Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information

Aqueous Furfural Hydrogenation on Ni/TiO_2 Catalysts: Nature of Support Phase Steers the Product Selectivity

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1. EXPERIMENTAL SECTION:

1.1. Materials. Nickel(II) acetate tetrahydrate ($Ni(CH_3COO)_2.4H_2O$)-98%,from Central Drug House (P) Ltd., Furfural ($C_5H_4O_2$)-99% and Tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$)-99%from Sigma Aldrich, Furfuryl alcohol ($C_5H_6O_2$)-98% from Avra synthesis Pvt. Ltd., Cyclopentanone (C_5H_8O)-99% from Spectrochem Pvt. Ltd., Cyclopentanol ($C_5H_{10}O$)-99%from Alfa Aesar, Hydrochloric acid (HCl, 37%) from Merck Life Science Pvt. Ltd., Titanium(IV) iso-propoxide ($C_{12}H_{28}O_4Ti$)-98% from Spectrochem Pvt. Ltd., Anatase TiO_2 (99.7% trace metals basis)from Sigma Aldrich, Hombikat UV-100~99%from Sachtleben Chemie GmbH, Anatase-rutile mixed phasesTiO_2(99.9% trace metals basis) from Sigma Aldrich, Degussa P25 (AEROXIDE TiO_2, 99.5% trace metals basis) from EVONIK industries, and deionized water from Merck were used without further purification.

1.2. Preparation of Supports.

Anatase and mixed phases supports were used as received. Rutile TiO_2 supports were synthesized from titanium iso-propoxide using sol-gel and hydrothermal methods as described below[1,2].

1.2.1. Sol-gel method. In a typical sol-gel synthesis procedure,42 mL of titanium iso-propoxide was hydrolyzed by the addition of 72 mL of 2 mol L^{-1} aqueous solution of hydrochloric acid under vigorous stirring. The hydrosol formed was then stirred at room temperature for 7 days. The resulting mixture was washed with water and methanol, followed by drying at 110°Cin air oven for 24 h. This was then followed by calcination in air at 450°C for 4 h, at a heating rate of 2 °C/min. The obtained product is labelled as RS.

1.2.2. Hydrothermal method. The sol-gel method process is followed till the hydrolysis step of hydrothermal procedure except that the stirring was restricted to 2 h till solution became

clear as opposed to 7 days as in the case of sol-gel method. Then the solution was transferred to a 250 ml Teflon-lined autoclave and heated at 180 °C for 12 h (ramp rate: 5 °C/min). After cooling down to room temperature, the precipitate was collected and washed with water and then with methanol. The sample was dried at 110 °C in air oven for 24 h, followed by calcination at 450°C for 4 h(ramp rate: 2 °C/min) giving the product named as RH.

1.3. Preparation of catalysts

1.3.1. Synthesis of catalysts. All Ni/TiO_2 were prepared by wetness impregnation method. In brief, 0.64 g $Ni(CH_3COO)_2.4H_2O$ was dissolved in 30 mL of deionized water in a beaker. The temperature was raised to 60 °C. 2.85 g TiO_2 support was added under stirring and water was allowed to evaporate. The sample was further dried at 100°C for overnight. The sample was then calcined in static air at 450°C for 6 h, followed by reduction in H_2 flow at 450°C for 6 h (ramp rate: 5 °C/min). It was cooled to room temperature in H_2 flow for further catalytic evaluation. The optimum nickel loading on all catalysts was 5 wt%. The prepared catalysts were designated as three letter abbreviation. For example, those catalysts prepared from anatase titania supports obtained from Aldrich and Hombikat are labelled as ATA and ATH, mixed phase titania supports obtained from Aldrich and EVONIK are labelled as ART and P25, and rutile titania supports synthesized from hydrothermal and sol-gel method are labelled as RTH and RTS, respectively.

1.3.2 Synthesis of RTH catalyst by hydrazine reduction method. 10 mL of ethanolic solution of $Ni(CH_3COO)_2.4H_2O$ was taken in a round flask attached with condenser. The temperature was raised to 80 °C. 5 ml 1M ethanolic NaOH solution was added under stirring, followed by 4 ml of hydrazine hydrate. 0.95 g TiO_2 support was added once the solution turns black. The sample was further stirred for 1h. The resultant catalyst is obtained after washing with water till pH is neutral. The nickel loading calculated from AAS shows 4.9 wt%.

1.4. Experimental procedure

Catalytic hydrogenation was carried out in 100 mL stainless steel autoclave batch reactor (Parr Instrument Company 4565). In a typical run, the autoclave was loaded with 5.2 mmol furfural in 50 mL water, and 100 mg catalyst. Before the reaction, the reactor was flushed and pressurized with hydrogen. The reactor was heated to the desired reaction temperature and then the reaction was initiated by switching on the stirrer at 500 rpm. The reaction was quenched after desired time by cooling reactor in a water-ice bath. The reaction solution was filtered and solid catalyst was separated to analyse products on Chemito GC 1000 gas chromatograph equipped with a Agilent HP-FFAP-19091F-413 capillary column (30 m x 0.32 mm) and a flame ionization detector.

1.5. Characterization of catalysts

Powder X-ray Diffraction (PXRD) patterns of samples were recorded using Bruker AXS D8 advance diffractometer at room temperature using Cu Kα radiation source (λ = 1.5406 Å) and scanning in the 2θ range of 10-80° with a step of 0.03°. The diffractograms were analyzed by comparing with the JCPDS-ICDD data.

The surface morphology of catalysts support was investigated using Hitachi S-4800 Field emission SEM. Energy Dispersive X-ray Analysis, equipped with the SEM unit was used to chemically characterize the samples. The micrographs of nanoparticles dispersed on support were observed by FEI Technai T20 TEM, operating at 200 kV.

N_2physisorption measurements on freshly prepared catalysts were carried out using a Micromeritics ASAP 2020 instrument at 77 K. Before measurements, catalysts were degassed under vacuum at 200°C for 8 h. Surface area was measured by BET method in the

range of 0.04-0.22 relative pressures (P/P_0) and pore volume and pore size distribution by BJH method.

The amount of Ni loaded on catalyst was measured by Shimadzu AA-7000 atomic absorption spectrometry.

BELCAT-II Chemisorption analyzer was used to perform both temperature programmed desorption of ammonia and temperature programmed reduction by hydrogen. In a typical NH_3-TPDexperiment, the reduced sample was pre-treated at 300 °C for 1 h under a He (99.9%) flow at a rate of 50 mL min^{-1}. After pre-treatment, the sample was saturated with anhydrous ammonia (5% NH_3 balance He) at 100 °C for 30 min and subsequently flushed with He at the same temperature to remove physisorbed ammonia. Then, the TPD analysis was carried out by heating the sample in He flow (30 mL min^{-1}) upto600°C at a rate of 10 °Cmin^{-1}, and the desorbed NH_3 was measured. The detector inNH_3-TPD is thermal conductivity detector (TCD). For H_2-TPR, the Ni impregnated sample calcined at 450 °C in air was taken. Prior to analysis, the sample was heated at 300 °C in high purity He gas (50 mL min^{-1}) for 1 h and then on cooling to 50 °C the gas was switched to Ar flow. After 15 min the flow was adjusted to 5 % H_2 in Ar (30 mL min^{-1}) at 50 °C and waited till baseline was stabilized. TPR of catalyst was recorded from 50 °C to 900 °C with a heating rate 10 °Cmin^{-1}. X-ray photoelectron spectra (XPS) of the reduced catalysts were obtained fromPHI5000VersaProbe III X-ray photoelectron spectroscopy using 1486.6 eV monochromatic Al-K_α radiation source. The binding energy of all catalyst atoms were calibrated with carbon 1s peak present at 284.8 eV.

1.6. Computational details

All electronic structure calculations were performed with Gaussian 16 program using density functional theory[3]. The geometry optimization of metal cluster and other molecules were

carried out using PBE functional, where metal atoms were treated with LANL2DZ basis set with effective core pseudopotential (ECP) and 6-31g** basis set was employed to describe all other atoms type[4,5,6]. The Grimme's D3 dispersion correction was also included in calculations[7]. Lowest energy icosahedra Ni geometry is obtained with spin multiplicity 9 and 8 for neutral and charged (-1) cluster. The Ni cluster was fixed at optimized coordinates for further catalytic studies. All calculations are done in aqueous medium using implicit solvent as conductor like polarizable continuum model (CPCM)[8]. The minima and transition states on potential energy surface were confirmed by the presence of all positive frequencies for minima and one negative frequency for the transition state geometry[9]. The transition states were connected to minima on potential energy surface by tracing intrinsic reaction coordinates[10]. The minima were characterized by all positive frequencies, whereas transition states exhibit one imaginary frequency. All structures were visualized using Chemcraft 1.8 software[11]. The zero-point energy corrected adsorption energy (E_{ads}) of a substrate on the metal cluster is given by,

$$E_{ads} = E_{M\text{-}S} + \Delta ZPVE - E_M - E_S$$

Where, ΔZPVE stands for zero-point vibrational energy correction. E_S, E_M, and $E_{M\text{-}S}$ are the total energy corresponding to the substrate, metal cluster and substrate adsorbed on a metal cluster system.

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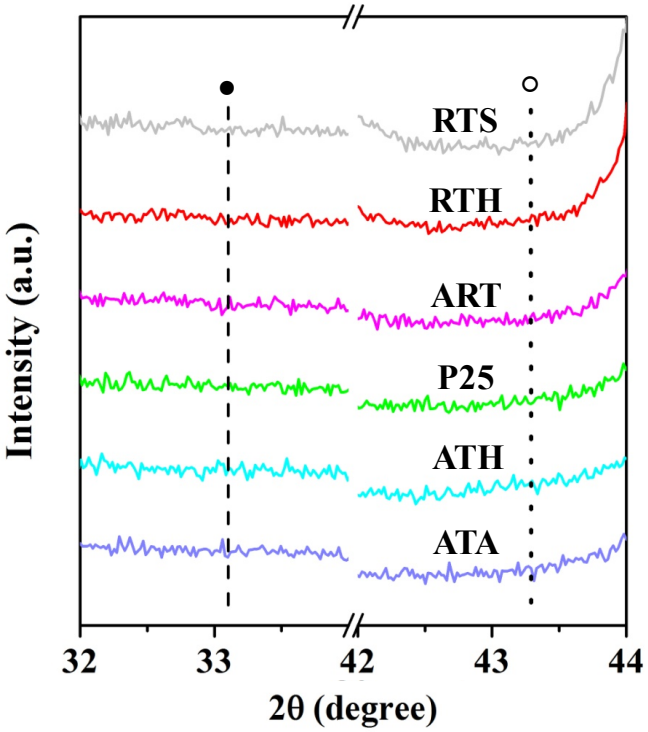

Figure S1. XRD pattern Ni/TiO_2 catalysts: (a) ATA, (b) ATH, (c) P25, (d) ART, (e) RTH, and (f) RTS showing (•) NiTiO3 (104) and (○) NiO (200) region. (JCPDS No. for $NiTiO_3$ and NiO is 33-0960 and 47-1049, repectively)

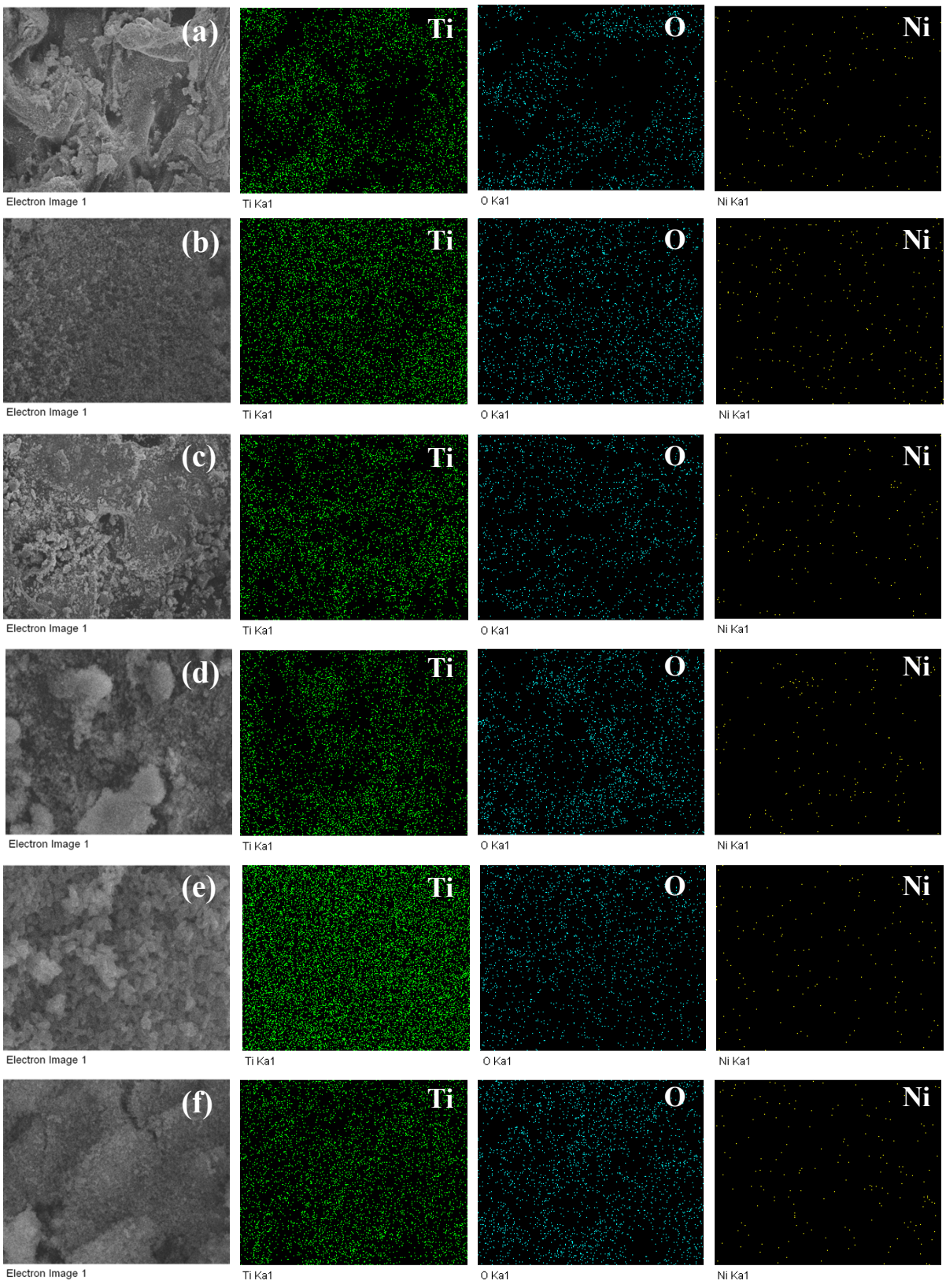

Figure S2. SEM images with EDX elemental mapping of Ni/TiO_2 catalysts: (a) ATA, (b) ATH, (c) P25, (d) ART, (e) RTH, and (f) RTS.

