0.82692700
Al	0	4.89760400	1.76115800	1.66325800
Al	0	5.78058000	-0.60083100	2.51590300
H	0	2.81392500	1.13922100	-2.35130900
H	0	5.10854800	-4.30409800	-0.66840600
H	0	9.08327200	1.49567300	-0.40057300
H	0	6.71734500	-4.50677900	2.28745700
H	0	1.84527200	-2.53392500	-0.25114400
H	0	5.58806600	3.90608900	0.52222100
H	0	4.58172600	3.75248800	-2.86182000
H	0	8.06175400	-1.18968000	1.90660600
H	0	4.34335700	-2.10696800	3.88388700
H	0	5.57198400	-2.88533400	3.31194000
H	0	5.17503900	3.29056300	3.58171500
H	0	6.41603400	1.39964200	3.73300900
H	0	6.34526200	0.23905700	4.81942600
H	0	7.32234600	-0.88639100	-3.11803400
H	0	3.61839800	-2.94831600	-2.28901100
H	0	2.38836400	-0.55637700	-3.26429900
H	0	6.10285600	1.21587800	-4.96458400
H	0	4.14746900	-2.27723000	-3.57861900
H	0	3.90555600	-0.40038500	-5.00083300
O	0	4.50755800	-0.85338300	-1.50319000
O	0	3.66634400	1.58973600	-2.44924200

O	0	5.74813400	-3.58742400	-0.71159200
O	0	8.75116500	0.59714500	-0.40231700
O	0	6.93342500	-1.53646000	-0.52083500
O	0	6.06706100	1.15230400	-1.49160700
O	0	2.62089600	-2.18343100	-0.70574600
O	0	5.98650000	-3.95030200	2.00780800
O	0	5.23096900	3.59176700	-2.16560800
O	0	4.83352300	-1.58054000	1.22592900
O	0	3.79331400	1.10042700	0.25957500
O	0	4.94989800	3.18872000	0.45906800
O	0	6.31374900	0.69334400	1.29540100
O	0	7.26888400	-1.68858800	2.13798100
O	0	5.30606800	-2.05025500	3.81812200
O	0	4.26311000	0.47171700	2.88718200
O	0	5.66300500	2.69251600	3.01380800
O	0	6.67150300	0.43594200	3.93316400
O	0	6.40430200	-1.17394600	-3.19837800
O	0	5.86614100	1.47666700	-4.07150500
O	0	4.36866300	-3.00579900	-2.92814300
O	0	3.88033200	-0.62810200	-4.06765000
H	0	3.41019100	0.10740400	2.57978300
Ir	0	7.01923100	3.03767200	-3.19883300
C	0	8.51443900	2.61039700	-4.16910900
C	0	7.87120500	4.51862900	-2.53605600
O	0	9.43653900	2.33130100	-4.79998400
O	0	8.37920200	5.46525600	-2.12215800
H	0	-4.85797400	-4.23817500	3.67084100
H	0	-6.19193700	-3.04418000	3.66509200
H	0	-5.96962400	-4.20933100	2.30135000
H	0	-5.62783300	-4.16419900	-2.98722300
H	0	-6.63799600	-3.80683200	-1.58715500
H	0	-6.80404600	-2.80119200	-3.06834900
H	0	-3.49196600	6.01089900	-2.44092500
H	0	-4.69152900	5.01332800	-3.36127500
H	0	-4.99087000	5.45232100	-1.66756100
H	0	-2.77489200	5.69306700	3.37025700
H	0	-4.38914000	5.32913100	2.73515100
H	0	-3.91870100	4.65102100	4.31111400
H	0	3.08636300	3.87505600	1.72946000
H	0	1.97668300	4.69159000	2.83464500
H	0	2.88749100	3.23756500	3.40465500
H	0	1.63687300	-4.98308700	1.74261900
H	0	0.83284900	-4.83437400	3.30676300
H	0	0.06090600	-5.80649500	2.00083500
H	0	1.07917100	-4.73816000	-2.96956000
H	0	-0.51353300	-5.56627400	-2.88116500
H	0	-0.09484000	-4.48259500	-4.26096600
H	0	2.32776100	3.41471000	-3.86948900
H	0	1.09771400	4.71662000	-3.67601800
H	0	2.29064500	4.47059800	-2.40173600

Al_8-NU-1000 (C_geminal)

Electronic Energy: -7257.801582
Enthalpy: -7256.792482
Free Energy: -7257.008563
ν_{CO} = 2106, 2178 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.86477900	-1.83934800	2.78869000
H	0	1.47112300	1.39538300	-0.21535600
H	0	-3.69403800	1.63852800	-3.92355600
H	0	-2.61998500	0.47082600	-3.98130100
H	0	-2.91537000	0.97981600	4.58085600
H	0	-5.73154300	0.94859000	0.81969900
H	0	-6.39228000	0.53125800	-1.25430200
H	0	-5.90083800	0.03215300	2.10242800
H	0	-2.56648200	-1.60491700	-2.84047300
H	0	-4.18020300	2.62503500	0.39305300
H	0	-0.50542000	0.63748200	-4.56021500
H	0	-1.00298800	-0.00800400	4.00961100
H	0	0.46292200	0.60141500	3.96952100
H	0	2.17464400	-1.73138500	1.72713100
O	0	-1.74659900	1.26723200	-1.39027100
O	0	-2.57417600	4.06353100	-1.09554200
O	0	-2.21616000	3.90788400	1.64576900
O	0	0.10664700	3.44683600	-1.47628700
O	0	0.66007800	1.82492200	-2.89996800
O	0	1.79133700	-0.49748000	-2.43491700
O	0	-0.04575800	-2.33202200	-2.74597700
O	0	0.52901100	-2.57226500	2.03715000
O	0	-1.42326200	-3.63330100	-1.57010800
O	0	-1.09428200	-3.77038900	1.09028500
O	0	-4.12503300	-2.99579300	-1.20315500
O	0	-3.75625800	-3.12089200	1.48470800
O	0	-4.57946700	-1.39780400	2.63966300
O	0	-5.09673000	-1.20594100	-2.11515000
O	0	-3.43714200	-0.57563400	0.19464500
O	0	-2.37857700	-1.09176400	-2.04730500
O	0	-1.04505500	0.05849300	-4.00995000

O	0	-3.57380200	0.69635300	-3.72990200
O	0	-0.04543200	-0.19951000	3.76257200
O	0	-0.57449700	-1.22289200	-0.22517000
O	0	0.60518700	0.96712400	-0.25047000
O	0	1.24824600	1.60785300	2.37706700
O	0	2.22073600	-0.80380100	1.43990000
O	0	0.45112300	3.33925700	1.22546700
O	0	-5.70488700	1.05279100	-0.82529400
O	0	-5.51152000	0.86785500	1.80163300
O	0	-3.50788700	1.94109000	0.31090200
O	0	-4.00113000	2.81833600	-2.27313500
O	0	-3.47607000	2.57811900	2.92095500
O	0	-2.65074500	0.25836800	3.99929500
O	0	-1.83244800	-1.27196300	2.01098700
O	0	-1.38397600	1.14388500	1.45770700
Zr	0	-2.35404600	-2.30980800	-0.05033200
Zr	0	-0.34443500	-0.11297900	-2.07752700
Zr	0	-3.78748000	0.59592100	-1.45764400
Zr	0	-3.26006300	0.47792200	2.03954200
Zr	0	-1.28058700	2.65049800	0.04051900
Zr	0	0.12010900	-0.30014000	1.47707100
H	0	2.15481100	-1.29718500	-1.93761600
Al	0	5.65124200	-1.83706500	-2.06848900
Al	0	5.02624900	0.67299200	-2.80373900
Al	0	3.61884700	-0.80025200	0.09394400
Al	0	7.08256300	0.18973500	-0.15422100
Al	0	4.75276500	2.16791800	-0.63128000
Al	0	6.09487800	-2.70059000	0.42406800
Al	0	4.97981900	1.48112700	2.00962100
Al	0	5.79683400	-1.05722600	2.53702500
H	0	2.84614800	1.29867200	-1.95930600
H	0	4.35248900	-3.50292300	-0.96509300
H	0	9.21273900	1.20276600	0.08323300
H	0	5.45066900	-3.87279800	2.38928700
H	0	1.88829300	-2.57407500	-0.29330100
H	0	5.79422700	3.73068800	1.09544800
H	0	4.55843100	4.29362800	-2.04838700
H	0	8.03440500	-1.84001100	1.70265000
H	0	4.31133600	-2.56509700	3.85043100
H	0	5.08425900	2.08059000	4.24229400
H	0	7.00187100	0.19238700	4.31559700
H	0	7.29882900	-0.37816800	-3.04192000
H	0	3.87181800	-3.01971100	-3.33345500
H	0	2.43016000	-0.30252300	-3.18065000
H	0	6.44724500	2.01788200	-4.19747800
H	0	4.30473300	-1.64397900	-4.00225700
H	0	3.85478500	0.35806400	-4.88575100
O	0	4.42803100	-0.67816000	-1.55948400
O	0	3.64120600	1.84398000	-2.03613800
O	0	5.31937900	-3.41470100	-1.10435500
O	0	8.79607200	0.38940600	-0.20247200
O	0	6.87678700	-1.55615400	-0.73372700
O	0	6.12951600	1.23123400	-1.24874700