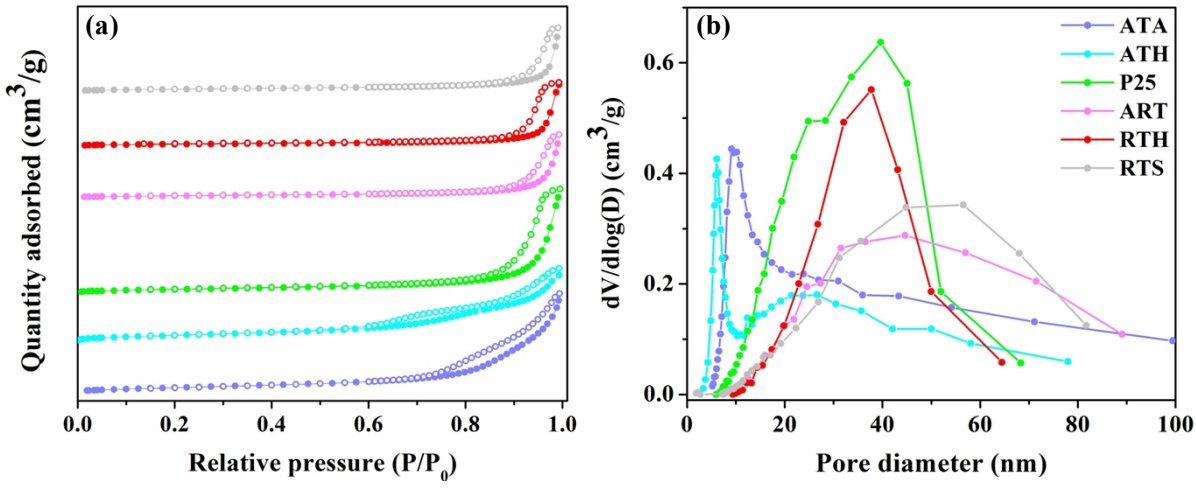

Figure S3. Nitrogen sorption isotherms and BJH pore size distribution of Ni catalysts. The adsorption and desorption in isotherm are represented as closed and open circles respectively.

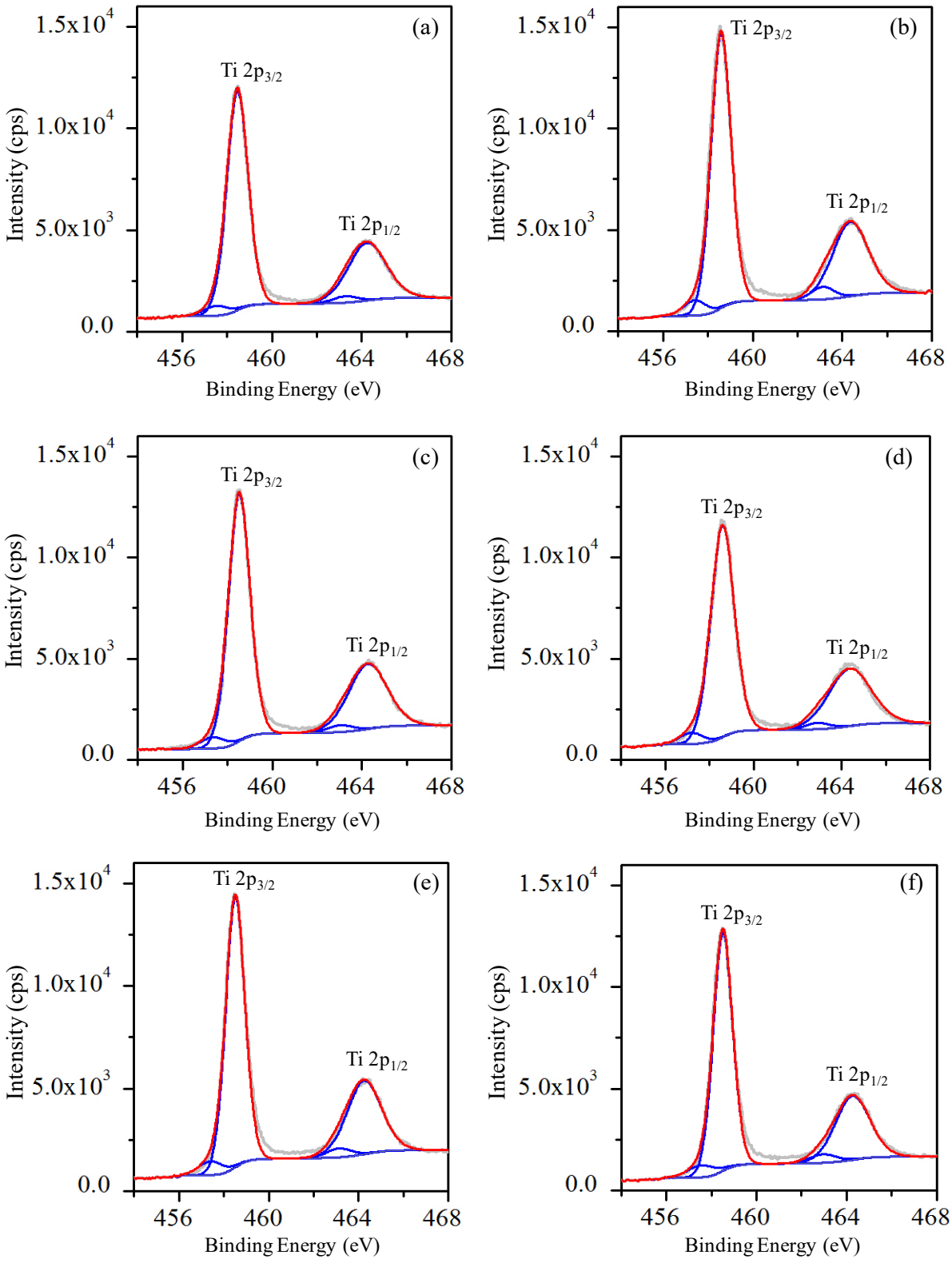

Figure S4. Ti 2p core level XP spectra for the Ni catalysts supported on (a) ATA, (b) ATH, (c) P25, (d) ART, (e) RTH and, (f) RTS.

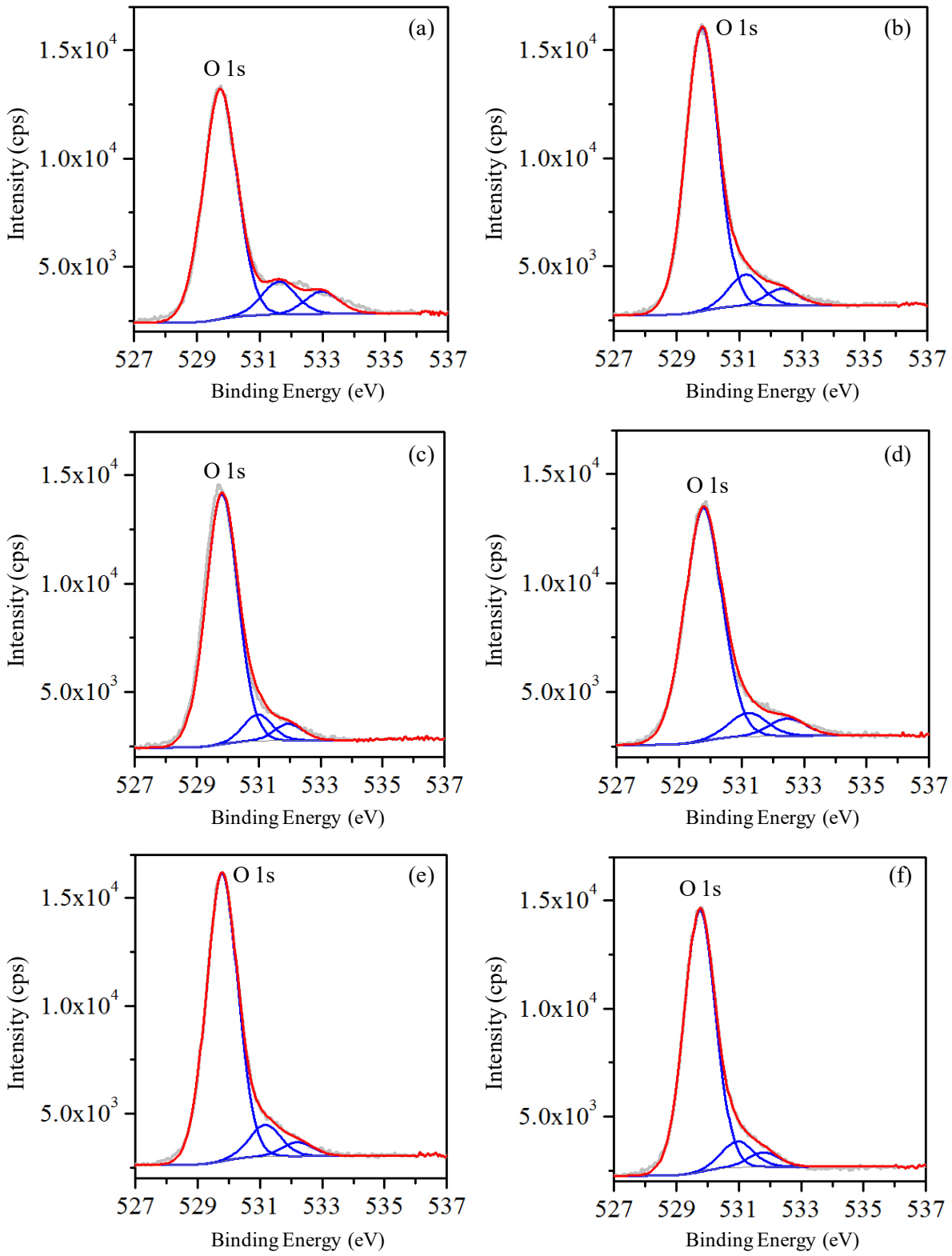

Figure S5. O 1s core level XP spectra for the Ni catalysts supported on (a) ATA, (b) ATH, (c) P25, (d) ART, (e) RTH and, (f) RTS.

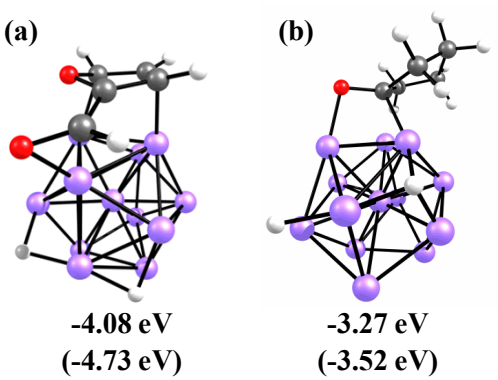

Figure S6. Co-adsorption of (a) FAL + 2H and, (b) CPO + 2H on Ni cluster. The adsorption energy on neutral Ni cluster is given below, where values in parentheses are for adsorption over charged (-1) cluster.

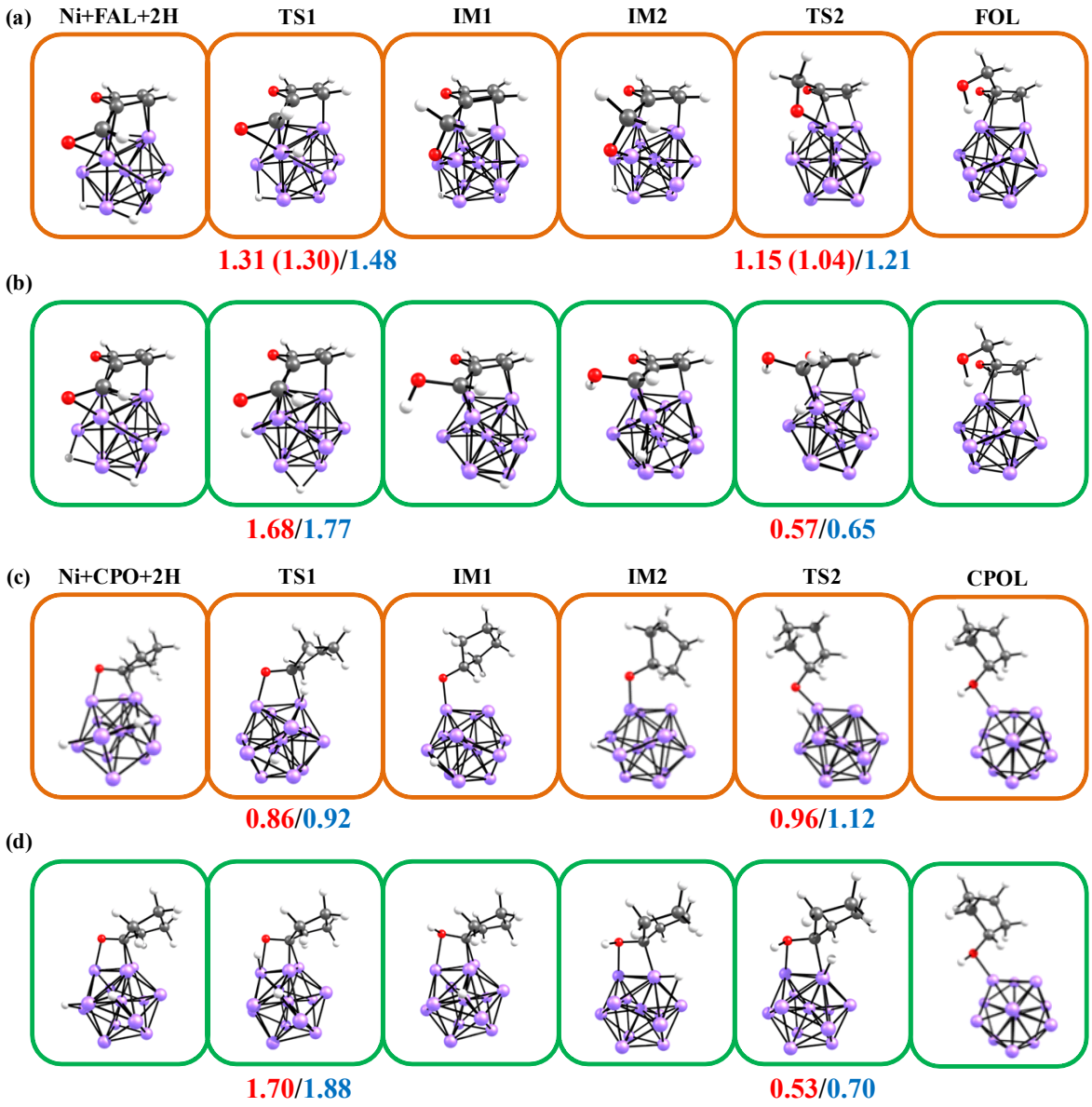

Figure S7. Initial, transition, intermediate and final state geometry during hydrogenation of (a and b) FAL to FOL and (c and d) CPO to CPOL over Ni cluster. Colour code: Figures in brown box (a and c) are corresponding to path a (addition of hydrogen first to carbon and then second hydrogen to oxygen of the carbonyl group). Figures in green box (b and d) are corresponding to path b (addition of hydrogen first to oxygen and then second hydrogen to carbon of the carbonyl group). Values in red and blue represent free energy barriers for reaction over neutral and charged (-1 electronic charge) Ni clusters, respectively. The values

in bracket (a) shows energy barrier for furfural hydrogenation along path a over relaxed neutral cluster. All values are in eV.

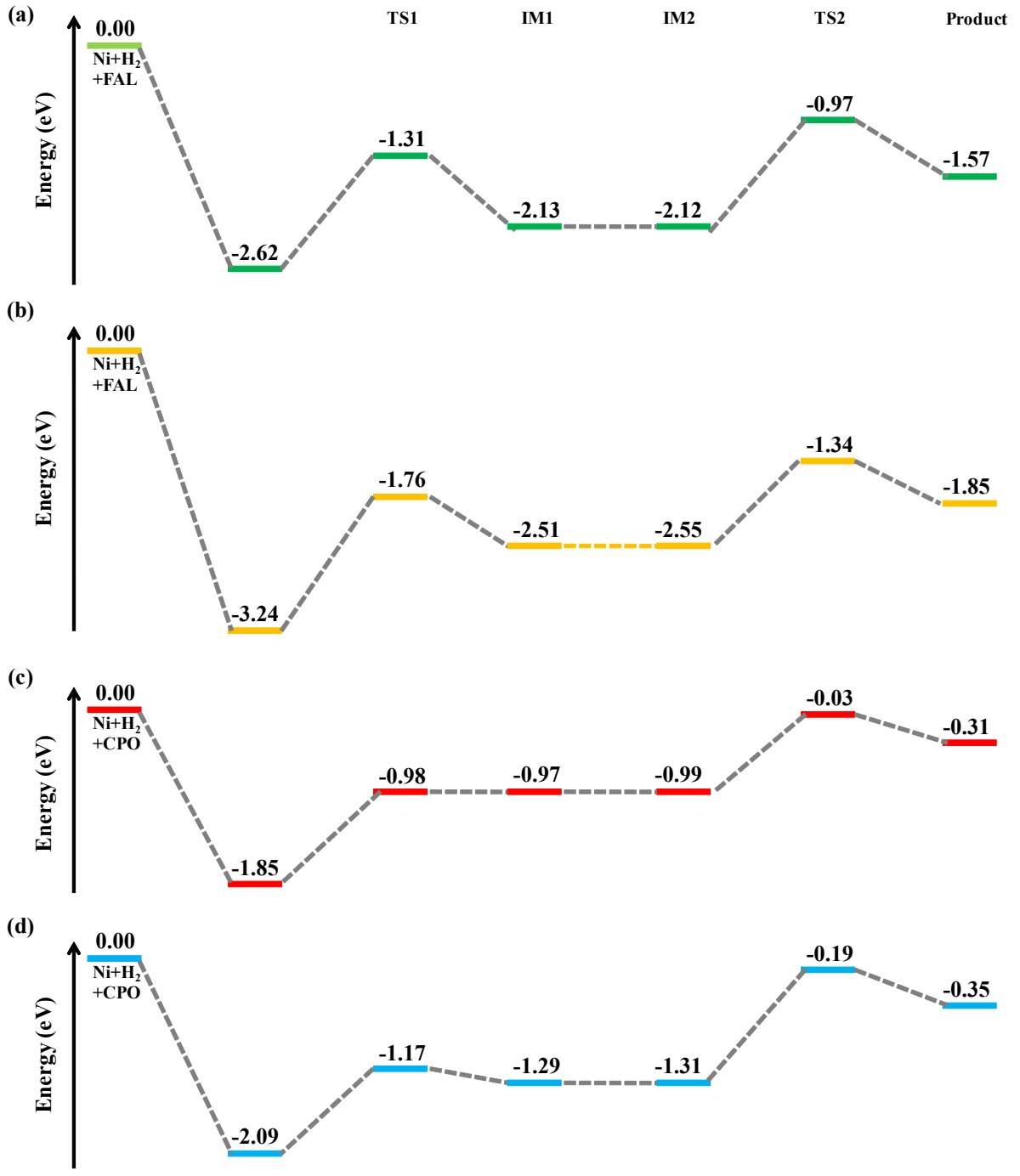

Figure S8. Free energy profile for furfural and cyclopentanone hydrogenation over (a and c) neutral and (b and d) charged Ni clusters along path a, respectively. The values are in eV.

Figure S9. XRD pattern of RH support loaded with 10 wt% Ni content. The enlarged region shows overlapped Rutile and Ni peak.

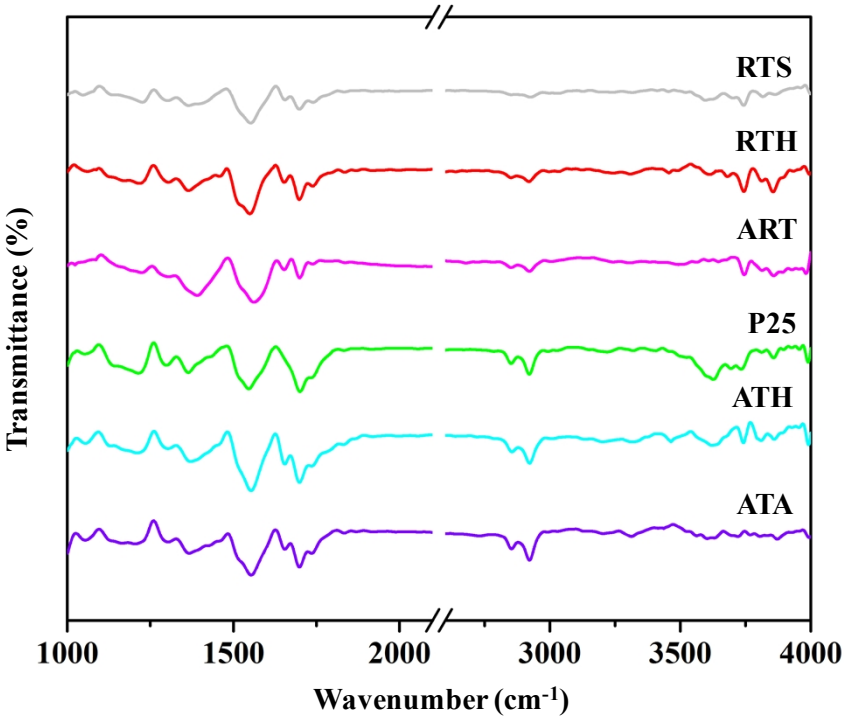

Figure S10. FTIR spectra of dried Ni catalysts after reaction at 140°C.

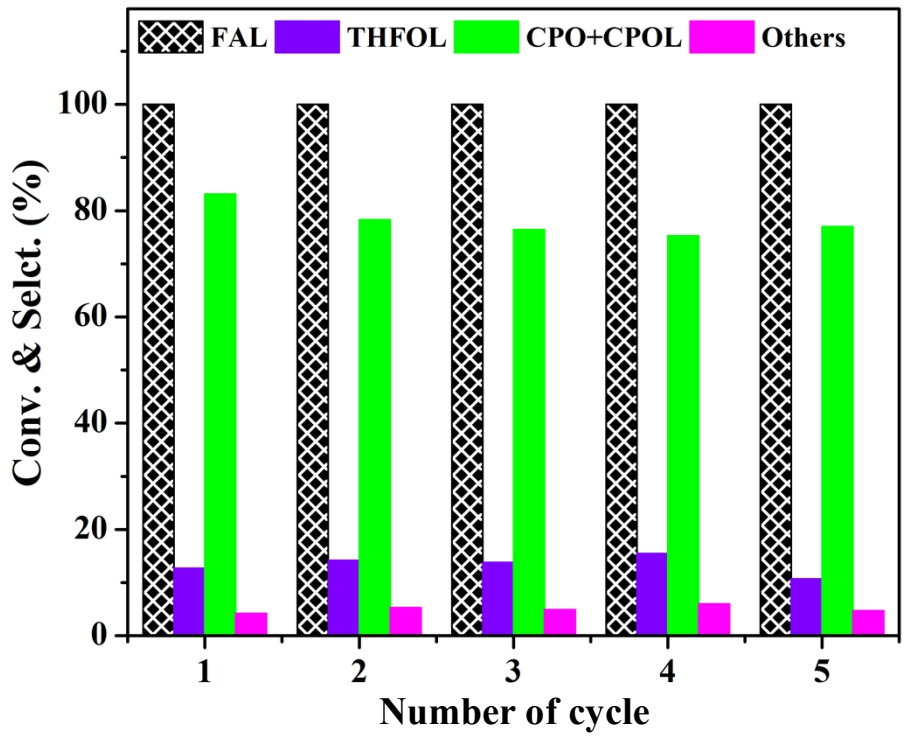

Figure S11. Recycling test over RTH catalyst. Reaction conditions: 5.2 mmol furfural, 50 mL water, 50 bar H_2, 140°C, 4h, 500 rpm.

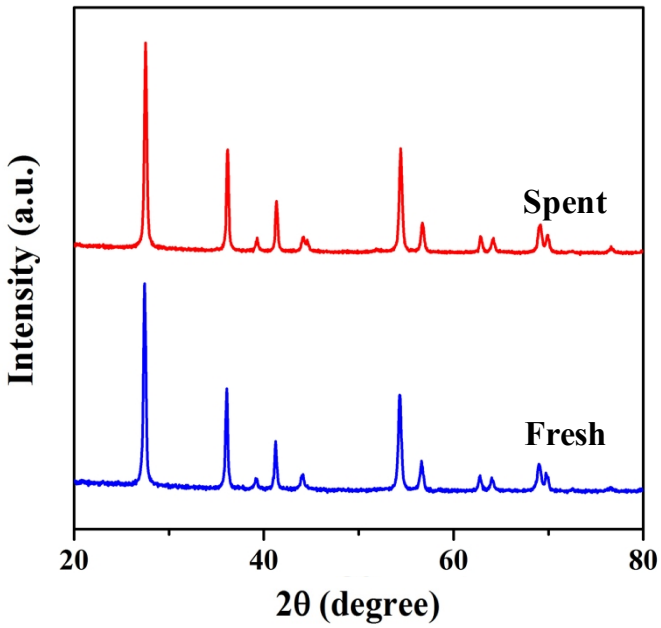

Figure S12. XRD pattern of fresh and spent (after 5 recycles) RTH catalyst.