O	0	2.68257700	-2.24114100	-0.72785600
O	0	5.65063300	-4.31534800	1.51340900
O	0	5.29562800	3.73266200	-1.77578900
O	0	4.77839100	-1.75969700	1.12562800
O	0	3.90291100	1.01117000	0.52829300
O	0	5.19070000	3.01498200	0.88429500
O	0	6.38673300	0.38373200	1.50740000
O	0	7.18602000	-2.28164400	1.83476400
O	0	5.25411100	-2.63998700	3.64787600
O	0	4.37006800	0.03473600	3.08264500
O	0	5.31614900	2.49334100	3.40734400
O	0	6.84887600	-0.72347400	4.05863800
O	0	6.40286800	-0.66219100	-3.25982900
O	0	5.58379100	2.10193100	-3.78476900
O	0	4.65637800	-2.51908000	-3.59592600
O	0	3.85201700	-0.12023200	-4.04944300
H	0	3.48338200	-0.22563700	2.77401200
H	0	-4.85948400	-4.22672900	3.68419500
H	0	-6.20145500	-3.04310800	3.65290500
H	0	-5.95770500	-4.22066700	2.30321300
H	0	-5.62782400	-4.16723700	-2.98272300
H	0	-6.64174000	-3.80251700	-1.58719000
H	0	-6.80095100	-2.80213500	-3.07254100
H	0	-3.49490100	6.01393600	-2.43019400
H	0	-4.68174700	5.01610700	-3.36664000
H	0	-4.99933900	5.44515300	-1.67416000
H	0	-2.77718300	5.69566300	3.36505600
H	0	-4.39368700	5.32429800	2.73836100
H	0	-3.91283800	4.65203100	4.31354600
H	0	5.53753900	3.22709300	-2.63728200
H	0	6.35972700	-4.94199100	1.71017600
Ir	0	6.40600300	-2.24542300	5.36214500
C	0	5.87192000	-3.71805900	6.33244700
C	0	7.49233200	-1.73255200	6.75896200
O	0	5.51828100	-4.64376400	6.91705400
O	0	8.17064900	-1.39679000	7.62280600
H	0	3.09808700	3.85462100	1.73776200
H	0	1.97521300	4.69481700	2.82064300
H	0	2.92086900	3.25341500	3.38943800
H	0	2.58183500	3.40799200	-3.49677700
H	0	1.17798900	4.36546700	-4.03868600
H	0	1.94310700	4.77888800	-2.48953600
H	0	0.99702200	-4.88386900	-2.76816000
H	0	-0.64773000	-5.51957100	-3.05005800
H	0	0.13547500	-4.40720900	-4.24194100
H	0	0.79195900	-4.85058900	3.31404400
H	0	0.08088600	-5.81017000	1.96628500
H	0	1.65382000	-4.96312500	1.77547800

Al_8-NU-1000 (geminal)

Electronic Energy: -7257.811525

Enthalpy: -7256.802219

Free Energy: -7257.017377

ν_{CO} = 2106, 2179 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.88403800	-1.89241400	2.72318000
H	0	1.51215200	1.32618600	-0.24227700
H	0	-3.68846500	1.63394200	-3.95633000
H	0	-2.60512000	0.46912000	-3.98654900
H	0	-2.75984800	1.17833900	4.47990500
H	0	-5.74197200	0.93218800	0.79646900
H	0	-6.39483700	0.52204700	-1.26670300
H	0	-5.91174500	0.03353000	2.09910500
H	0	-2.56726700	-1.59935700	-2.84299400
H	0	-4.19400100	2.62353200	0.39495000
H	0	-0.50450500	0.62478900	-4.55998900
H	0	0.53422100	0.47304100	4.00937200
H	0	2.23997100	-1.67662100	1.79288600
O	0	-1.75387800	1.27194700	-1.38794800
O	0	-2.57189400	4.06106600	-1.09878200
O	0	-2.23215800	3.91034800	1.63535900
O	0	0.11272400	3.45682300	-1.47404300
O	0	0.64428100	1.82909900	-2.89792500
O	0	1.77935200	-0.50981800	-2.43540700
O	0	-0.06343700	-2.32926800	-2.75761900
O	0	0.53734300	-2.57274500	2.01913900
O	0	-1.41913800	-3.63311300	-1.56304900
O	0	-1.10740800	-3.76704300	1.10625200
O	0	-4.12172500	-2.99368700	-1.20858500
O	0	-3.77549600	-3.10783300	1.46530300
O	0	-4.55024400	-1.40100000	2.67769800
O	0	-5.09855500	-1.20505700	-2.11821500
O	0	-3.45878200	-0.56547600	0.18586600
O	0	-2.38630600	-1.08622500	-2.04798800
O	0	-1.05304400	0.06032100	-4.00356400
O	0	-3.56479000	0.69725400	-3.74223300
O	0	0.03968200	-0.29571500	3.69232300
O	0	-0.58252000	-1.22255300	-0.22656500

O	0	0.60919200	0.96830500	-0.24556400
O	0	1.25271300	1.61452900	2.37966500
O	0	2.24433600	-0.77030500	1.44195000
O	0	0.44821700	3.35032900	1.23728300
O	0	-5.71332000	1.05242100	-0.83867500
O	0	-5.51224800	0.85655300	1.77868600
O	0	-3.52015000	1.94179600	0.30631800
O	0	-4.00488700	2.81927100	-2.27348300
O	0	-3.45477700	2.56918400	2.93426200
O	0	-2.70947500	0.30687300	4.06503000
O	0	-1.85397600	-1.27535900	1.97864700
O	0	-1.39702500	1.14414100	1.45014300
Zr	0	-2.34072200	-2.31142900	-0.06205600
Zr	0	-0.34556200	-0.11844100	-2.06808000
Zr	0	-3.79428300	0.60425900	-1.47979700
Zr	0	-3.26389900	0.46711200	1.98121400
Zr	0	-1.27100100	2.64901900	0.03138800
Zr	0	0.13347800	-0.29759200	1.51059100
H	0	2.09782700	-1.28468900	-1.85901700
Al	0	5.71205200	-2.07568900	-1.81809900
Al	0	5.04128200	0.32132500	-2.94224500
Al	0	3.64896100	-0.81138100	0.09311900
Al	0	7.07204000	0.23311800	-0.25376100
Al	0	4.70089800	2.08660200	-0.97661500
Al	0	6.25393300	-2.64945100	0.78677500
Al	0	4.89397100	1.71947600	1.70165100
Al	0	5.77257900	-0.66003900	2.53521300
H	0	2.83217800	1.13027000	-2.24235600
H	0	5.07287400	-4.29046000	-0.73814800
H	0	9.15098100	1.37065300	-0.12551100
H	0	5.55878800	-2.97710300	3.25420900
H	0	1.87237100	-2.56551300	-0.26449400
H	0	5.66229100	3.83992900	0.55410900
H	0	4.58640900	4.00283500	-2.67819300
H	0	8.05317000	-1.22587000	1.75958800
H	0	4.43000700	-2.18023900	4.02668100
H	0	5.06166500	3.10387800	3.70391400
H	0	7.31720500	-0.87475300	-3.13757200
H	0	3.60480300	-2.92412200	-2.32305900
H	0	6.53794700	1.44457300	-4.44446300
H	0	4.11543900	-2.21232100	-3.60225400
H	0	3.86607200	-0.29043700	-4.95287400
O	0	4.50877600	-0.81211600	-1.50733500
O	0	3.65540000	1.62640800	-2.36552900
O	0	5.71860100	-3.57872800	-0.76600600
O	0	8.78446200	0.48948400	-0.20299900
O	0	6.93118600	-1.55455600	-0.54415200
O	0	6.12950500	1.14708700	-1.45341000
O	0	2.64118800	-2.20706300	-0.72412000
O	0	6.01173300	-4.00082400	1.94137900
O	0	5.32351400	3.51888900	-2.28351300
O	0	4.83644700	-1.61153500	1.21714600
O	0	3.80979700	1.07474000	0.30750000

O	0	4.97945700	3.16781900	0.46287400
O	0	6.31368300	0.66350100	1.32676300
O	0	7.29169500	-1.71075400	2.10505900
O	0	5.36496300	-2.14308200	3.78941600
O	0	4.27361100	0.41629200	2.92137300
O	0	5.61910400	2.67348200	3.05249700
O	0	6.65143100	0.38563700	3.97198900
O	0	6.39234300	-1.13281500	-3.22476900
O	0	5.65990200	1.59019300	-4.08388200
O	0	4.35109600	-2.95596800	-2.96823000
O	0	3.82238600	-0.59018300	-4.03909000
H	0	3.41954300	0.05347100	2.61661800
H	0	-4.95599700	-3.92439000	3.95093800
H	0	-6.38786200	-3.07090700	3.35307100
H	0	-5.67594700	-4.44257300	2.40796400
H	0	-5.62683500	-4.14506200	-3.01385600
H	0	-6.61764300	-3.83347600	-1.58968400
H	0	-6.81994000	-2.79651000	-3.04624600
H	0	-3.50293200	6.02137300	-2.40359000
H	0	-4.65627600	5.02276200	-3.37983900
H	0	-5.02105800	5.42709400	-1.69228400
H	0	-2.79503400	5.71413700	3.32022100
H	0	-4.42759500	5.29157400	2.76765600
H	0	-3.86757900	4.66212400	4.33175900
H	0	5.60733000	2.89424900	-3.04026000
H	0	6.75497500	-4.54001200	2.22162700
H	0	3.10376400	3.85430600	1.74050700
H	0	1.98201700	4.69893800	2.81448200
H	0	2.86843000	3.24521600	3.41965600
H	0	2.44397700	3.38900200	-3.72266000
H	0	1.10662400	4.57964300	-3.84495600
H	0	2.14409100	4.61498900	-2.41411600
H	0	1.07261200	-4.75319700	-2.94402500
H	0	-0.53125000	-5.56217600	-2.90052900
H	0	-0.06608200	-4.47142100	-4.26127600
H	0	0.75640700	-4.86400600	3.31934000
H	0	0.09757900	-5.81212000	1.93871400
H	0	1.66928100	-4.94413700	1.81130100
H	0	7.61105600	0.38473600	3.86923300
H	0	6.35582700	1.33579200	3.78555400
Ir	0	-1.40517200	-1.04421900	4.98636400
C	0	-2.76726300	-1.70718400	6.04253100
C	0	-0.19591500	-2.24970500	5.67769700
O	0	0.58214200	-3.00038600	6.06624900
O	0	-3.63425200	-2.11837000	6.67326400
H	0	2.40036700	-0.51193500	-3.23109500