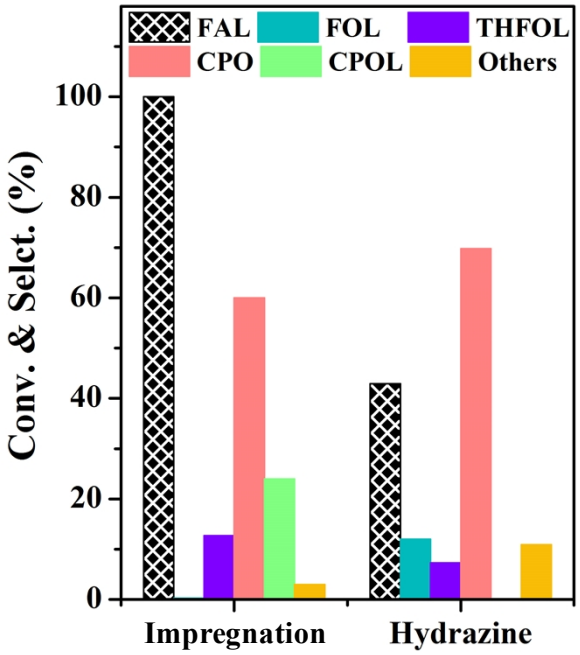

Figure S13. Furfural hydrogenation over RTH catalysts prepared from imprgnation method and hydrazine reduction method. Reaction conditions: 5.2 mmol furfural, 50 mL water, 50 bar H_2, 140°C, 4h, 500 rpm.

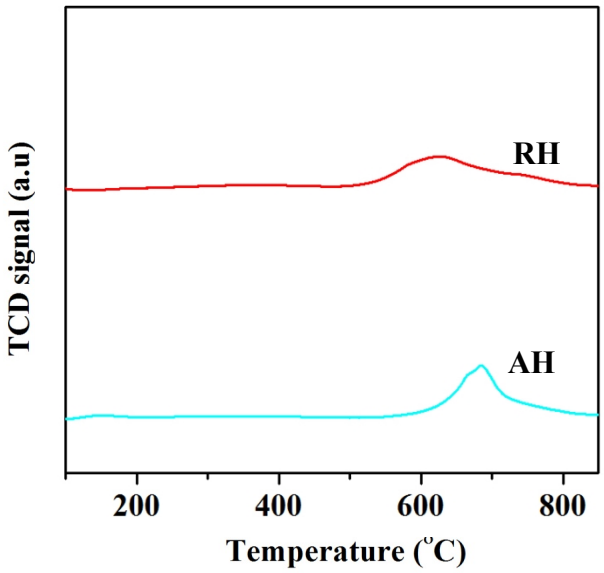

Figure S14. H_2-TPR profiles of bare anatase (AH) and rutile (RH) titania supports of ATH and RTH catalysts, respectively.

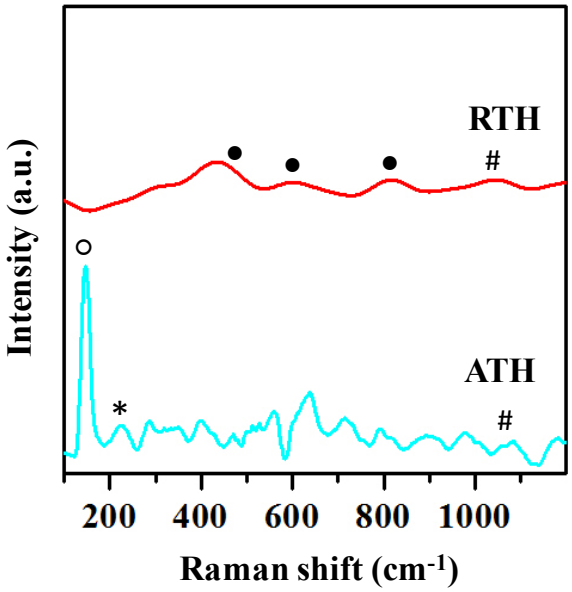

Figure S15. Raman spectra of ATH and RTH catalysts showing presence of (○) anatase phase, (•) rutile phase, (*) $NiTiO_3$ and (#) NiO.

Table S1. Physico-chemical properties of catalysts support

Catalyst	A:R (%)[a]	D (nm)[b]	S_{BET}(m^2/g)	V_p (cm^3/g)[c]	D_p (nm)[c]
ATA	100:0	19.4/-	62	0.28	16.1
ATH	100:0	15.9/-	66	0.21	11.1
P25	77:23	23.1/31.8	40	0.29	26.0
ART	48:52	47.7/54.4	23	0.17	34.6
RTH	0:100	-/29.9	22	0.17	31.4
RTS	0:100	-/22.5	23	0.17	33.8

[a]Percentage of anatase:rutile phases calculated using (101) and (110) XRD peaks intensities;[b]crystallite size of (101) and (110) plane of anatase and rutile phase calculated using Scherrer equation;[c]pore volume and diameter obtained from BJH analysis

Table S2. Desorption temperature (°C) of NH_3 from titania catalysts based on their desorption strength

Catalyst	Weak	Medium	Strong
ATA	190	328	403,463
ATH	193	337	410,475
P25	201	307	350,410
ART	190	296	351,422
RTH	189	292	338,404
RTS	185	286	347,388

Table S3. Binding energy values, atomic ratios of titania catalysts determined from XPS

Catalyst	Binding energy (eV)				$\frac{Ti^{3+}}{(Ti^{3+}+Ti^{4+})}$	Ni/Ti
	Ni^{0}	Ni^{2+}	Ti^{3+}	Ti^{4+}		
ATA	852.2	855.8	457.8	458.5	0.101	0.424
ATH	852.2	855.5	457.9	458.6	0.118	0.512
P25	852.3	855.6	457.3	458.5	0.062	0.630
ART	852.4	855.5	457.5	458.6	0.059	0.802
RTH	852.6	855.8	458.0	458.5	0.052	0.920
RTS	852.5	855.7	457.9	458.5	0.067	1.212

Table S4. Ni leaching (ppm) in the solution after reaction at different temperature.

Catalyst	Ni leaching		Carbon balance	
	100°C	**140°C**	**100°C**	**140°C**
ATA	1.5	2.2	94.1	92.9
ATH	1.8	3.6	93.3	95.2
P25	1.4	0.4	94.8	95.7
ART	2.6	0.3	98.5	98.4
RTH	1.2	0.3	97.7	97.1
RTS	2.5	0.6	97.9	96.3

Cartesian coordinates

Cartesian coordinates (Angstroms) and energies (Hartree) of the adsorbed species on Ni cluster along reaction coordinates.

1. FAL to FOL on neutral Ni cluster (path a)
    a. Ni + FAL+2H

        E+ZPE=-2545.619714

        G=-2545.663595

Ni	1.506629000	-0.924052000	1.022357000
Ni	-0.778447000	-1.281485000	1.987863000
Ni	-2.425586000	-1.335050000	0.112106000
Ni	-1.184186000	-1.017015000	-2.041289000
Ni	1.243532000	-0.746652000	-1.463221000
Ni	1.519886000	1.291373000	-0.034598000
Ni	0.263980000	0.994243000	2.058990000
Ni	-2.133657000	0.685957000	1.455888000
Ni	-2.426088000	0.904408000	-1.006852000
Ni	-0.194546000	1.233535000	-1.990100000
Ni	-0.746197000	2.332189000	0.190397000
Ni	-0.431842000	0.018534000	-0.017420000
Ni	-0.200267000	-2.313701000	-0.151042000
C	3.077821000	-1.510490000	-1.082253000
C	3.164867000	-1.999403000	0.288994000
C	3.532083000	-0.888866000	1.122329000
C	3.620845000	0.244666000	0.233128000
O	3.637645000	-0.179571000	-1.088068000

H	3.409316000	-2.098029000	-1.948913000
H	3.171786000	-3.056655000	0.556524000
H	3.857813000	-0.901035000	2.164207000
C	3.416403000	1.651966000	0.490125000
H	3.581644000	1.994235000	1.530743000
O	3.158087000	2.499521000	-0.474704000
H	-0.390936000	2.767376000	-1.365715000
H	-1.237474000	2.163352000	1.805178000

b. TS1

E+ZPE=-2545.570702

G=-2545.615413

Ni	1.414998000	-1.189363000	0.886298000
Ni	-0.919928000	-1.608627000	1.701682000
Ni	-2.496093000	-1.218629000	-0.195700000
Ni	-1.161356000	-0.558967000	-2.210244000
Ni	1.248999000	-0.529085000	-1.523822000
Ni	1.562411000	1.184731000	0.281027000
Ni	0.220143000	0.555030000	2.239631000
Ni	-2.165669000	0.490212000	1.520761000
Ni	-2.354996000	1.189391000	-0.861668000
Ni	-0.071375000	1.590201000	-1.701083000
Ni	-0.660341000	2.275043000	0.635716000
Ni	-0.440084000	0.030788000	-0.003970000
Ni	-0.307612000	-2.241334000	-0.578251000
C	3.023296000	-1.523068000	-1.193877000

C	3.103549000	-2.102212000	0.137659000
C	3.440152000	-1.032342000	1.046453000
C	3.538838000	0.154414000	0.240303000
O	3.557722000	-0.183917000	-1.106320000
H	3.358432000	-2.037622000	-2.102606000
H	3.158555000	-3.174709000	0.332629000
H	3.750413000	-1.103297000	2.090598000
C	3.565309000	1.622483000	0.574022000
H	4.276015000	1.869687000	1.400318000
O	3.425461000	2.460015000	-0.439260000
H	-1.254118000	2.643203000	-0.988565000
H	2.483585000	1.735365000	1.474343000

c. IM1

E+ZPE=-2545.601080

G=-2545.645537

Ni	1.566324000	-0.689007000	1.023209000
Ni	-0.646426000	-0.987854000	2.166184000
Ni	-2.390352000	-1.357288000	0.417318000
Ni	-1.283284000	-1.297613000	-1.828954000
Ni	1.155303000	-0.867869000	-1.441297000
Ni	1.423361000	1.360257000	-0.320667000
Ni	0.301673000	1.310061000	1.864297000
Ni	-2.111427000	0.838645000	1.454475000
Ni	-2.547373000	0.703409000	-0.993563000
Ni	-0.385550000	0.973720000	-2.148213000

Ni	-0.867425000	2.340610000	-0.104837000
Ni	-0.465264000	0.033220000	-0.013419000
Ni	-0.142551000	-2.285508000	0.157245000
C	2.988588000	-1.606659000	-1.031453000
C	3.025673000	-1.990587000	0.377298000
C	3.630018000	-0.882470000	1.088083000
C	3.947793000	0.090810000	0.116274000
O	3.749497000	-0.393851000	-1.146710000
H	3.207322000	-2.305051000	-1.853345000
H	2.911000000	-3.017582000	0.727987000
H	3.918761000	-0.829392000	2.139883000
C	4.183817000	1.571633000	0.211306000
H	5.090824000	1.839515000	-0.375561000
O	3.065769000	2.293143000	-0.273570000
H	-1.708310000	2.129522000	-1.613156000
H	4.406722000	1.798335000	1.277575000

d. IM2

E+ZPE=-2545.600857

G=-2545.645250

Ni	-1.579247000	-0.697186000	-1.006082000
Ni	0.628009000	-1.023779000	-2.147782000
Ni	2.381618000	-1.369972000	-0.410604000
Ni	1.291402000	-1.272003000	1.842747000
Ni	-1.151677000	-0.838670000	1.469483000
Ni	-1.420897000	1.367240000	0.316312000

Ni	-0.312080000	1.283968000	-1.878276000
Ni	2.101520000	0.810262000	-1.479584000
Ni	2.555033000	0.712747000	0.967237000
Ni	0.407526000	1.004543000	2.128727000
Ni	0.871864000	2.341805000	0.066185000
Ni	0.464636000	0.033730000	0.013202000
Ni	0.133648000	-2.286917000	-0.119083000
C	-2.988126000	-1.609101000	1.039142000
C	-3.043358000	-2.004262000	-0.363993000
C	-3.630948000	-0.892818000	-1.082208000
C	-3.906493000	0.102062000	-0.116950000
O	-3.724611000	-0.382241000	1.151587000
H	-3.206538000	-2.296563000	1.869618000
H	-2.937899000	-3.033606000	-0.709624000
H	-3.930976000	-0.845305000	-2.130947000
C	-4.154503000	1.580477000	-0.219519000
H	-5.071898000	1.838919000	0.356087000
O	-3.050701000	2.317938000	0.272836000
H	1.661774000	2.152136000	1.620351000
H	-4.369307000	1.799199000	-1.289224000

e. TS2

E+ZPE=-2545.558802

G=-2545.603118

Ni	0.992353000	-1.622992000	0.964485000
Ni	-1.456502000	-1.557831000	1.496695000

Ni	-2.684794000	-0.713425000	-0.501093000
Ni	-1.019306000	-0.246432000	-2.313155000
Ni	1.250577000	-0.793634000	-1.395861000
Ni	1.716581000	0.690340000	0.566533000
Ni	0.053658000	0.261596000	2.328196000
Ni	-2.192366000	0.771422000	1.377066000
Ni	-1.954435000	1.639357000	-0.945076000
Ni	0.436276000	1.569576000	-1.518858000
Ni	-0.246386000	2.227799000	0.796248000
Ni	-0.444144000	0.034113000	-0.005292000
Ni	-0.738428000	-2.171919000	-0.753344000
C	2.932371000	-1.777109000	-0.956500000
C	2.903432000	-2.006473000	0.488119000
C	3.350699000	-0.753327000	1.089238000
C	3.663507000	0.134053000	0.024081000
O	3.637408000	-0.542998000	-1.199221000
H	3.198490000	-2.546964000	-1.690382000
H	3.031882000	-2.998093000	0.943565000
H	3.612673000	-0.595394000	2.135558000
C	4.115228000	1.573746000	0.008473000
H	4.566700000	1.787696000	-0.982390000
O	2.996500000	2.422263000	0.296801000
H	1.864341000	2.090539000	-0.587202000
H	4.896876000	1.739588000	0.776550000

f. FOL

E+ZPE=-2545.579669

G=-2545.625067

Ni	1.284067000	-0.976648000	1.245139000
Ni	-0.925894000	-0.438971000	2.297734000
Ni	-2.702585000	-0.667433000	0.557609000
Ni	-1.619044000	-1.355556000	-1.595107000
Ni	0.847035000	-1.527969000	-1.159732000
Ni	1.712518000	0.720009000	-0.475065000
Ni	0.615047000	1.413260000	1.613907000
Ni	-1.833554000	1.533639000	1.169151000
Ni	-2.287087000	1.036434000	-1.228393000
Ni	-0.137501000	0.480043000	-2.287390000
Ni	-0.222464000	2.305254000	-0.578264000
Ni	-0.470629000	0.039694000	-0.024850000
Ni	-0.795381000	-2.197340000	0.604676000
C	2.776851000	-1.871424000	-0.954041000
C	2.850427000	-2.169423000	0.475302000
C	3.311723000	-0.985574000	1.146218000
C	3.509591000	0.029979000	0.118396000
O	3.475830000	-0.617504000	-1.158404000
H	3.057560000	-2.599523000	-1.730897000
H	2.819767000	-3.182137000	0.880942000
H	3.727689000	-0.912791000	2.154983000
C	4.435527000	1.210826000	0.228622000
H	5.393601000	1.011653000	-0.284045000