Al_8-NU-1000 (opposite)

Electronic Energy: -7257.812846

Enthalpy: -7256.802919

Free Energy: -7257.016662

ν_{CO} = 2106, 2180 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.87185000	-1.84785700	2.77076900
H	0	1.52895800	1.31363300	-0.24663500
H	0	-3.70148900	1.63563400	-3.94734300
H	0	-2.60071200	0.48394800	-3.99328400
H	0	-2.92689000	0.95126100	4.58805600
H	0	-6.34290300	0.29146000	-1.16139200
H	0	-5.91036500	0.10433900	2.18153300
H	0	-2.57163600	-1.59535000	-2.85851400
H	0	-4.10792700	2.66839000	0.39250000
H	0	-0.49623900	0.63266400	-4.57563000
H	0	-1.01597200	-0.01504700	3.99127400
H	0	0.45301700	0.58672300	3.96147300
H	0	2.23048500	-1.66659100	1.81933200
O	0	-1.73943500	1.26238200	-1.40826000
O	0	-2.55303000	4.05727700	-1.12537400
O	0	-2.22000700	3.90814600	1.63755800
O	0	0.11734400	3.44946900	-1.47067300
O	0	0.64661800	1.82937700	-2.90524500
O	0	1.79271500	-0.51818100	-2.45082100
O	0	-0.06219500	-2.32976400	-2.76362700
O	0	0.53790100	-2.57016800	2.01297000
O	0	-1.41627100	-3.63106500	-1.56222800
O	0	-1.10336500	-3.77102300	1.10276200
O	0	-4.11058500	-2.99909700	-1.23156400
O	0	-3.77607500	-3.11949200	1.46307600
O	0	-4.56392700	-1.40381500	2.65157100
O	0	-5.11274400	-1.19716300	-2.08490000
O	0	-3.43614700	-0.57297700	0.17510100
O	0	-2.37960400	-1.08618200	-2.06361500
O	0	-1.04159500	0.06136100	-4.02279700
O	0	-3.55607700	0.70267800	-3.73130500
O	0	-0.05518000	-0.21216300	3.74912900
O	0	-0.57992100	-1.22845400	-0.24099700
O	0	0.62742400	0.95150800	-0.26328100

O	0	1.24171900	1.61763500	2.39190900
O	0	2.23521000	-0.75488900	1.48272100
O	0	0.46071900	3.34739900	1.22426600
O	0	-5.77981300	1.03072800	-0.89525300
O	0	-5.43752200	0.90395600	1.91326900
O	0	-3.47517800	1.94436000	0.29266100
O	0	-4.03705500	2.81635600	-2.23697700
O	0	-3.47109600	2.58177200	2.92481500
O	0	-2.63980000	0.25328100	3.98918900
O	0	-1.84241600	-1.27843100	1.99447100
O	0	-1.37653300	1.13929700	1.44317900
Zr	0	-2.35201200	-2.31691500	-0.05045700
Zr	0	-0.33014500	-0.12581900	-2.09375500
Zr	0	-3.73324700	0.59878700	-1.46119300
Zr	0	-3.30095000	0.47086800	2.04275000
Zr	0	-1.26630100	2.64316900	0.04746900
Zr	0	0.11283700	-0.30681600	1.46425200
H	0	2.11037300	-1.27869200	-1.85630300
Al	0	5.71772500	-2.07396700	-1.77623300
Al	0	5.05489600	0.31687300	-2.91632100
Al	0	3.64611500	-0.79834100	0.12279300
Al	0	7.07107600	0.24398100	-0.22245800
Al	0	4.69736600	2.09145300	-0.96368300
Al	0	6.24971200	-2.63268400	0.83367800
Al	0	4.88771800	1.74146300	1.71810800
Al	0	5.76470400	-0.63230600	2.56830000
H	0	2.83526100	1.12611700	-2.24109000
H	0	5.07461900	-4.28466000	-0.68641900
H	0	9.14976900	1.38295800	-0.09773500
H	0	5.54904800	-2.94488100	3.29960900
H	0	1.85810100	-2.53895400	-0.23701500
H	0	5.65631000	3.85313100	0.55673200
H	0	4.58984900	4.00102800	-2.67385300
H	0	8.04679300	-1.20456000	1.80305400
H	0	4.41268300	-2.14162500	4.05226600
H	0	5.06182800	3.15365400	3.70355900
H	0	7.33194900	-0.88186900	-3.09302700
H	0	3.61321300	-2.92526400	-2.29603300
H	0	6.55799700	1.43731400	-4.41493400
H	0	4.13727800	-2.22130900	-3.57391200
H	0	3.90334100	-0.30693500	-4.93603000
O	0	4.51165000	-0.81064000	-1.47767100
O	0	3.66082100	1.62049100	-2.35550200
O	0	5.71724500	-3.57025100	-0.71498000
O	0	8.78296100	0.50156700	-0.17130900
O	0	6.93155700	-1.54587500	-0.50079900
O	0	6.12949900	1.15053500	-1.42853600
O	0	2.63152500	-2.18428500	-0.69187300
O	0	6.00497100	-3.97754900	1.99548400
O	0	5.32420000	3.51714000	-2.27399300
O	0	4.83042300	-1.59277800	1.25355000
O	0	3.80256100	1.08694600	0.32518300
O	0	4.97349400	3.18029800	0.47038300

O	0	6.30734900	0.68263300	1.35224700
O	0	7.28384700	-1.68646000	2.14942900
O	0	5.35116100	-2.10821500	3.82933400
O	0	4.26468400	0.44542600	2.94260100
O	0	5.61478400	2.70154400	3.06326700
O	0	6.63914600	0.42113700	4.00094800
O	0	6.40690400	-1.13827300	-3.18334500
O	0	5.67653700	1.58087900	-4.06190800
O	0	4.36572200	-2.96116300	-2.93257100
O	0	3.84871900	-0.60306200	-4.02158400
H	0	3.41208700	0.07914300	2.63698900
H	0	-4.85738300	-4.30568100	3.58966000
H	0	-6.13158700	-3.05069800	3.73380300
H	0	-6.04217500	-4.13725400	2.29523100
H	0	-5.62728800	-4.15157500	-3.00466700
H	0	-6.62250500	-3.82364800	-1.58683900
H	0	-6.81717100	-2.79951500	-3.05229600
H	0	-3.48635000	6.00422600	-2.46500500
H	0	-4.71694900	5.00899800	-3.34751000
H	0	-4.97113000	5.46686100	-1.65142900
H	0	-2.79258800	5.71183000	3.33578900
H	0	-4.41891100	5.29954800	2.75797700
H	0	-3.88331200	4.65598000	4.32512300
H	0	5.61242500	2.88997000	-3.02722500
H	0	6.74871800	-4.51300600	2.28161900
H	0	3.10295700	3.85605700	1.74026400
H	0	1.98084300	4.69887700	2.81345100
H	0	2.86736300	3.24685200	3.42117500
H	0	2.45544300	3.38724000	-3.70545200
H	0	1.11094800	4.56293900	-3.86356100
H	0	2.12821600	4.63026600	-2.41863400
H	0	1.07457000	-4.74962200	-2.95174300
H	0	-0.52650400	-5.56325600	-2.89498400
H	0	-0.07423200	-4.47459800	-4.26129200
H	0	0.81756400	-4.84018000	3.30967100
H	0	0.06794200	-5.80768500	1.98777600
H	0	1.64388600	-4.97529400	1.75612400
H	0	7.59926000	0.41989700	3.90303100
H	0	6.34398000	1.37065000	3.80899500
Ir	0	-6.50969100	2.18907000	0.68123300
C	0	-7.04823800	3.19357800	2.13171100
C	0	-7.38333300	3.31625300	-0.49075500
O	0	-7.35556700	3.81484900	3.04710000
O	0	-7.90628600	4.01413000	-1.23832000
H	0	2.42680400	-0.52363300	-3.23755100

Table S8. XYZ Cartesian Coordinates of Selected Optimized Al_8-NU-1000 Isomers at the M06-2X Density Functional.

Al_8-NU-1000 (A)

Electronic Energy: -7257.879044
Enthalpy: -7256.870762
Free Energy: -7257.082930
ν_{CO} = 2157, 2245 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.88034600	-1.86597400	2.76732400
H	0	1.52518200	1.34254700	-0.21072700
H	0	-3.64532800	1.57746300	-3.98306100
H	0	-2.48547700	0.43407000	-3.92137300
H	0	-2.82116000	1.01849400	4.52749300
H	0	-5.66373600	0.94430400	0.68087700
H	0	-6.36220100	0.46357000	-1.17758700
H	0	-5.94921500	0.10087200	2.04120200
H	0	-2.56115500	-1.61694000	-2.84071500
H	0	-4.17144300	2.63440800	0.38418200
H	0	-0.56008600	0.69704100	-4.51778700
H	0	-1.15761300	-0.01862700	3.92807500
H	0	0.34200700	0.56447800	4.02830300
H	0	2.30074200	-1.60485400	1.89444800
O	0	-1.73729200	1.26219800	-1.38956800
O	0	-2.55871800	4.05853300	-1.11109600
O	0	-2.21712600	3.90460400	1.64170200
O	0	0.12502200	3.44501300	-1.46098800
O	0	0.62906400	1.83159300	-2.90353300
O	0	1.76642300	-0.52705800	-2.46457600
O	0	-0.07405200	-2.32511300	-2.75946900
O	0	0.54717800	-2.56460800	1.98120500
O	0	-1.40388400	-3.63487400	-1.54889600
O	0	-1.11304400	-3.76582300	1.11821800
O	0	-4.11726700	-2.99566900	-1.21305600
O	0	-3.77322900	-3.11655500	1.46604300

O	0	-4.55746100	-1.39903300	2.64759400
O	0	-5.09296000	-1.20349600	-2.10694500
O	0	-3.43475700	-0.57345900	0.18185400
O	0	-2.37383600	-1.10575800	-2.04544000
O	0	-1.08032400	0.07471600	-3.99553300
O	0	-3.49011100	0.66666000	-3.69835500
O	0	-0.15006800	-0.21008500	3.72172700
O	0	-0.57421000	-1.22570400	-0.22909400
O	0	0.63623400	0.95371400	-0.24636400
O	0	1.25069300	1.61533800	2.38608600
O	0	2.23225100	-0.70032500	1.54324800
O	0	0.45224600	3.34240800	1.23116700
O	0	-5.69169900	1.03456100	-0.78482100
O	0	-5.47332500	0.87533700	1.71153800
O	0	-3.49687900	1.95237200	0.29684800
O	0	-4.01136200	2.81575400	-2.25121800
O	0	-3.47163700	2.57461700	2.91458600
O	0	-2.61267700	0.25701500	3.97361300
O	0	-1.85046200	-1.29036400	1.99501600
O	0	-1.38732900	1.14105800	1.44810100
Zr	0	-2.35543200	-2.31825200	-0.05129300
Zr	0	-0.33578400	-0.12971100	-2.05597100
Zr	0	-3.76145700	0.60129600	-1.47839300
Zr	0	-3.28149900	0.46621300	2.00716500
Zr	0	-1.27901000	2.64929200	0.03704300
Zr	0	0.09952600	-0.29949100	1.48867300
H	0	2.08705000	-1.30129900	-1.82905000
Al	0	5.60010700	-1.95545200	-1.95282800
Al	0	4.97267700	0.48470300	-2.89300200
Al	0	3.56262500	-0.75905800	0.06581600
Al	0	6.94741600	0.21525000	-0.25664800
Al	0	4.58432300	2.20167000	-0.96000600
Al	0	6.07398300	-2.70772800	0.64049400
Al	0	4.83162400	1.75111900	1.68488700
Al	0	5.66101400	-0.72314900	2.51886400
H	0	2.74241600	1.12321300	-2.20140600
H	0	4.19167600	-3.49202200	-0.77800000
H	0	9.00464000	1.37762100	-0.15113300
H	0	1.66443500	-2.35019300	-0.18991600
H	0	5.62655400	3.87076300	0.57725300
H	0	4.44160700	4.14389300	-2.53437700
H	0	7.91914000	-1.44938200	1.84018900
H	0	4.60871400	-2.54472800	3.78210700
H	0	5.13751100	3.20049300	3.68463200
H	0	6.25170900	1.39946000	3.69671200
H	0	7.27745400	-0.50421900	-2.96400100
H	0	4.02137500	-3.29442500	-3.30410200
H	0	2.38331100	-0.49903600	-3.24238000
H	0	6.44486900	1.83909800	-4.25738200
H	0	4.34357500	-1.81833000	-3.94353600
H	0	3.91940800	-0.06847300	-5.01304400
O	0	4.36189900	-0.73997100	-1.57443700
O	0	3.52453100	1.68228400	-2.33269900

O	0	5.14565500	-3.37345200	-0.90678800
O	0	8.65836100	0.48935800	-0.25350700
O	0	6.80359800	-1.56352700	-0.61856000
O	0	6.01071000	1.22461500	-1.40186900
O	0	2.45963700	-2.07931500	-0.66709600
O	0	6.35329000	-4.29452400	1.28585500
O	0	5.15413000	3.58785100	-2.19544700
O	0	4.69780000	-1.62577700	1.20459800
O	0	3.71576500	1.12980900	0.31612500
O	0	4.91967200	3.21875400	0.52372300
O	0	6.18520000	0.62167500	1.32687700
O	0	7.07101000	-1.82891400	2.10276600
O	0	4.94025400	-1.66264900	3.98454900
O	0	4.05055900	0.48863600	2.87830900
O	0	5.60049300	2.61260800	3.08357600
O	0	6.47847100	0.41488400	3.93224100
O	0	6.38744000	-0.79964700	-3.19165800
O	0	5.53330900	1.90147500	-3.95392500
O	0	4.74681200	-2.69155800	-3.50888700
O	0	3.87946500	-0.43840800	-4.12384200
H	0	3.23762200	0.12730200	2.39086800
H	0	-4.85329900	-4.24200700	3.65873300
H	0	-6.17884500	-3.03801000	3.67024400
H	0	-5.97630000	-4.19309000	2.29572800
H	0	-5.62280800	-4.12274800	-3.03625500
H	0	-6.59524500	-3.84929200	-1.58850600
H	0	-6.82800600	-2.78630300	-3.02251100
H	0	-3.48871300	6.00476100	-2.43588000
H	0	-4.68161200	5.00648700	-3.36211900
H	0	-4.99284500	5.44301900	-1.66898100
H	0	-2.79707700	5.71246400	3.31095000
H	0	-4.43417700	5.27683600	2.77189100
H	0	-3.85213600	4.65379500	4.33159700
H	0	5.40597000	2.92289100	-3.05017400
H	0	6.91277200	-4.30382000	2.06633700
Ir	0	3.64810000	-0.25305800	4.83753700
C	0	3.35990500	-1.06372600	6.44086600
C	0	2.48740800	1.05419400	5.31821200
O	0	3.17708400	-1.57208400	7.44420700
O	0	1.71348500	1.85978300	5.57054300
H	0	7.43462700	0.32477000	4.01739800
H	0	2.44969100	3.38577200	-3.70460300
H	0	1.10108200	4.56345400	-3.85260100
H	0	2.12504100	4.62096200	-2.41212900
H	0	3.04494100	3.94429600	1.71777400
H	0	1.95357100	4.65190100	2.91827300
H	0	2.92248600	3.20132800	3.35711700
H	0	0.92405400	-4.96625000	-2.67027300
H	0	-0.71453400	-5.47199500	-3.14607300
H	0	0.25408300	-4.37245500	-4.20813500
H	0	0.90299400	-4.79892600	3.28675100
H	0	0.02147300	-5.78989000	2.06423400
H	0	1.59494100	-5.02076900	1.67510500

Al_8-NU-1000 (A_2)

Electronic Energy: -7257.879302

Enthalpy: -7256.868591

Free Energy: -7257.082300

ν_{CO} = 2171, 2256 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100
C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.86728000	-1.85386100	2.77427600
H	0	1.47511000	1.41420600	-0.20393500
H	0	-3.64682200	1.57856700	-3.97669800
H	0	-2.48999700	0.43515100	-3.91692400
H	0	-2.79971500	1.02334700	4.53199800
H	0	-5.66315700	0.94358600	0.69392500
H	0	-6.36652000	0.46375500	-1.16995200
H	0	-5.94275900	0.09490100	2.04963000
H	0	-2.56295200	-1.61944500	-2.83306300
H	0	-4.17498700	2.63544700	0.39070500
H	0	-0.56294300	0.70864400	-4.50746100
H	0	-1.12313300	-0.00149200	3.93462300
H	0	0.41431100	0.52427400	4.03962000
H	0	2.16097300	-1.71759200	1.72566500
O	0	-1.74660300	1.26579500	-1.38942400
O	0	-2.56069800	4.05916600	-1.11052600
O	0	-2.22339800	3.90703900	1.63828600
O	0	0.11026100	3.44457600	-1.47250300
O	0	0.64924100	1.82423600	-2.89607500
O	0	1.75962300	-0.50106400	-2.38825300
O	0	-0.06256800	-2.32722800	-2.75350300
O	0	0.53859100	-2.56944600	2.00783300
O	0	-1.40863600	-3.63249300	-1.55428800
O	0	-1.10477800	-3.76663500	1.10726200
O	0	-4.11716200	-2.99411100	-1.21160400
O	0	-3.77054600	-3.11475100	1.46686200
O	0	-4.55289700	-1.40067700	2.65444400
O	0	-5.09479600	-1.20314000	-2.10524200
O	0	-3.43366000	-0.57095000	0.18732800
O	0	-2.37484700	-1.10556300	-2.03982500
O	0	-1.07896900	0.07702500	-3.99232100
O	0	-3.49355100	0.66622500	-3.69541700
O	0	-0.12137900	-0.21692900	3.72218300