O	3.908786000	2.413517000	-0.374400000
H	2.964380000	2.462712000	-0.054421000
H	4.648543000	1.362028000	1.305220000

2. FAL to FOL on neutral Ni cluster (path b)
   a. Ni + FAL+2H

      E+ZPE=-2545.619714

      G=-2545.663595

Ni	1.506629000	-0.924052000	1.022357000
Ni	-0.778447000	-1.281485000	1.987863000
Ni	-2.425586000	-1.335050000	0.112106000
Ni	-1.184186000	-1.017015000	-2.041289000
Ni	1.243532000	-0.746652000	-1.463221000
Ni	1.519886000	1.291373000	-0.034598000
Ni	0.263980000	0.994243000	2.058990000
Ni	-2.133657000	0.685957000	1.455888000
Ni	-2.426088000	0.904408000	-1.006852000
Ni	-0.194546000	1.233535000	-1.990100000
Ni	-0.746197000	2.332189000	0.190397000
Ni	-0.431842000	0.018534000	-0.017420000
Ni	-0.200267000	-2.313701000	-0.151042000
C	3.077821000	-1.510490000	-1.082253000
C	3.164867000	-1.999403000	0.288994000
C	3.532083000	-0.888866000	1.122329000
C	3.620845000	0.244666000	0.233128000
O	3.637645000	-0.179571000	-1.088068000

H	3.409316000	-2.098029000	-1.948913000
H	3.171786000	-3.056655000	0.556524000
H	3.857813000	-0.901035000	2.164207000
C	3.416403000	1.651966000	0.490125000
H	3.581644000	1.994235000	1.530743000
O	3.158087000	2.499521000	-0.474704000
H	-0.390936000	2.767376000	-1.365715000
H	-1.237474000	2.163352000	1.805178000

b. TS1

E+ZPE=-2545.557691

G=-2545.601910

Ni	1.476910000	-0.927495000	1.047966000
Ni	-0.802836000	-1.134634000	2.064684000
Ni	-2.480016000	-1.240469000	0.217901000
Ni	-1.261845000	-1.104541000	-1.967598000
Ni	1.183608000	-0.893149000	-1.440248000
Ni	1.558888000	1.217942000	-0.145193000
Ni	0.325476000	1.104408000	1.973450000
Ni	-2.091322000	0.846271000	1.429511000
Ni	-2.414526000	0.924124000	-1.037925000
Ni	-0.191528000	1.104911000	-2.071271000
Ni	-0.658502000	2.353899000	0.049930000
Ni	-0.439023000	0.024136000	-0.023227000
Ni	-0.297729000	-2.318801000	-0.013846000
C	2.989152000	-1.601700000	-1.025531000

C	3.099698000	-2.043674000	0.373340000
C	3.517043000	-0.925465000	1.160764000
C	3.632702000	0.185431000	0.222314000
O	3.635580000	-0.291740000	-1.084345000
H	3.342770000	-2.240152000	-1.849442000
H	3.094312000	-3.092773000	0.673693000
H	3.883778000	-0.921073000	2.188326000
C	3.484662000	1.576772000	0.456712000
H	3.614443000	1.951501000	1.482072000
O	3.300764000	2.460539000	-0.567282000
H	1.962078000	2.724893000	-0.499724000
H	-1.139168000	2.294214000	1.736769000

c. IM1

E+ZPE=-2545.586382

G=-2545.631338

Ni	1.229943000	-1.250464000	1.087542000
Ni	-1.149993000	-1.283457000	1.872540000
Ni	-2.636964000	-0.978398000	-0.110246000
Ni	-1.199941000	-0.758042000	-2.151010000
Ni	1.188804000	-0.910203000	-1.394690000
Ni	1.670893000	0.983304000	0.170734000
Ni	0.227617000	0.788720000	2.152961000
Ni	-2.135694000	0.899367000	1.371833000
Ni	-2.200844000	1.284388000	-1.087585000
Ni	0.123087000	1.298868000	-1.895781000

Ni	-0.413946000	2.363244000	0.305012000
Ni	-0.451703000	0.041668000	-0.021288000
Ni	-0.578864000	-2.288014000	-0.281315000
C	2.963349000	-1.717528000	-1.043788000
C	2.935972000	-2.176227000	0.345112000
C	3.252786000	-1.053304000	1.182999000
C	3.516424000	0.061368000	0.257960000
O	3.659227000	-0.434312000	-1.045378000
H	3.330527000	-2.359143000	-1.856211000
H	2.929163000	-3.230091000	0.632618000
H	3.608566000	-1.074565000	2.215469000
C	3.599796000	1.457215000	0.512096000
H	3.768837000	1.760824000	1.557210000
O	4.190915000	2.273994000	-0.473046000
H	3.720524000	3.127634000	-0.431185000
H	-0.595783000	2.281259000	1.979340000

d. IM2

E+ZPE=-2545.588462

G=-2545.633246

Ni	-1.221244000	-1.409309000	-0.893637000
Ni	1.188513000	-1.677367000	-1.516610000
Ni	2.586782000	-0.989964000	0.437937000
Ni	1.059051000	-0.294721000	2.295738000
Ni	-1.295136000	-0.537862000	1.457139000
Ni	-1.624067000	0.980217000	-0.508295000

Ni	-0.087026000	0.327459000	-2.309124000
Ni	2.234585000	0.535574000	-1.438636000
Ni	2.189660000	1.442461000	0.882484000
Ni	-0.169100000	1.695111000	1.531608000
Ni	0.520773000	2.238433000	-0.814140000
Ni	0.451903000	0.049457000	0.010606000
Ni	0.472368000	-2.174830000	0.767072000
C	-2.956615000	-1.617620000	1.169226000
C	-2.948405000	-2.211269000	-0.159053000
C	-3.215154000	-1.153777000	-1.106072000
C	-3.466110000	0.046336000	-0.308590000
O	-3.571980000	-0.307739000	1.058655000
H	-3.300385000	-2.147794000	2.065622000
H	-2.999482000	-3.286904000	-0.343264000
H	-3.551457000	-1.259730000	-2.139884000
C	-3.591559000	1.422898000	-0.649458000
H	-3.903639000	1.694661000	-1.663336000
O	-4.060038000	2.342045000	0.302515000
H	-3.590734000	2.123081000	1.134600000
H	-1.128785000	2.512426000	-0.879423000

e. TS2

E+ZPE=-2545.567565

G=-2545.612272

Ni	1.188150000	-1.423600000	0.907210000
Ni	-1.214795000	-1.597545000	1.588458000

Ni	-2.634831000	-0.935589000	-0.358702000
Ni	-1.128845000	-0.350391000	-2.270832000
Ni	1.235883000	-0.634814000	-1.475086000
Ni	1.650457000	0.937322000	0.429515000
Ni	0.136612000	0.393339000	2.284503000
Ni	-2.196776000	0.641880000	1.455995000
Ni	-2.176407000	1.467374000	-0.895560000
Ni	0.174044000	1.626522000	-1.602698000
Ni	-0.447799000	2.270135000	0.737122000
Ni	-0.461545000	0.053238000	-0.012463000
Ni	-0.563814000	-2.194082000	-0.690793000
C	2.963339000	-1.620274000	-1.179727000
C	2.913930000	-2.217616000	0.152282000
C	3.217091000	-1.175087000	1.107094000
C	3.486196000	0.011349000	0.314975000
O	3.621586000	-0.328505000	-1.035193000
H	3.355504000	-2.162622000	-2.049506000
H	2.941371000	-3.295648000	0.330677000
H	3.517693000	-1.286896000	2.150868000
C	3.636257000	1.422534000	0.648378000
H	4.044829000	1.631876000	1.644474000
O	4.255845000	2.238601000	-0.314766000
H	3.837665000	2.002510000	-1.168535000
H	2.293240000	2.198447000	0.926960000

f. FOL

E+ZPE=-2545.579669

G=-2545.625067

Ni	1.284067000	-0.976648000	1.245139000
Ni	-0.925894000	-0.438971000	2.297734000
Ni	-2.702585000	-0.667433000	0.557609000
Ni	-1.619044000	-1.355556000	-1.595107000
Ni	0.847035000	-1.527969000	-1.159732000
Ni	1.712518000	0.720009000	-0.475065000
Ni	0.615047000	1.413260000	1.613907000
Ni	-1.833554000	1.533639000	1.169151000
Ni	-2.287087000	1.036434000	-1.228393000
Ni	-0.137501000	0.480043000	-2.287390000
Ni	-0.222464000	2.305254000	-0.578264000
Ni	-0.470629000	0.039694000	-0.024850000
Ni	-0.795381000	-2.197340000	0.604676000
C	2.776851000	-1.871424000	-0.954041000
C	2.850427000	-2.169423000	0.475302000
C	3.311723000	-0.985574000	1.146218000
C	3.509591000	0.029979000	0.118396000
O	3.475830000	-0.617504000	-1.158404000
H	3.057560000	-2.599523000	-1.730897000
H	2.819767000	-3.182137000	0.880942000
H	3.727689000	-0.912791000	2.154983000
C	4.435527000	1.210826000	0.228622000
H	5.393601000	1.011653000	-0.284045000

O	3.908786000	2.413517000	-0.374400000
H	2.964380000	2.462712000	-0.054421000
H	4.648543000	1.362028000	1.305220000

3. FAL to FOL on charged (-1) Ni cluster (path a)
   a. Ni + FAL+2H

      E+ZPE=-2545.733606

      G=-2545.777336

Ni	-1.120644000	-1.073895000	-2.031095000
Ni	-0.185326000	1.223981000	-1.993234000
Ni	1.473951000	1.414373000	-0.098030000
Ni	1.507518000	-0.911105000	1.115389000
Ni	-0.108383000	-2.368227000	-0.142849000
Ni	-2.320787000	-1.347056000	0.082393000
Ni	-2.410126000	0.814893000	-1.041974000
Ni	-0.847346000	2.302899000	0.153385000
Ni	0.157172000	1.009659000	2.043567000
Ni	-0.793880000	-1.272878000	1.997042000
Ni	-2.204533000	0.693480000	1.427809000
Ni	-0.379177000	-0.002504000	-0.004746000
Ni	1.290478000	-0.782532000	-1.504048000
C	3.101464000	-1.474206000	-1.000072000
C	3.188157000	-1.927970000	0.389256000
C	3.510564000	-0.789489000	1.206535000
C	3.551514000	0.334200000	0.298334000
O	3.601790000	-0.110685000	-1.018731000

H	3.524456000	-2.063566000	-1.826838000
H	3.264755000	-2.979227000	0.671029000
H	3.863391000	-0.777377000	2.240146000
C	3.337799000	1.741534000	0.533461000
H	3.460606000	2.086760000	1.579050000
O	3.134924000	2.594571000	-0.446647000
H	-0.492543000	2.747844000	-1.400193000
H	-1.301045000	2.179602000	1.793750000

b. TS1

E+ZPE=-2545.678789

G=-2545.722791

Ni	-1.097722000	-0.725542000	-2.178579000
Ni	-0.128794000	1.521090000	-1.766321000
Ni	1.486771000	1.386589000	0.170914000
Ni	1.455306000	-1.098123000	1.011780000
Ni	-0.151815000	-2.313708000	-0.490697000
Ni	-2.353069000	-1.297799000	-0.158747000
Ni	-2.381978000	1.012623000	-0.937997000
Ni	-0.826134000	2.269128000	0.506041000
Ni	0.112439000	0.682164000	2.195680000
Ni	-0.872305000	-1.547711000	1.777114000
Ni	-2.238399000	0.509013000	1.487375000
Ni	-0.389627000	0.007292000	0.004569000
Ni	1.303745000	-0.564597000	-1.560351000
C	3.047214000	-1.503493000	-1.075539000