O	0	-0.56303500	-1.22064300	-0.22511800
O	0	0.60692400	0.98845200	-0.24279400
O	0	1.25721700	1.60349400	2.35867900
O	0	2.21581100	-0.78322100	1.46605400
O	0	0.43845600	3.33770700	1.23477400
O	0	-5.69568000	1.03407500	-0.77684500
O	0	-5.47107800	0.87302500	1.72254700
O	0	-3.50089300	1.95318600	0.30156500
O	0	-4.01350700	2.81541700	-2.25028200
O	0	-3.46701600	2.57343300	2.91873100
O	0	-2.58437400	0.26404700	3.97769100
O	0	-1.84108700	-1.28472100	1.99706500
O	0	-1.39145100	1.14582900	1.45303700
Zr	0	-2.35285900	-2.30746100	-0.04910400
Zr	0	-0.34450100	-0.11877800	-2.04629100
Zr	0	-3.76665700	0.60554200	-1.47322800
Zr	0	-3.27516800	0.46966400	2.01571600
Zr	0	-1.27872300	2.65518400	0.04373700
Zr	0	0.11095200	-0.27874900	1.49278700
H	0	2.11288000	-1.30343500	-1.84532000
Al	0	5.48427800	-1.91659300	-2.12141200
Al	0	4.92871900	0.61602300	-2.82516900
Al	0	3.56814600	-0.77591800	0.09165200
Al	0	6.87518700	0.01937500	-0.19919400
Al	0	4.75022900	2.17567300	-0.69152800
Al	0	6.06327900	-2.79870500	0.41471400
Al	0	4.87866400	1.50723200	1.98875500
Al	0	5.79570800	-1.06175200	2.60062200
H	0	2.80016300	1.27729500	-1.94664500
H	0	4.12401300	-3.39117600	-0.94018500
H	0	9.27253000	0.75423200	-0.44795300
H	0	5.45934000	-3.52995100	2.78444600
H	0	1.74098300	-2.46089800	-0.26102200
H	0	5.83645100	3.68419200	1.05126700
H	0	4.64725800	4.26544900	-2.09744500
H	0	7.87353900	-2.39268700	2.25582600
H	0	4.16108500	-2.85681100	3.30584900
H	0	5.13001200	2.09174800	4.20319900
H	0	6.39960500	-0.70287400	4.86233000
H	0	7.15448900	-0.48287700	-3.12639700
H	0	3.69662100	-3.03595500	-3.39830400
H	0	2.38732100	-0.32654900	-3.14782200
H	0	6.35927600	1.98167400	-4.23600000
H	0	4.12702100	-1.58951300	-4.00989800
H	0	3.71138300	0.28236700	-4.91886300
O	0	4.33017100	-0.68670800	-1.58476900
O	0	3.59313800	1.82028100	-2.06971600
O	0	5.08682000	-3.40783600	-1.12406600
O	0	8.56340700	0.53176200	0.15657300
O	0	6.81154900	-1.65476600	-0.86262100
O	0	6.08961400	1.14773200	-1.31320300
O	0	2.55808200	-2.18877000	-0.70022400
O	0	5.98826100	-4.31858600	1.32955300
O	0	5.33120500	3.62423600	-1.86733700
O	0	4.82850700	-1.63944700	1.04006900
O	0	3.87135100	1.03299500	0.48491300
O	0	5.18275700	3.01430500	0.83108600
O	0	6.40796900	0.50578700	1.51279800

O	0	7.15759600	-2.04021800	1.72110100
O	0	5.12170100	-2.81124900	3.39425600
O	0	4.32251000	0.03756100	3.02692200
O	0	5.20380400	2.55007500	3.36045700
O	0	6.80576400	-0.64107000	3.99466100
O	0	6.24582300	-0.72475000	-3.33289900
O	0	5.50542100	2.06332200	-3.80119800
O	0	4.47310900	-2.51368500	-3.64083300
O	0	3.73546000	-0.16639300	-4.06634300
H	0	3.44163300	-0.23023800	2.71044900
H	0	-4.85796200	-4.19345300	3.71217000
H	0	-6.21675200	-3.03509900	3.62204000
H	0	-5.92782100	-4.23970800	2.30497600
H	0	-5.62264400	-4.14000700	-3.01303400
H	0	-6.61383400	-3.82649800	-1.58606400
H	0	-6.81371300	-2.78995500	-3.04292300
H	0	-3.48911000	6.00519300	-2.43377400
H	0	-4.68047500	5.00768300	-3.36293300
H	0	-4.99387200	5.44144400	-1.66953100
H	0	-2.78550900	5.70137400	3.33392000
H	0	-4.41509500	5.29565600	2.75419300
H	0	-3.87785900	4.65014000	4.32243800
H	0	5.49309400	3.06090900	-2.76746900
H	0	5.58612100	-5.08860500	0.91980500
Ir	0	8.32667900	1.30884400	2.13479500
C	0	7.92569200	1.80187800	3.85039700
C	0	9.97005900	2.00873200	2.38535900
O	0	7.74744900	2.11126600	4.93041300
O	0	11.01197200	2.46098400	2.52735700
H	0	3.12786700	3.79963400	1.75977600
H	0	1.98026800	4.70871700	2.75865400
H	0	2.87085900	3.27775000	3.42757300
H	0	2.54013300	3.39523400	-3.56371200
H	0	1.14077100	4.43167800	-3.97832100
H	0	2.00175300	4.72476100	-2.45456600
H	0	0.94451400	-4.94315100	-2.69428200
H	0	-0.69864100	-5.48395100	-3.11902600
H	0	0.22049300	-4.38010900	-4.21806300
H	0	0.88044200	-4.80822800	3.29287900
H	0	0.03126700	-5.79342300	2.04541800
H	0	1.60386100	-5.01212700	1.68873200

Al_8-NU-1000 (C)

Electronic Energy: -7257.89269

Enthalpy: -7256.881214

Free Energy: -7257.094501

ν_{CO} = 2165, 2242 cm^{-1}

C	-1	1.68441900	3.94341500	-3.15514000
C	-1	0.64899900	-4.90821600	2.22466600
C	-1	2.37165700	3.70494900	2.55374400
C	-1	0.00185000	-4.64437900	-3.17737000
C	-1	-5.46152400	-3.56982100	3.03745400
C	-1	-4.20580600	5.17837100	-2.39073300
C	-1	-6.09808400	-3.34300700	-2.42691100
C	-1	-3.54711000	4.91457400	3.31258500

C	-1	1.27407100	2.82442300	2.03809500
C	-1	0.75416700	3.00364000	-2.46953500
C	-1	-3.54118900	3.93046700	-1.89896000
C	-1	-5.03722900	-2.44266000	-1.88258700
C	-1	-4.54348500	-2.62142800	2.33674300
C	-1	-0.02842400	-3.67128600	1.74594600
C	-1	-3.03318900	3.71325000	2.58679300
C	-1	-0.52889700	-3.45027300	-2.44888800
H	0	-1.87700600	-1.86218200	2.76966400
H	0	1.51883800	1.34313100	-0.21664400
H	0	-3.64165400	1.57934700	-3.97965200
H	0	-2.48456700	0.43523200	-3.91849300
H	0	-2.80741500	1.02448000	4.52627300
H	0	-5.66119500	0.94392700	0.68757000
H	0	-6.36153200	0.46186000	-1.17254400
H	0	-5.94161000	0.09415800	2.04338200
H	0	-2.56237000	-1.61708600	-2.83759500
H	0	-4.17039900	2.63578600	0.38707800
H	0	-0.55879500	0.71250500	-4.50770900
H	0	-1.12830600	-0.00980400	3.93114000
H	0	0.39253700	0.54520400	4.01046400
H	0	2.27705800	-1.60493200	1.86822100
O	0	-1.74006600	1.26409600	-1.38837300
O	0	-2.56013000	4.05820600	-1.11028700
O	0	-2.21735100	3.90492500	1.64250600
O	0	0.11809400	3.45090700	-1.46951100
O	0	0.64098700	1.82518600	-2.89212400
O	0	1.76737800	-0.52894400	-2.38274200
O	0	-0.07584300	-2.32618600	-2.76687300
O	0	0.54748900	-2.56745900	1.98772300
O	0	-1.40636700	-3.63104200	-1.55067200
O	0	-1.11280700	-3.76629200	1.11888800
O	0	-4.11732600	-2.99572500	-1.21286000
O	0	-3.77429200	-3.11617300	1.46504500
O	0	-4.55327700	-1.40037300	2.65301700
O	0	-5.09418600	-1.20340200	-2.10543600
O	0	-3.43394700	-0.57217900	0.18462500
O	0	-2.37604600	-1.10425300	-2.04324700
O	0	-1.07424000	0.07911800	-3.99425500
O	0	-3.48852800	0.66733100	-3.69742900
O	0	-0.12591800	-0.22035700	3.72378900
O	0	-0.56934200	-1.23020200	-0.23026600
O	0	0.62134000	0.97000100	-0.24167400
O	0	1.23762600	1.61899100	2.39098200
O	0	2.21798300	-0.69131000	1.54491800
O	0	0.45410700	3.34511500	1.22771600
O	0	-5.69224600	1.03472300	-0.78045600
O	0	-5.47042200	0.87303500	1.71742500
O	0	-3.49668500	1.95300300	0.29962000
O	0	-4.01216400	2.81549100	-2.25164400
O	0	-3.47078100	2.57466300	2.91719100
O	0	-2.59148800	0.26283900	3.97558800
O	0	-1.84687500	-1.28905900	1.99570400
O	0	-1.38820600	1.14366200	1.45130000
Zr	0	-2.35561800	-2.31411200	-0.05116400
Zr	0	-0.33801700	-0.12771200	-2.05000900
Zr	0	-3.76185800	0.60472400	-1.47573200
Zr	0	-3.27524100	0.46839500	2.01068600

Zr	0	-1.27256900	2.65061800	0.03919400
Zr	0	0.10469900	-0.29617800	1.48473600
H	0	2.08649500	-1.28638100	-1.71016400
Al	0	5.66103400	-2.03743900	-1.72883900
Al	0	4.97269700	0.31952500	-2.86274100
Al	0	3.57653400	-0.68824800	0.14806200
Al	0	6.98671800	0.35055800	-0.26723800
Al	0	4.57072900	2.23512900	-1.04171600
Al	0	6.20100500	-2.48257000	0.89000700
Al	0	4.81705900	1.85984900	1.65818700
Al	0	5.72114200	-0.46553100	2.57036500
H	0	2.74759500	1.11885900	-2.30674200
H	0	4.98510100	-4.18165700	-0.52148100
H	0	9.01704000	1.56639400	-0.22593200
H	0	6.67248600	-4.27668100	2.45859500
H	0	1.73361600	-2.38945500	-0.16308300
H	0	5.55349000	3.97047400	0.50151000
H	0	4.38612300	3.72338800	-2.87793800
H	0	7.99032000	-1.00996900	1.87358600
H	0	4.33935300	-1.96078600	3.96271000
H	0	5.54868500	-2.74395000	3.28570000
H	0	5.13850000	3.33469400	3.61996600
H	0	6.30211500	1.59577900	3.65408000
H	0	6.29810400	0.44728900	4.81015300
H	0	7.25175700	-0.79757300	-3.06003100
H	0	3.60042600	-2.93869900	-2.32144300
H	0	2.37295100	-0.58113700	-3.17435900
H	0	5.85709000	1.30761200	-4.99337900
H	0	4.15090300	-2.13796900	-3.53688700
H	0	3.84205300	-0.47073700	-4.95063400
O	0	4.42924500	-0.78517500	-1.45126400
O	0	3.57790600	1.60369100	-2.43670500
O	0	5.64873700	-3.49011300	-0.60290000
O	0	8.68667800	0.67267700	-0.33519600
O	0	6.87754200	-1.44969900	-0.49038900
O	0	6.00542200	1.22867600	-1.48844100
O	0	2.52136400	-2.08095200	-0.63108000
O	0	5.92206400	-3.76049400	2.14824200
O	0	5.06843100	3.64383900	-2.19899400
O	0	4.76612600	-1.45858600	1.27867900
O	0	3.70055300	1.19491600	0.27395900
O	0	4.89922900	3.26711300	0.44519700
O	0	6.23532000	0.80164600	1.29936300
O	0	7.23182500	-1.53678500	2.15981500
O	0	5.29560600	-1.90112800	3.83830200
O	0	4.17901700	0.61509500	2.90933400
O	0	5.63575200	2.78811200	3.00686500
O	0	6.59405900	0.62218200	3.90913300
O	0	6.33807300	-1.09768000	-3.14384400
O	0	5.76381100	1.51329600	-4.06079800
O	0	4.37777000	-2.91987600	-2.91720700
O	0	3.83342700	-0.65244600	-4.00631300
H	0	3.32445000	0.24477400	2.61099800
Ir	0	6.87104100	3.16933200	-3.27428000
C	0	8.35657700	2.79520900	-4.24291000
C	0	7.67209600	4.68096300	-2.68030100
O	0	9.28655900	2.55936600	-4.86364200
O	0	8.16254100	5.64596700	-2.31393100

H	0	-4.85461800	-4.22204900	3.68115100
H	0	-6.19479700	-3.03661100	3.65060600
H	0	-5.95635300	-4.21281900	2.29927800
H	0	-5.62255600	-4.13310200	-3.02236400
H	0	-6.60642200	-3.83570600	-1.58697500
H	0	-6.81956300	-2.78851300	-3.03477000
H	0	-3.48940400	6.00550600	-2.43279700
H	0	-4.67900300	5.00763600	-3.36363700
H	0	-4.99506800	5.44097100	-1.67067300
H	0	-2.79697600	5.71241000	3.31097200
H	0	-4.43381600	5.27749200	2.77172700
H	0	-3.85290700	4.65393800	4.33143600
H	0	3.03869300	3.95008200	1.71338700
H	0	1.95310900	4.65216300	2.91729000
H	0	2.92363800	3.19525100	3.35269700
H	0	1.63480800	-4.97691800	1.74346100
H	0	0.82298100	-4.83076800	3.30599000
H	0	0.05614900	-5.79865100	1.99521700
H	0	1.05716000	-4.77899500	-2.89993600
H	0	-0.56321300	-5.54712400	-2.92596800
H	0	-0.02697300	-4.45152500	-4.25699300
H	0	2.29669200	3.41263600	-3.89075400
H	0	1.09481100	4.73344100	-3.64200400
H	0	2.31339900	4.43609800	-2.40074500

Al_8-NU-1000 (C_geminal)

Electronic Energy: -7257.873005

Enthalpy: -7256.862545

Free Energy: -7257.075314

ν_{CO} = 2176, 2250 cm^{-1}

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.87216800	-1.85783300	2.77289400
H	1.48777300	1.40537300	-0.19140300
H	-3.63903500	1.57857300	-3.97677900
H	-2.48383800	0.43205000	-3.91632500
H	-2.80703100	1.02602200	4.52908100
H	-5.66111100	0.94325500	0.69009100
H	-6.36106300	0.46049300	-1.17221000
H	-5.94000300	0.09212800	2.04435500
H	-2.55960100	-1.61909100	-2.83340700

H	-4.17303800	2.63529300	0.38789400
H	-0.56005300	0.70584500	-4.50619900
H	-1.12679600	-0.00353100	3.93665900
H	0.40107900	0.53990700	4.02689300
H	2.21745000	-1.67902800	1.78837500
O	-1.74135600	1.26390800	-1.38807400
O	-2.56034900	4.05903800	-1.11067400
O	-2.22063100	3.90644200	1.64050800
O	0.11692200	3.44455700	-1.46790700
O	0.63786400	1.82797900	-2.90136600
O	1.76759800	-0.51004700	-2.39787500
O	-0.06564200	-2.32729700	-2.75556900
O	0.53822800	-2.56930500	2.00635300
O	-1.40736600	-3.63404100	-1.55297500
O	-1.10680800	-3.76759300	1.10935100
O	-4.11756800	-2.99460400	-1.21150300
O	-3.77079800	-3.11551800	1.46737100
O	-4.55416800	-1.40065500	2.65365600
O	-5.09392300	-1.20346000	-2.10656300
O	-3.43353500	-0.57188100	0.18649900
O	-2.37234900	-1.10590500	-2.03954200
O	-1.07573200	0.07303800	-3.99200200
O	-3.48805000	0.66584000	-3.69568300
O	-0.12505600	-0.21622600	3.72863400
O	-0.56288100	-1.22261800	-0.22527400
O	0.61924500	0.97849600	-0.24008100
O	1.24044500	1.61099300	2.37717300
O	2.21448200	-0.74870600	1.51068200
O	0.44774600	3.33831800	1.22512200
O	-5.69251700	1.03386700	-0.77966800
O	-5.47075800	0.87255300	1.71927500
O	-3.49866200	1.95319400	0.30027600
O	-4.01238400	2.81540200	-2.25145700
O	-3.46935600	2.57423000	2.91782300
O	-2.59169200	0.26408900	3.97847400
O	-1.84318500	-1.28614400	1.99779500
O	-1.39061500	1.14515400	1.45331200
Zr	-2.35143200	-2.30858700	-0.04932100
Zr	-0.33680300	-0.12143500	-2.04712300
Zr	-3.76183500	0.60492600	-1.47425700
Zr	-3.27414500	0.46970200	2.01361800
Zr	-1.27515700	2.65292000	0.04377300
Zr	0.11183100	-0.28581700	1.49538500
H	2.12278400	-1.30160900	-1.80218100
Al	5.59945500	-1.82945400	-2.05794600
Al	4.94380900	0.64966900	-2.80589300
Al	3.55944300	-0.71899300	0.11082100
Al	7.00565200	0.27429900	-0.21943400
Al	4.63788500	2.23627000	-0.73481200
Al	6.06953600	-2.59081800	0.46895200
Al	4.92050200	1.61340800	1.92430000
Al	5.75902600	-0.88775800	2.52370400
H	2.74549100	1.20956400	-1.99761100
H	4.35805000	-3.55346700	-0.89518400
H	9.11146400	1.32775100	-0.01197500
H	5.47493900	-3.62045300	2.48288000
H	1.74206200	-2.40350100	-0.23387100
H	5.73174800	3.81835100	0.93320300