C	3.131991000	-2.023271000	0.286558000
C	3.470047000	-0.913518000	1.149975000
C	3.535305000	0.241262000	0.305694000
O	3.542200000	-0.137939000	-1.028465000
H	3.458299000	-2.044152000	-1.939083000
H	3.232193000	-3.085785000	0.517144000
H	3.785161000	-0.941666000	2.195275000
C	3.466898000	1.714143000	0.597513000
H	4.151620000	2.028507000	1.421556000
O	3.310153000	2.522046000	-0.452786000
H	-1.437418000	2.547489000	-1.093499000
H	2.366856000	1.800329000	1.461513000

c. IM1

E+ZPE=-2545.706244

G=-2545.750585

Ni	-1.224009000	-1.291372000	-1.854163000
Ni	-0.333021000	1.008800000	-2.121689000
Ni	1.407969000	1.437810000	-0.342536000
Ni	1.542642000	-0.733114000	1.124126000
Ni	-0.101009000	-2.347060000	0.118211000
Ni	-2.320036000	-1.338094000	0.332062000
Ni	-2.503122000	0.679807000	-1.024622000
Ni	-0.916139000	2.316182000	-0.082083000
Ni	0.199566000	1.261896000	1.892232000
Ni	-0.708356000	-1.024166000	2.150440000

Ni	-2.181672000	0.844164000	1.430261000
Ni	-0.411069000	0.014979000	0.000028000
Ni	1.202517000	-0.908057000	-1.479463000
C	3.021568000	-1.573384000	-0.983460000
C	3.064464000	-1.943632000	0.432538000
C	3.597631000	-0.797052000	1.142476000
C	3.857779000	0.193963000	0.169182000
O	3.711503000	-0.310068000	-1.094697000
H	3.331461000	-2.265463000	-1.782619000
H	3.032420000	-2.976777000	0.783014000
H	3.894336000	-0.726331000	2.191900000
C	4.106878000	1.674062000	0.264486000
H	5.037375000	1.920268000	-0.297967000
O	3.019769000	2.424881000	-0.243296000
H	-1.667135000	2.102560000	-1.677074000
H	4.312160000	1.893811000	1.336800000

d. IM2

E+ZPE=-2545.707166

G=-2545.751857

Ni	-1.227917000	-1.321859000	-1.830847000
Ni	-0.369807000	0.987581000	-2.135615000
Ni	1.383963000	1.459044000	-0.380178000
Ni	1.565831000	-0.692269000	1.108025000
Ni	-0.068436000	-2.340204000	0.139802000
Ni	-2.298631000	-1.359155000	0.367859000

Ni	-2.524477000	0.640703000	-1.008165000
Ni	-0.950748000	2.308767000	-0.101794000
Ni	0.203160000	1.291660000	1.870092000
Ni	-0.670162000	-1.003588000	2.163815000
Ni	-2.176433000	0.836796000	1.440829000
Ni	-0.411714000	0.015216000	-0.000791000
Ni	1.194947000	-0.903743000	-1.489588000
C	3.013136000	-1.557397000	-0.982500000
C	3.052729000	-1.929509000	0.436906000
C	3.611650000	-0.793568000	1.145444000
C	3.885431000	0.190936000	0.169189000
O	3.731338000	-0.308781000	-1.093738000
H	3.317468000	-2.258469000	-1.777165000
H	3.012368000	-2.964083000	0.783470000
H	3.915922000	-0.729459000	2.193098000
C	4.113100000	1.673807000	0.258862000
H	5.039894000	1.935511000	-0.301764000
O	3.014651000	2.401640000	-0.258223000
H	-1.806209000	2.131475000	-1.596005000
H	4.308207000	1.906029000	1.330198000

e. TS2

E+ZPE=-2545.663157

G=-2545.707256

Ni	-0.905444000	-0.288308000	-2.326913000
Ni	0.519380000	1.559987000	-1.492082000

Ni	1.706797000	0.804054000	0.610715000
Ni	0.914031000	-1.652749000	1.088089000
Ni	-0.677222000	-2.232739000	-0.770643000
Ni	-2.576950000	-0.699831000	-0.594112000
Ni	-1.895963000	1.598901000	-1.040436000
Ni	-0.335786000	2.240793000	0.761716000
Ni	-0.110802000	0.298176000	2.318031000
Ni	-1.544398000	-1.528956000	1.464355000
Ni	-2.282425000	0.835414000	1.289078000
Ni	-0.403126000	0.004941000	0.007332000
Ni	1.328450000	-0.840116000	-1.387692000
C	2.896925000	-1.872208000	-0.739394000
C	2.854410000	-1.975352000	0.718163000
C	3.282474000	-0.670326000	1.217540000
C	3.591230000	0.141438000	0.090718000
O	3.578112000	-0.639894000	-1.085562000
H	3.197336000	-2.697225000	-1.396613000
H	3.029773000	-2.920262000	1.252656000
H	3.557353000	-0.441264000	2.247716000
C	4.143743000	1.542047000	-0.022426000
H	4.583670000	1.658031000	-1.036202000
O	3.106515000	2.490475000	0.241312000
H	1.956546000	2.123166000	-0.580662000
H	4.962439000	1.691467000	0.711229000

f. FOL

E+ZPE=-2545.680850

G=-2545.726073

Ni	-1.630469000	-1.342136000	-1.583820000
Ni	-0.103615000	0.480408000	-2.285811000
Ni	1.729645000	0.736937000	-0.562245000
Ni	1.249276000	-1.026020000	1.321688000
Ni	-0.824723000	-2.251220000	0.603550000
Ni	-2.637659000	-0.609546000	0.521263000
Ni	-2.245304000	1.046672000	-1.224577000
Ni	-0.221916000	2.301875000	-0.571771000
Ni	0.580214000	1.391196000	1.612361000
Ni	-0.961120000	-0.418514000	2.297529000
Ni	-1.828615000	1.610952000	1.155884000
Ni	-0.421108000	0.019098000	-0.006341000
Ni	0.808630000	-1.622591000	-1.202805000
C	2.735701000	-1.851710000	-0.925105000
C	2.823527000	-2.142819000	0.510911000
C	3.269791000	-0.954988000	1.187626000
C	3.463730000	0.074284000	0.168624000
O	3.413174000	-0.564796000	-1.120599000
H	3.105458000	-2.570892000	-1.676040000
H	2.846501000	-3.160859000	0.906373000
H	3.715674000	-0.895185000	2.185109000
C	4.433696000	1.219674000	0.285116000
H	5.405790000	0.966776000	-0.177707000

O	3.981144000	2.425374000	-0.364869000
H	2.994885000	2.444299000	-0.181982000
H	4.607902000	1.385483000	1.367615000

4. FAL to FOL on charged (-1) Ni cluster (path b)

   a. Ni + FAL+2H

   E+ZPE=-2545.733025

   G=-2545.776759

Ni	-1.084290000	-1.217144000	-1.959602000
Ni	-0.328339000	1.141999000	-2.058880000
Ni	1.365964000	1.549329000	-0.214301000
Ni	1.593245000	-0.711417000	1.102384000
Ni	0.065021000	-2.342640000	-0.044629000
Ni	-2.213023000	-1.476739000	0.194605000
Ni	-2.489712000	0.616649000	-1.022283000
Ni	-1.022176000	2.256129000	0.073571000
Ni	0.131917000	1.147956000	1.974757000
Ni	-0.645564000	-1.199096000	2.066710000
Ni	-2.207172000	0.635318000	1.435417000
Ni	-0.377181000	-0.001226000	-0.010974000
Ni	1.309612000	-0.722666000	-1.517493000
C	3.069145000	-1.464350000	-0.982930000
C	3.183214000	-1.895167000	0.421085000
C	3.572375000	-0.762101000	1.214035000
C	3.547904000	0.354376000	0.294025000
O	3.595218000	-0.100983000	-1.022156000

H	3.511031000	-2.072987000	-1.787719000
H	3.236971000	-2.944171000	0.716569000
H	3.958486000	-0.748426000	2.235510000
C	3.257745000	1.750805000	0.506986000
H	3.338373000	2.107637000	1.552982000
O	3.090932000	2.599220000	-0.486346000
H	0.154943000	2.530921000	-1.135761000
H	-2.223704000	2.299094000	1.227328000

b. TS1

E+ZPE=-2545.668020

G=-2545.711773

Ni	-1.188986000	-1.166502000	-1.954551000
Ni	-0.233888000	1.118539000	-2.068841000
Ni	1.482420000	1.394320000	-0.220589000
Ni	1.511440000	-0.866542000	1.114831000
Ni	-0.146650000	-2.370617000	-0.026284000
Ni	-2.343198000	-1.311515000	0.196852000
Ni	-2.435848000	0.788029000	-1.037316000
Ni	-0.837393000	2.305289000	0.052048000
Ni	0.211058000	1.117638000	1.966378000
Ni	-0.764339000	-1.153805000	2.073126000
Ni	-2.161423000	0.802179000	1.421431000
Ni	-0.387349000	0.000055000	-0.012503000
Ni	1.236830000	-0.874811000	-1.506554000
C	3.023966000	-1.512706000	-0.976259000

C	3.121761000	-1.953937000	0.433918000
C	3.533185000	-0.835455000	1.230075000
C	3.624577000	0.282385000	0.294823000
O	3.661493000	-0.187748000	-1.010355000
H	3.455099000	-2.148717000	-1.768291000
H	3.158554000	-3.006843000	0.721688000
H	3.922710000	-0.839436000	2.249788000
C	3.417031000	1.662737000	0.518530000
H	3.490006000	2.047991000	1.544985000
O	3.273671000	2.545154000	-0.521159000
H	1.968905000	2.876055000	-0.484452000
H	-2.194594000	2.450353000	1.037088000

c. IM1

E+ZPE=-2545.694675

G=-2545.739019

Ni	1.036463000	-0.647495000	2.232653000
Ni	-0.267028000	1.410153000	1.771336000
Ni	-1.668911000	1.053715000	-0.310288000
Ni	-1.119455000	-1.360373000	-1.181479000
Ni	0.535162000	-2.325662000	0.447092000
Ni	2.546371000	-0.933346000	0.329280000
Ni	2.101530000	1.323413000	1.136942000
Ni	0.495164000	2.316507000	-0.438460000
Ni	-0.015762000	0.659849000	-2.208544000
Ni	1.302514000	-1.382627000	-1.742331000

Ni	2.245175000	0.878646000	-1.291615000
Ni	0.403960000	0.012929000	0.007402000
Ni	-1.293939000	-0.884512000	1.404843000
C	-3.017617000	-1.673146000	0.941800000
C	-2.896144000	-2.118244000	-0.455715000
C	-3.145281000	-0.979927000	-1.301196000
C	-3.484294000	0.124419000	-0.392250000
O	-3.713799000	-0.384268000	0.898592000
H	-3.480972000	-2.324488000	1.696802000
H	-2.944773000	-3.170914000	-0.750003000
H	-3.448314000	-0.996099000	-2.351454000
C	-3.587192000	1.534407000	-0.598915000
H	-3.811282000	1.904991000	-1.606611000
O	-4.187471000	2.351417000	0.387103000
H	-3.808913000	2.044549000	1.236481000
H	1.052729000	2.086212000	-2.064416000

d. IM2

E+ZPE=-2545.694190

G=-2545.738020

Ni	0.927743000	-0.289920000	2.326073000
Ni	-0.238822000	1.724614000	1.475313000
Ni	-1.591185000	1.098016000	-0.570948000
Ni	-1.176268000	-1.455263000	-0.998301000
Ni	0.374765000	-2.216546000	0.828058000
Ni	2.468256000	-0.979920000	0.555142000

Ni	2.140595000	1.402588000	0.955490000
Ni	0.632031000	2.220789000	-0.818839000
Ni	0.081028000	0.295539000	-2.312644000
Ni	1.261102000	-1.702083000	-1.451414000
Ni	2.338348000	0.535812000	-1.361354000
Ni	0.399567000	0.017589000	-0.004945000
Ni	-1.385605000	-0.534382000	1.458882000
C	-2.963062000	-1.654169000	1.011631000
C	-2.948382000	-2.179291000	-0.349768000
C	-3.152564000	-1.059880000	-1.240645000
C	-3.387961000	0.110456000	-0.394099000
O	-3.528833000	-0.313940000	0.960974000
H	-3.359675000	-2.219186000	1.864910000
H	-3.087129000	-3.237139000	-0.588261000
H	-3.481150000	-1.102576000	-2.281947000
C	-3.545902000	1.500926000	-0.678626000
H	-3.916388000	1.805104000	-1.664433000
O	-4.005355000	2.368157000	0.336303000
H	-3.415345000	2.191152000	1.101718000
H	-0.963150000	2.549352000	-1.155477000

e. TS2

E+ZPE=-2545.670093

G=-2545.714072

Ni	1.011228000	-0.369745000	2.296601000
Ni	-0.212808000	1.656543000	1.562489000

Ni	-1.614120000	1.089406000	-0.468260000
Ni	-1.169375000	-1.436979000	-1.011584000
Ni	0.446657000	-2.243820000	0.737401000
Ni	2.510575000	-0.960189000	0.455723000
Ni	2.155336000	1.398014000	0.962407000
Ni	0.582252000	2.260363000	-0.733179000
Ni	0.019888000	0.387653000	-2.288116000
Ni	1.257440000	-1.621866000	-1.543345000
Ni	2.299643000	0.629183000	-1.392652000
Ni	0.410121000	0.022254000	-0.003657000
Ni	-1.322023000	-0.620056000	1.486779000
C	-2.962835000	-1.662909000	1.030358000
C	-2.925430000	-2.192292000	-0.333808000
C	-3.181284000	-1.087838000	-1.231944000
C	-3.409113000	0.071411000	-0.390512000
O	-3.558988000	-0.330871000	0.948854000
H	-3.405293000	-2.231299000	1.859654000
H	-3.035499000	-3.255227000	-0.565863000
H	-3.486614000	-1.136187000	-2.279559000
C	-3.597660000	1.493662000	-0.672036000
H	-4.069868000	1.718572000	-1.637275000
O	-4.198541000	2.262279000	0.348644000
H	-3.658283000	2.085049000	1.148386000
H	-2.321064000	2.294292000	-1.014668000

f. FOL

E+ZPE=-2545.680850

G=-2545.726073

Ni	-1.630469000	-1.342136000	-1.583820000
Ni	-0.103615000	0.480408000	-2.285811000
Ni	1.729645000	0.736937000	-0.562245000
Ni	1.249276000	-1.026020000	1.321688000
Ni	-0.824723000	-2.251220000	0.603550000
Ni	-2.637659000	-0.609546000	0.521263000
Ni	-2.245304000	1.046672000	-1.224577000
Ni	-0.221916000	2.301875000	-0.571771000
Ni	0.580214000	1.391196000	1.612361000
Ni	-0.961120000	-0.418514000	2.297529000
Ni	-1.828615000	1.610952000	1.155884000
Ni	-0.421108000	0.019098000	-0.006341000
Ni	0.808630000	-1.622591000	-1.202805000
C	2.735701000	-1.851710000	-0.925105000
C	2.823527000	-2.142819000	0.510911000
C	3.269791000	-0.954988000	1.187626000
C	3.463730000	0.074284000	0.168624000
O	3.413174000	-0.564796000	-1.120599000
H	3.105458000	-2.570892000	-1.676040000
H	2.846501000	-3.160859000	0.906373000
H	3.715674000	-0.895185000	2.185109000
C	4.433696000	1.219674000	0.285116000
H	5.405790000	0.966776000	-0.177707000