H	4.37548600	4.26063800	-2.20613100
H	7.98991200	-1.59510100	1.66998200
H	4.34438600	-2.39329700	3.87686100
H	5.08218400	2.23058900	4.14194500
H	6.94761900	0.47659600	4.20284700
H	7.22842200	-0.32459200	-3.00201600
H	3.90026200	-3.06365800	-3.34966600
H	2.38725800	-0.38334500	-3.16284200
H	6.32641700	2.07126600	-4.18827300
H	4.26830700	-1.57638000	-3.95637400
H	3.85442200	0.16661300	-4.93447000
O	4.36650300	-0.67098300	-1.54547700
O	3.51818100	1.78275400	-2.11344300
O	5.30699200	-3.38124100	-1.03237400
O	8.72107600	0.49491200	-0.28357800
O	6.83654000	-1.48767500	-0.74253700
O	6.03372700	1.28557200	-1.32485400
O	2.54742900	-2.11889200	-0.68673300
O	5.68270700	-4.13070400	1.63281900
O	5.11635700	3.70213900	-1.93900100
O	4.72949200	-1.65527400	1.14040300
O	3.79936900	1.10518400	0.47752200
O	5.10354500	3.11152700	0.76458400
O	6.31895800	0.51514500	1.42694700
O	7.17513100	-2.08392700	1.85036600
O	5.28337000	-2.45107800	3.65260200
O	4.31409100	0.19813200	3.03663800
O	5.33421100	2.62980700	3.30491000
O	6.80736200	-0.45674300	4.00889500
O	6.34580200	-0.62646500	-3.25222400
O	5.43486200	2.10386900	-3.82720000
O	4.65950100	-2.50780800	-3.56799600
O	3.83045500	-0.24301700	-4.06192800
H	3.43284600	-0.07664600	2.72043200
H	-4.85810400	-4.19412200	3.71167200
H	-6.21653700	-3.03519100	3.62246700
H	-5.92832000	-4.23913300	2.30474900
H	-5.62242900	-4.13979400	-3.01315200
H	-6.61400000	-3.82667400	-1.58626000
H	-6.81371700	-2.79002200	-3.04302200
H	-3.48908900	6.00521100	-2.43321900
H	-4.67963000	5.00772000	-3.36336600
H	-4.99452000	5.44136900	-1.67020900
H	-2.78806800	5.70392900	3.32882100
H	-4.41947600	5.29156300	2.75823100
H	-3.87224900	4.65084700	4.32450400
H	5.33438200	3.11639100	-2.81950100
H	6.43214600	-4.69732700	1.86184300
Ir	6.52004100	-2.01540800	5.33576300
C	6.12470300	-3.49924500	6.31393600
C	7.63090200	-1.48140600	6.67349600
O	5.86613100	-4.43330900	6.91827700
O	8.32483900	-1.14359900	7.51269700
H	3.08985500	3.86864300	1.73731000
H	1.96289100	4.68393900	2.83365000
H	2.91202400	3.24603500	3.38632800
H	2.52289400	3.39145800	-3.59335700
H	1.13075100	4.45874900	-3.95487100

H	2.02209300	4.70746600	-2.44389900
H	0.94010800	-4.94811200	-2.68900500
H	-0.70236700	-5.48129800	-3.12528000
H	0.22836300	-4.37802300	-4.21576300
H	0.81627400	-4.83274800	3.30717600
H	0.05942300	-5.79965700	1.99028700
H	1.63642800	-4.97549100	1.74595500

Al_8-NU-1000 (geminal)

Electronic Energy: -7257.885389

Enthalpy: -7256.874432

Free Energy: -7257.086325

ν_{CO} = 2173, 2248 cm^{-1}

C	1.68444800	3.94340000	-3.15512100
C	0.64900500	-4.90821400	2.22466400
C	2.37166400	3.70494700	2.55373300
C	0.00185700	-4.64437500	-3.17737100
C	-5.46152300	-3.56982200	3.03745400
C	-4.20580500	5.17837200	-2.39073100
C	-6.09808300	-3.34300800	-2.42691100
C	-3.54710600	4.91457500	3.31258600
C	1.27405600	2.82442600	2.03808400
C	0.75414900	3.00362100	-2.46954200
C	-3.54119800	3.93046700	-1.89895400
C	-5.03723600	-2.44266000	-1.88258800
C	-4.54349000	-2.62143200	2.33674400
C	-0.02842600	-3.67127100	1.74594700
C	-3.03319100	3.71324400	2.58679900
C	-0.52889300	-3.45025300	-2.44888900
H	-1.90520400	-1.95297900	2.68076700
H	1.49613000	1.36772400	-0.20474500
H	-3.63049100	1.57497000	-3.99582600
H	-2.46294200	0.43016600	-3.91820400
H	-2.74888400	1.18764000	4.44274500
H	-5.67228300	0.93465100	0.66400300
H	-6.36441300	0.45404400	-1.18248300
H	-5.95739300	0.10051200	2.03962300
H	-2.55551000	-1.61541000	-2.83797000
H	-4.17999300	2.63588900	0.38610800
H	-0.55529600	0.69341900	-4.50626000
H	0.53669900	0.44761600	4.02252000
H	2.26889000	-1.61993500	1.84562500
O	-1.74796200	1.26400300	-1.38679900
O	-2.55944200	4.05551100	-1.11171900
O	-2.22936100	3.90573100	1.63533100
O	0.12186600	3.44974100	-1.46436100
O	0.62831000	1.83130400	-2.89989000
O	1.76364900	-0.51006800	-2.39134600
O	-0.06933300	-2.32640800	-2.75481100
O	0.53759900	-2.56962800	2.00509500
O	-1.40810400	-3.63449700	-1.55216800
O	-1.11563600	-3.76331900	1.11863400
O	-4.11597100	-2.99345800	-1.21473800
O	-3.77916200	-3.10411900	1.45818500
O	-4.54029300	-1.40313800	2.67963000

O	-5.09305800	-1.20352200	-2.11246600
O	-3.45290400	-0.56815000	0.17644300
O	-2.37418600	-1.10385300	-2.04152600
O	-1.07773800	0.07191500	-3.98525000
O	-3.47714600	0.66646500	-3.70329200
O	0.02584100	-0.30206900	3.68966100
O	-0.56741400	-1.22401500	-0.22291800
O	0.60235200	0.98824400	-0.22910500
O	1.24860500	1.61682100	2.37959300
O	2.22034200	-0.71114500	1.50719900
O	0.44384600	3.34886500	1.23962600
O	-5.70008200	1.03216500	-0.78945900
O	-5.47782400	0.86757000	1.69889500
O	-3.50742100	1.95218100	0.29710300
O	-4.01537300	2.81632500	-2.25268200
O	-3.46076100	2.57028200	2.92576200
O	-2.73338200	0.30700700	4.04622100
O	-1.86362200	-1.28929900	1.98047300
O	-1.40672200	1.14342400	1.46120700
Zr	-2.34239300	-2.30595500	-0.06319900
Zr	-0.33130100	-0.12689000	-2.03652800
Zr	-3.76586200	0.60888100	-1.49200100
Zr	-3.28814200	0.46223000	1.97806100
Zr	-1.26989800	2.64397500	0.03833600
Zr	0.10993900	-0.28551600	1.53050800
H	2.09588000	-1.29112100	-1.73867900
Al	5.63897300	-1.97550500	-1.83375800
Al	4.96303100	0.42468300	-2.88794500
Al	3.57176500	-0.70809000	0.11824800
Al	6.98745700	0.32137700	-0.25539800
Al	4.60365500	2.19924900	-0.97604700
Al	6.18099300	-2.52391000	0.77958400
Al	4.81932200	1.80157200	1.70002100
Al	5.71608000	-0.55843200	2.55372400
H	2.74715300	1.11842300	-2.18946800
H	4.89043800	-4.12342200	-0.67475200
H	9.05725300	1.44743100	-0.03649200
H	5.54828300	-2.87818100	3.16948500
H	1.72441100	-2.37978900	-0.21265200
H	5.62882800	3.90039000	0.56221400
H	4.44255000	4.08637000	-2.63165400
H	7.98087000	-1.08526500	1.69090000
H	4.43075100	-2.10308700	4.02801000
H	5.07867300	3.15969800	3.72902300
H	7.25294800	-0.66756100	-3.04546600
H	3.63563100	-2.93120100	-2.56561000
H	6.43043300	1.70562200	-4.32357000
H	4.17602300	-1.96852800	-3.68024100
H	3.85738600	-0.24207600	-4.95130800
O	4.41085300	-0.74167300	-1.49484700
O	3.54000200	1.65715800	-2.33976100
O	5.58350500	-3.46017700	-0.74612300
O	8.70517600	0.56941600	-0.19474300
O	6.86931100	-1.46383500	-0.56882800
O	6.03545700	1.23460400	-1.45000800
O	2.51903400	-2.08594900	-0.67846000
O	5.94181500	-3.85284400	1.97987300
O	5.16798700	3.55639900	-2.27789700

O	4.76682500	-1.50069300	1.22496000
O	3.71535600	1.17308000	0.31485000
O	4.92160400	3.25161300	0.48308700
O	6.23906900	0.75713700	1.31412500
O	7.24657100	-1.59151300	2.06880100
O	5.35495600	-2.05188900	3.75503400
O	4.19907800	0.52166000	2.92750800
O	5.61243200	2.71750400	3.06373000
O	6.56821000	0.50687600	3.93990400
O	6.34256200	-0.94962100	-3.19753300
O	5.52334200	1.77834700	-4.01062600
O	4.43256500	-2.80195300	-3.11334000
O	3.81701800	-0.53488500	-4.03433300
H	3.34284100	0.15877500	2.62494400
H	-4.98635500	-3.86358600	3.98550300
H	-6.41041700	-3.07970900	3.28493200
H	-5.62187400	-4.46622800	2.43067500
H	-5.62464200	-4.09417300	-3.07299400
H	-6.56597900	-3.88486600	-1.59426000
H	-6.84973700	-2.78087000	-2.98947400
H	-3.49562100	6.01154200	-2.41118400
H	-4.65838800	5.01303300	-3.37442300
H	-5.01245800	5.42643700	-1.68495100
H	-2.81647000	5.72885100	3.26997200
H	-4.46372900	5.24560400	2.80194600
H	-3.80879800	4.66448400	4.34650000
H	5.40854000	2.88114600	-3.08722000
H	6.70049800	-4.36948000	2.26752400
H	3.05682900	3.92732600	1.72188500
H	1.95744000	4.66206600	2.89497500
H	2.90637500	3.20522000	3.37015800
H	2.43821100	3.38395400	-3.71918100
H	1.09922700	4.57683000	-3.83865200
H	2.13959800	4.60777700	-2.40884100
H	0.95104400	-4.93595800	-2.70327900
H	-0.69459700	-5.48660900	-3.11087500
H	0.21367900	-4.38120500	-4.21962800
H	0.72683200	-4.87024400	3.32011000
H	0.10315800	-5.80503900	1.91658600
H	1.67402200	-4.92862000	1.82975900
H	7.52987700	0.49506800	3.86136200
H	6.26005100	1.47164700	3.70538000
Ir	-1.44808900	-1.09660200	4.95606500
C	-2.80157200	-1.78509000	5.96537800
C	-0.28338500	-2.32126000	5.63066900
O	0.45913600	-3.09355300	6.02347700
O	-3.65795400	-2.22435000	6.57718400
H	2.37339100	-0.50783500	-3.18345200