O	3.981144000	2.425374000	-0.364869000
H	2.994885000	2.444299000	-0.181982000
H	4.607902000	1.385483000	1.367615000

5. CPO to CPOL on neutral Ni cluster (path a)

   a. Ni + CPO+2H

      E+ZPE=-2472.824296

      G=-2472.869355

Ni	2.013125000	1.885071000	-0.091137000
Ni	1.479338000	0.699183000	2.050948000
Ni	1.040571000	-1.704674000	1.533619000
Ni	1.306909000	-2.044028000	-0.934876000
Ni	1.889228000	0.185329000	-1.932384000
Ni	0.009761000	1.784446000	-1.507134000
Ni	-0.275460000	2.081449000	0.918589000
Ni	-0.802871000	-0.151755000	1.886412000
Ni	-0.984419000	-1.843167000	0.071393000
Ni	-0.441590000	-0.717491000	-2.046600000
Ni	-1.784694000	0.494413000	-0.319514000
Ni	0.500846000	0.036125000	-0.048724000
Ni	2.765114000	-0.457706000	0.323579000
C	-3.758584000	0.077351000	-1.224253000
C	-4.208757000	-0.328636000	1.184462000
C	-4.810381000	1.017993000	0.752965000
C	-5.010476000	0.852955000	-0.769536000
H	-2.947666000	0.872113000	-1.548900000

H	-3.856143000	-0.536624000	-2.132670000
H	-5.002538000	-1.091631000	1.321841000
H	-3.617935000	-0.285534000	2.116640000
H	-5.741437000	1.277116000	1.281444000
H	-4.071569000	1.819915000	0.937296000
H	-5.903259000	0.231461000	-0.965555000
H	-5.144532000	1.812360000	-1.295820000
C	-3.339588000	-0.750600000	-0.004543000
O	-2.894182000	-1.999093000	-0.083232000
H	-1.685522000	1.236199000	1.341501000
H	-0.153214000	-1.478480000	2.658685000

b. TS1

E+ZPE=-2472.791785

G=-2472.837718

Ni	2.071418000	1.825747000	0.348066000
Ni	1.452755000	0.227164000	2.175922000
Ni	0.990194000	-2.002784000	1.150270000
Ni	1.321372000	-1.818266000	-1.325784000
Ni	1.972493000	0.556215000	-1.813972000
Ni	0.110069000	2.073392000	-1.108359000
Ni	-0.242508000	1.858510000	1.317019000
Ni	-0.844584000	-0.514239000	1.778965000
Ni	-0.995657000	-1.781578000	-0.357812000
Ni	-0.370297000	-0.248020000	-2.176224000
Ni	-1.738356000	0.606675000	-0.267357000

Ni	0.525535000	0.044492000	-0.040443000
Ni	2.768483000	-0.568987000	0.276205000
C	-3.806524000	0.264169000	-1.152720000
C	-4.662778000	-0.596940000	0.989473000
C	-5.159373000	0.841381000	0.813357000
C	-5.054690000	1.066579000	-0.712825000
H	-2.979580000	0.987540000	-1.516444000
H	-3.961261000	-0.376226000	-2.035668000
H	-5.413060000	-1.318736000	0.611300000
H	-4.410820000	-0.873877000	2.026339000
H	-6.175992000	1.008661000	1.202409000
H	-4.476080000	1.532281000	1.342750000
H	-5.948928000	0.651214000	-1.209620000
H	-4.994394000	2.133273000	-0.982857000
C	-3.434633000	-0.670923000	0.050804000
O	-2.913273000	-1.894233000	-0.217155000
H	-2.612615000	-0.029324000	0.940626000
H	0.401200000	-1.219585000	2.648010000

c. IM1

E+ZPE=-2472.789316

G=-2472.837212

Ni	2.521497000	1.374801000	0.457590000
Ni	2.009143000	-0.697368000	1.770037000
Ni	0.865920000	-2.324955000	0.259315000
Ni	0.659190000	-1.286315000	-2.010772000

Ni	1.669559000	1.007179000	-1.873943000
Ni	0.379602000	2.367710000	-0.216308000
Ni	0.547623000	1.322753000	2.005110000
Ni	-0.422000000	-0.965910000	1.830469000
Ni	-1.317000000	-1.334572000	-0.463571000
Ni	-0.810061000	0.673726000	-1.788557000
Ni	-1.498015000	0.925865000	0.603254000
Ni	0.587307000	0.055368000	-0.022729000
Ni	2.661791000	-0.891225000	-0.577581000
C	-4.387233000	0.434667000	-1.081621000
C	-5.199395000	-0.850879000	0.782774000
C	-5.979605000	0.486267000	0.808129000
C	-5.384502000	1.354302000	-0.353813000
H	-3.540805000	0.971207000	-1.555389000
H	-4.888000000	-0.170741000	-1.861552000
H	-5.741399000	-1.615972000	0.194523000
H	-5.010846000	-1.273667000	1.783848000
H	-7.062901000	0.324354000	0.687139000
H	-5.844517000	1.000318000	1.775020000
H	-6.163883000	1.749700000	-1.025154000
H	-4.850233000	2.225911000	0.064827000
C	-3.894770000	-0.526186000	0.020780000
O	-3.164493000	-1.631671000	-0.401797000
H	-3.278612000	0.118677000	0.759438000
H	0.842632000	-2.023034000	2.109393000

d. IM2

E+ZPE=-2472.789780

G=-2472.837783

Ni	-2.604223000	1.319424000	-0.113158000
Ni	-2.649939000	-1.176898000	0.099095000
Ni	-0.653385000	-1.893418000	1.417389000
Ni	0.652297000	0.148766000	2.045548000
Ni	-0.550294000	2.128844000	1.080093000
Ni	-0.606858000	1.911785000	-1.412654000
Ni	-1.853169000	-0.117963000	-2.027806000
Ni	-0.664156000	-2.062229000	-1.019990000
Ni	1.406122000	-1.285042000	0.127144000
Ni	1.471416000	1.166082000	-0.040505000
Ni	0.657331000	-0.174455000	-1.986745000
Ni	-0.581554000	0.050048000	-0.010425000
Ni	-1.838761000	0.174537000	1.967703000
C	3.805862000	0.852860000	-0.157981000
C	5.565530000	-0.851850000	-0.379907000
C	6.012594000	0.272036000	0.575011000
C	5.188643000	1.483111000	0.097256000
H	3.207190000	1.448977000	-0.906520000
H	3.262112000	0.785454000	0.821887000
H	5.738946000	-1.866465000	0.014484000
H	6.119098000	-0.765057000	-1.332944000
H	5.729458000	0.023973000	1.615210000

H	7.100144000	0.452501000	0.561625000
H	5.154321000	2.311528000	0.824642000
H	5.613033000	1.881240000	-0.843265000
C	4.041472000	-0.622895000	-0.638481000
O	3.242951000	-1.574067000	0.031702000
H	3.838605000	-0.669269000	-1.734272000
H	-0.566276000	-3.115352000	0.230845000

e. TS2

E+ZPE=-2472.752983

G=-2472.802588

Ni	-2.892752000	0.031029000	-0.827654000
Ni	-1.714508000	-2.096019000	-0.223165000
Ni	-0.135205000	-1.617805000	1.651701000
Ni	-0.318300000	0.809568000	2.238419000
Ni	-2.011474000	1.825348000	0.689228000
Ni	-1.199209000	1.598167000	-1.667348000
Ni	-0.979162000	-0.787123000	-2.228535000
Ni	0.673381000	-1.779121000	-0.649162000
Ni	1.597087000	-0.003794000	0.834035000
Ni	0.444823000	2.096248000	0.283957000
Ni	1.058843000	0.517546000	-1.553830000
Ni	-0.645357000	0.050418000	-0.013969000
Ni	-2.313351000	-0.510419000	1.538453000
C	4.408932000	1.088550000	-0.223418000
C	5.499481000	-1.105740000	-0.483661000

C	6.407594000	-0.182876000	0.347359000
C	5.946126000	1.220490000	-0.093611000
H	3.988800000	1.697918000	-1.043617000
H	3.890288000	1.406657000	0.700480000
H	5.454859000	-2.148339000	-0.128755000
H	5.853317000	-1.121109000	-1.532288000
H	6.204543000	-0.327083000	1.424830000
H	7.483905000	-0.358360000	0.184453000
H	6.252867000	2.019792000	0.601375000
H	6.391606000	1.455654000	-1.077745000
C	4.106779000	-0.432223000	-0.421114000
O	3.342019000	-0.963908000	0.668105000
H	3.531303000	-0.600187000	-1.361524000
H	2.184024000	-1.596130000	0.114994000

f. CPOL

E+ZPE=-2472.764041

G=-2472.812995

Ni	2.981814000	0.395503000	0.473193000
Ni	1.789724000	-1.668653000	1.245273000
Ni	0.032415000	-2.239985000	-0.435073000
Ni	0.116233000	-0.542026000	-2.273473000
Ni	1.929673000	1.093815000	-1.695335000
Ni	1.347460000	2.227968000	0.458601000
Ni	1.223691000	0.552529000	2.255917000
Ni	-0.552562000	-1.081579000	1.636044000

Ni	-1.643467000	-0.378915000	-0.490238000
Ni	-0.481854000	1.633675000	-1.290370000
Ni	-0.891703000	1.347159000	1.158451000
Ni	0.667806000	0.048093000	-0.014522000
Ni	2.191524000	-1.334023000	-1.142781000
C	-4.478349000	1.113274000	0.282652000
C	-5.772286000	-0.920304000	0.673274000
C	-6.464612000	-0.144120000	-0.461586000
C	-5.913093000	1.290213000	-0.295218000
H	-4.310091000	1.737623000	1.176017000
H	-3.675443000	1.376280000	-0.432524000
H	-5.813575000	-2.018057000	0.571309000
H	-6.224943000	-0.659941000	1.647782000
H	-6.153759000	-0.563575000	-1.434444000
H	-7.563986000	-0.193096000	-0.412542000
H	-5.919712000	1.857114000	-1.239984000
H	-6.539620000	1.849183000	0.421005000
C	-4.339226000	-0.377029000	0.650951000
O	-3.583563000	-1.019299000	-0.446697000
H	-3.767171000	-0.541789000	1.581937000
H	-3.458962000	-1.961300000	-0.204649000

6. CPO to CPOL on neutral Ni cluster (path b)
    a. Ni + CPO+2H

       E+ZPE=-2472.828914

       G=-2472.873489

Ni	-1.792377000	1.991221000	0.375458000
Ni	-2.487982000	0.197911000	-1.230834000
Ni	-1.661034000	-1.996962000	-0.370391000
Ni	-0.447033000	-1.593292000	1.783515000
Ni	-0.518119000	0.876114000	2.227223000
Ni	0.661949000	2.071779000	0.370904000
Ni	-0.507395000	1.638982000	-1.750337000
Ni	-0.459135000	-0.819412000	-2.144626000
Ni	0.841702000	-1.939925000	-0.343587000
Ni	1.521937000	-0.213377000	1.267984000
Ni	1.546416000	0.312588000	-1.176565000
Ni	-0.442322000	0.048351000	0.034804000
Ni	-2.472372000	-0.275362000	1.167052000
C	3.725032000	-0.292674000	1.204282000
C	3.743301000	0.034074000	-1.268085000
C	4.834696000	0.892821000	-0.592336000
C	4.365475000	1.061922000	0.866500000
H	3.048783000	-0.211006000	2.144661000
H	4.456371000	-1.061736000	1.514034000
H	4.117880000	-0.662684000	-2.033992000
H	3.057212000	0.760065000	-1.876666000
H	5.783173000	0.327053000	-0.612109000
H	5.009904000	1.855914000	-1.098307000
H	5.181509000	1.342069000	1.551362000
H	3.582086000	1.840755000	0.921453000