Al_8-NU-1000 (opposite)

Electronic Energy: -7257.886169

Enthalpy: -7256.875205

Free Energy: -7257.087432

ν_{CO} = 2174, 2249 cm^{-1}

C	-1	1.68444800	3.94340000	-3.15512100

C	-1	0.64900500	-4.90821400	2.22466400
C	-1	2.37166400	3.70494700	2.55373300
C	-1	0.00185700	-4.64437500	-3.17737100
C	-1	-5.46152300	-3.56982200	3.03745400
C	-1	-4.20580500	5.17837200	-2.39073100
C	-1	-6.09808300	-3.34300800	-2.42691100
C	-1	-3.54710600	4.91457500	3.31258600
C	-1	1.27405600	2.82442600	2.03808400
C	-1	0.75414900	3.00362100	-2.46954200
C	-1	-3.54119800	3.93046700	-1.89895400
C	-1	-5.03723600	-2.44266000	-1.88258800
C	-1	-4.54349000	-2.62143200	2.33674400
C	-1	-0.02842600	-3.67127100	1.74594700
C	-1	-3.03319100	3.71324400	2.58679900
C	-1	-0.52889300	-3.45025300	-2.44888900
H	0	-1.88404700	-1.86766400	2.76172000
H	0	1.50740700	1.36138400	-0.20515100
H	0	-3.64294500	1.57315400	-3.99135000
H	0	-2.46534800	0.43726400	-3.92377700
H	0	-2.82019600	1.00996500	4.53661700
H	0	-6.32144100	0.28598000	-1.15902400
H	0	-5.91371500	0.10871300	2.16299500
H	0	-2.56348200	-1.61628900	-2.84225100
H	0	-4.05564200	2.72102500	0.38286800
H	0	-0.55124000	0.69686100	-4.51755900
H	0	-1.15007600	-0.00500700	3.92929900
H	0	0.38746500	0.52308700	4.03273600
H	0	2.26223500	-1.61203500	1.87675600
O	0	-1.73524300	1.26014600	-1.40540500
O	0	-2.55015400	4.05007500	-1.12590100
O	0	-2.22410100	3.90384000	1.63371600
O	0	0.12414900	3.44574400	-1.46358800
O	0	0.63196600	1.83067100	-2.90355300
O	0	1.77302700	-0.51802600	-2.39236100
O	0	-0.06889900	-2.32655600	-2.75947600
O	0	0.54190500	-2.56712200	1.99241100
O	0	-1.40572300	-3.63196800	-1.55076400
O	0	-1.11207900	-3.76723800	1.11580800
O	0	-4.10990300	-2.99611200	-1.22814800
O	0	-3.78587500	-3.11361200	1.45173800
O	0	-4.54591500	-1.40585000	2.66209600
O	0	-5.10341400	-1.19843500	-2.08985100
O	0	-3.44025200	-0.56633600	0.17392700
O	0	-2.37331500	-1.10412500	-2.04834400
O	0	-1.07213100	0.07183600	-3.99900200
O	0	-3.47448200	0.66772500	-3.69774300
O	0	-0.14199400	-0.22580500	3.72430200
O	0	-0.57078300	-1.22508000	-0.23183100
O	0	0.61610800	0.97629100	-0.23992700
O	0	1.23642000	1.62031300	2.39103900
O	0	2.21152700	-0.69612600	1.55846500
O	0	0.45533400	3.34765600	1.22722400
O	0	-5.76257200	1.03513300	-0.91584700
O	0	-5.42810600	0.90156300	1.90234200
O	0	-3.47703900	1.95465100	0.28652500
O	0	-4.03714100	2.81641700	-2.23330300
O	0	-3.47280300	2.57970400	2.91957300
O	0	-2.59187700	0.26090400	3.97408600

O	0	-1.85708500	-1.29211400	1.98941400
O	0	-1.39036800	1.14252000	1.45410100
Zr	0	-2.35249100	-2.31087300	-0.04924400
Zr	0	-0.32372500	-0.13229000	-2.05626800
Zr	0	-3.73102000	0.60625500	-1.48031500
Zr	0	-3.31248800	0.46645900	2.01766500
Zr	0	-1.26078500	2.63528200	0.04696200
Zr	0	0.09558400	-0.29331900	1.49468800
H	0	2.09995100	-1.28166300	-1.72157000
Al	0	5.64648900	-1.97046200	-1.78146700
Al	0	4.97146200	0.42133400	-2.85367500
Al	0	3.56838100	-0.69217300	0.15723800
Al	0	6.98498900	0.33868200	-0.21503400
Al	0	4.59719900	2.20680500	-0.95578900
Al	0	6.17820600	-2.50145700	0.83726800
Al	0	4.81014500	1.82889000	1.72446900
Al	0	5.70619300	-0.52445000	2.59661700
H	0	2.74664900	1.11444400	-2.17853400
H	0	4.90108500	-4.11733800	-0.61328400
H	0	9.05253500	1.47058000	-0.00236900
H	0	5.53776200	-2.84026200	3.22701500
H	0	1.71631500	-2.36230100	-0.17291700
H	0	5.62118700	3.91749900	0.57038100
H	0	4.43824800	4.08356200	-2.62303500
H	0	7.97356900	-1.05604100	1.74489800
H	0	4.41561200	-2.05870400	4.07324500
H	0	5.07487700	3.21141500	3.73927300
H	0	7.26443300	-0.66731700	-2.99400500
H	0	3.65069800	-2.93691700	-2.52532600
H	0	6.44152200	1.69793000	-4.29126000
H	0	4.19905600	-1.97941400	-3.64000700
H	0	3.88404400	-0.25893600	-4.92180600
O	0	4.41281700	-0.73835000	-1.45563000
O	0	3.54151600	1.65243800	-2.32080800
O	0	5.58856500	-3.44847000	-0.68492100
O	0	8.70177800	0.59096100	-0.15450800
O	0	6.87019200	-1.44903300	-0.51508900
O	0	6.03299300	1.24191400	-1.41724200
O	0	2.50979900	-2.06096400	-0.63556500
O	0	5.93601100	-3.82303100	2.04510300
O	0	5.16321800	3.55678600	-2.26349200
O	0	4.76079000	-1.47761100	1.27102700
O	0	3.70631600	1.18853400	0.34117300
O	0	4.91384500	3.26819900	0.49654600
O	0	6.23050000	0.78185200	1.34865000
O	0	7.23844600	-1.56026100	2.12379600
O	0	5.34169100	-2.01034700	3.80642400
O	0	4.18810000	0.55703500	2.95801600
O	0	5.60451000	2.75288000	3.08187900
O	0	6.55419200	0.54983800	3.97756000
O	0	6.35501700	-0.95157100	-3.14785600
O	0	5.53270600	1.76913200	-3.98300400
O	0	4.45252100	-2.80816600	-3.06540700
O	0	3.83707300	-0.54852500	-4.00404200
H	0	3.33225500	0.19039700	2.65825300
H	0	-4.85190500	-4.28803300	3.60289300
H	0	-6.13642800	-3.04240000	3.71856900
H	0	-6.02693600	-4.14415100	2.29252800

H	0	-5.62232100	-4.13154200	-3.02400700
H	0	-6.60397400	-3.83724000	-1.58632100
H	0	-6.82188700	-2.78927400	-3.03282400
H	0	-3.52391500	6.03223100	-2.32777600
H	0	-4.57781200	5.03880300	-3.41223000
H	0	-5.07681200	5.37046500	-1.74638100
H	0	-2.81293200	5.72650400	3.28243100
H	0	-4.45665200	5.25410800	2.79408300
H	0	-3.82184200	4.65993100	4.34198900
H	0	5.40915900	2.87768000	-3.06808500
H	0	6.69466600	-4.33639700	2.33870500
H	0	3.05046200	3.93862200	1.72019200
H	0	1.95433200	4.65731100	2.90495000
H	0	2.91132000	3.20187700	3.36499300
H	0	2.44501800	3.38257900	-3.70882800
H	0	1.10207500	4.56714500	-3.84991700
H	0	2.13020800	4.61691700	-2.41140900
H	0	0.95641000	-4.92978900	-2.71042400
H	0	-0.69007800	-5.48962600	-3.10277600
H	0	0.20405500	-4.38356400	-4.22216700
H	0	0.80652600	-4.83705600	3.30902300
H	0	0.06365400	-5.79993500	1.98139900
H	0	1.64211700	-4.96844400	1.75765100
H	0	7.51623100	0.53694800	3.90416600
H	0	6.24726000	1.51365400	3.73548300
Ir	0	-6.45459400	2.24769200	0.66171100
C	0	-6.95304100	3.27560200	2.08106300
C	0	-7.26964800	3.40287200	-0.48811100
O	0	-7.24513900	3.92277000	2.97351900
O	0	-7.76237100	4.13163800	-1.21458100
H	0	2.39660400	-0.52156800	-3.17538600

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