C	3.063576000	-0.750960000	-0.122832000
O	2.756860000	-2.053913000	-0.298128000
H	0.531936000	0.514690000	-2.637918000
H	-1.174824000	-2.306106000	-1.909492000

b. TS1

E+ZPE=-2472.766882

G=-2472.811192

Ni	1.738385000	-2.022772000	0.390399000
Ni	2.555771000	-0.205961000	-1.129942000
Ni	1.731843000	1.984810000	-0.256553000
Ni	0.397893000	1.555118000	1.820046000
Ni	0.392807000	-0.925598000	2.202058000
Ni	-0.713277000	-2.047380000	0.256162000
Ni	0.575017000	-1.588726000	-1.789444000
Ni	0.599938000	0.879708000	-2.121105000
Ni	-0.769485000	1.984082000	-0.360992000
Ni	-1.570327000	0.232439000	1.166478000
Ni	-1.477545000	-0.229089000	-1.288453000
Ni	0.450160000	-0.041645000	0.030895000
Ni	2.424243000	0.207225000	1.275474000
C	-3.763737000	0.458768000	1.162425000
C	-3.772247000	-0.199512000	-1.231614000
C	-4.736479000	-1.116636000	-0.437488000
C	-4.352314000	-0.960076000	1.053131000
H	-3.086365000	0.564646000	2.096649000

H	-4.518898000	1.249196000	1.333526000
H	-4.292972000	0.449630000	-1.955211000
H	-3.073542000	-0.836741000	-1.890030000
H	-5.767694000	-0.758084000	-0.596685000
H	-4.702349000	-2.167738000	-0.765450000
H	-5.205211000	-1.124680000	1.731163000
H	-3.561440000	-1.686495000	1.317067000
C	-3.059947000	0.677285000	-0.183822000
O	-2.830512000	2.018209000	-0.585258000
H	-0.558484000	-0.587818000	-2.695890000
H	-1.872447000	1.691565000	-1.529547000

c. IM1

E+ZPE=-2472.784056

G=-2472.828451

Ni	1.794608000	-1.964486000	0.484408000
Ni	2.470940000	-0.301033000	-1.263278000
Ni	1.682978000	1.958792000	-0.547616000
Ni	0.513075000	1.727563000	1.654768000
Ni	0.571865000	-0.703667000	2.276270000
Ni	-0.659690000	-2.019079000	0.538137000
Ni	0.466094000	-1.755788000	-1.633659000
Ni	0.432106000	0.668505000	-2.205796000
Ni	-0.818807000	1.932406000	-0.464991000
Ni	-1.478980000	0.333306000	1.283513000
Ni	-1.562814000	-0.366778000	-1.113747000

Ni	0.455644000	-0.037108000	0.030408000
Ni	2.512620000	0.346309000	1.093205000
C	-3.741678000	0.314390000	1.206077000
C	-3.782146000	-0.121057000	-1.228397000
C	-4.715198000	-1.121978000	-0.501172000
C	-4.262777000	-1.115370000	0.976691000
H	-3.097858000	0.378081000	2.157702000
H	-4.549439000	1.047586000	1.391211000
H	-4.338427000	0.584700000	-1.873397000
H	-3.101966000	-0.650652000	-1.999612000
H	-5.753765000	-0.756765000	-0.575477000
H	-4.685784000	-2.129979000	-0.943821000
H	-5.067231000	-1.395962000	1.674805000
H	-3.419333000	-1.817821000	1.117666000
C	-3.030708000	0.642312000	-0.114454000
O	-2.940786000	2.101388000	-0.354345000
H	-0.696112000	-0.846856000	-2.543446000
H	-3.198674000	2.256375000	-1.288727000

d. IM2

E+ZPE=-2472.768054

G=-2472.814057

Ni	-2.030948000	1.899766000	0.002096000
Ni	-1.867326000	0.329289000	-1.943267000
Ni	-1.322151000	-1.947901000	-1.074292000
Ni	-1.146186000	-1.820027000	1.421386000

Ni	-1.568341000	0.565822000	2.075856000
Ni	0.190410000	2.017064000	1.041946000
Ni	0.043275000	1.855784000	-1.409503000
Ni	0.423654000	-0.527162000	-2.026992000
Ni	0.932137000	-1.863782000	0.011489000
Ni	0.757025000	-0.353752000	1.946591000
Ni	1.758739000	0.500872000	-0.175858000
Ni	-0.528181000	0.030637000	0.035120000
Ni	-2.817990000	-0.462690000	0.164564000
C	4.136171000	-0.364230000	1.170575000
C	4.463681000	-0.118503000	-1.201649000
C	5.179322000	1.087763000	-0.549640000
C	4.953582000	0.934687000	0.990946000
H	3.443674000	-0.329648000	2.033440000
H	4.808091000	-1.237035000	1.320750000
H	5.178446000	-0.960436000	-1.336325000
H	4.028400000	0.113104000	-2.188937000
H	6.248702000	1.110891000	-0.815230000
H	4.727460000	2.028394000	-0.902802000
H	5.901873000	0.896569000	1.551407000
H	4.378460000	1.794383000	1.373002000
C	3.414256000	-0.519252000	-0.166453000
O	3.004687000	-1.946702000	-0.333226000
H	2.354176000	1.854680000	-0.465519000
H	2.935848000	-2.089850000	-1.302489000

e. TS2

E+ZPE=-2472.748401

G=-2472.794421

Ni	2.054586000	-1.851547000	-0.424579000
Ni	1.979812000	0.171767000	-1.900450000
Ni	1.391956000	2.151129000	-0.495290000
Ni	1.100102000	1.381730000	1.870833000
Ni	1.494256000	-1.096682000	1.901382000
Ni	-0.212652000	-2.210501000	0.447391000
Ni	0.048288000	-1.420035000	-1.868728000
Ni	-0.305841000	1.045551000	-1.862461000
Ni	-0.910426000	1.812660000	0.428131000
Ni	-0.823697000	-0.149744000	1.910284000
Ni	-1.724342000	-0.413126000	-0.404477000
Ni	0.549609000	-0.038776000	0.024832000
Ni	2.830295000	0.379021000	0.381585000
C	-4.054201000	-0.014866000	1.178587000
C	-4.871419000	0.478274000	-1.017207000
C	-5.568975000	-0.836602000	-0.604368000
C	-5.053975000	-1.143468000	0.840637000
H	-3.232185000	-0.349768000	1.842848000
H	-4.558219000	0.837707000	1.675297000
H	-5.465684000	1.354330000	-0.693316000
H	-4.697695000	0.565174000	-2.103064000
H	-6.664896000	-0.741131000	-0.650719000

H	-5.286639000	-1.652253000	-1.291272000
H	-5.872061000	-1.187699000	1.576536000
H	-4.539944000	-2.119239000	0.864429000
C	-3.568486000	0.469283000	-0.192873000
O	-3.032823000	1.846772000	-0.085878000
H	-3.064625000	-0.654818000	-0.987749000
H	-2.867639000	2.137309000	-1.011320000

f. CPOL

E+ZPE=-2472.764041

G=-2472.812995

Ni	2.981814000	0.395503000	0.473193000
Ni	1.789724000	-1.668653000	1.245273000
Ni	0.032415000	-2.239985000	-0.435073000
Ni	0.116233000	-0.542026000	-2.273473000
Ni	1.929673000	1.093815000	-1.695335000
Ni	1.347460000	2.227968000	0.458601000
Ni	1.223691000	0.552529000	2.255917000
Ni	-0.552562000	-1.081579000	1.636044000
Ni	-1.643467000	-0.378915000	-0.490238000
Ni	-0.481854000	1.633675000	-1.290370000
Ni	-0.891703000	1.347159000	1.158451000
Ni	0.667806000	0.048093000	-0.014522000
Ni	2.191524000	-1.334023000	-1.142781000
C	-4.478349000	1.113274000	0.282652000
C	-5.772286000	-0.920304000	0.673274000

C	-6.464612000	-0.144120000	-0.461586000
C	-5.913093000	1.290213000	-0.295218000
H	-4.310091000	1.737623000	1.176017000
H	-3.675443000	1.376280000	-0.432524000
H	-5.813575000	-2.018057000	0.571309000
H	-6.224943000	-0.659941000	1.647782000
H	-6.153759000	-0.563575000	-1.434444000
H	-7.563986000	-0.193096000	-0.412542000
H	-5.919712000	1.857114000	-1.239984000
H	-6.539620000	1.849183000	0.421005000
C	-4.339226000	-0.377029000	0.650951000
O	-3.583563000	-1.019299000	-0.446697000
H	-3.767171000	-0.541789000	1.581937000
H	-3.458962000	-1.961300000	-0.204649000

7. CPO to CPOL on charged (-1) Ni cluster (path a)
   a. Ni + CPO+2H

      E+ZPE=-2472.923643

      G=-2472.969288

Ni	2.797154000	-0.678930000	-0.180844000
Ni	2.141102000	1.267033000	1.206956000
Ni	-0.173190000	0.872588000	2.148385000
Ni	-0.975008000	-1.450869000	1.229902000
Ni	0.908798000	-2.323684000	-0.178475000
Ni	1.205899000	-0.757030000	-2.035805000
Ni	1.964170000	1.418483000	-1.238209000

Ni	0.142676000	2.342851000	0.148999000
Ni	-1.737638000	0.694722000	0.149958000
Ni	-1.066492000	-1.229020000	-1.247459000
Ni	-0.406883000	1.079184000	-1.886474000
Ni	0.505461000	0.012604000	0.086748000
Ni	1.537277000	-1.090830000	1.920888000
C	-3.773917000	1.111317000	-0.551003000
C	-4.167112000	-1.117500000	0.500355000
C	-5.400728000	-0.214139000	0.705973000
C	-4.852488000	1.221311000	0.549587000
H	-2.920514000	1.889471000	-0.354409000
H	-4.104743000	1.398358000	-1.563622000
H	-4.409379000	-2.122527000	0.117960000
H	-3.606967000	-1.240081000	1.447440000
H	-6.138420000	-0.415517000	-0.092248000
H	-5.907269000	-0.373018000	1.672598000
H	-5.637595000	1.954523000	0.301531000
H	-4.376273000	1.547419000	1.491382000
C	-3.311680000	-0.359486000	-0.535718000
O	-2.936068000	-0.995258000	-1.648452000
H	-0.376463000	-2.915981000	0.724024000
H	-1.611390000	-0.008483000	1.939815000

b. TS1

E+ZPE=-2472.890367

G=-2472.935441

Ni	2.820951000	-0.643892000	-0.340073000
Ni	2.208905000	1.079424000	1.332777000
Ni	-0.083242000	0.554177000	2.264542000
Ni	-0.918497000	-1.610071000	1.037377000
Ni	0.925165000	-2.268874000	-0.530637000
Ni	1.184081000	-0.447954000	-2.145674000
Ni	1.972144000	1.586652000	-1.058809000
Ni	0.190187000	2.300373000	0.493953000
Ni	-1.697657000	0.675525000	0.301922000
Ni	-1.070299000	-1.029546000	-1.377935000
Ni	-0.416059000	1.347568000	-1.690023000
Ni	0.539529000	0.002574000	0.083372000
Ni	1.611535000	-1.356650000	1.710083000
C	-3.832888000	1.049601000	-0.418167000
C	-4.679377000	-1.085421000	0.542286000
C	-5.832168000	-0.086289000	0.332165000
C	-5.122515000	1.279957000	0.390513000
H	-3.042658000	1.839840000	-0.145753000
H	-3.981559000	1.179644000	-1.503311000
H	-4.865799000	-2.089723000	0.129905000
H	-4.471050000	-1.196546000	1.621332000
H	-6.282721000	-0.227729000	-0.667268000
H	-6.637594000	-0.189847000	1.077682000
H	-5.729878000	2.108784000	-0.008935000
H	-4.865773000	1.525444000	1.437376000

C	-3.450923000	-0.457641000	-0.192966000
O	-2.991614000	-1.148113000	-1.270344000
H	0.398560000	-2.656874000	1.164373000
H	-2.550218000	-0.609903000	0.869840000

c. IM1

E+ZPE=-2472.892005

G=-2472.939916

Ni	2.755282000	-0.566996000	-0.812259000
Ni	2.460126000	1.116234000	0.982905000
Ni	0.429023000	0.510571000	2.362919000
Ni	-0.585260000	-1.663561000	1.297955000
Ni	0.906571000	-2.246624000	-0.632564000
Ni	0.772027000	-0.399015000	-2.232325000
Ni	1.714368000	1.645198000	-1.296768000
Ni	0.277992000	2.285266000	0.606795000
Ni	-1.563159000	0.604946000	0.783166000
Ni	-1.255167000	-1.057767000	-1.021565000
Ni	-0.745606000	1.341332000	-1.419530000
Ni	0.596293000	0.003988000	0.090342000
Ni	2.021619000	-1.341404000	1.431774000
C	-4.384661000	0.834342000	-0.872307000
C	-5.120109000	-1.108689000	0.356461000
C	-5.939229000	0.094315000	0.892178000
C	-5.316709000	1.368183000	0.227058000
H	-3.559738000	1.525603000	-1.132374000

H	-4.941804000	0.593597000	-1.798994000
H	-5.662730000	-1.632510000	-0.453074000
H	-4.874144000	-1.858200000	1.127522000
H	-7.006505000	-0.008926000	0.637145000
H	-5.883655000	0.163575000	1.991486000
H	-6.082907000	2.063094000	-0.152987000
H	-4.714710000	1.922860000	0.970357000
C	-3.849951000	-0.486964000	-0.273554000
O	-3.133405000	-1.322491000	-1.108281000
H	0.722580000	-2.722579000	1.087562000
H	-3.220252000	-0.174401000	0.666883000

d. IM2

E+ZPE=-2472.891813

G=-2472.940473

Ni	-2.752375000	0.569988000	-0.824983000
Ni	-2.470266000	-1.123132000	0.963101000
Ni	-0.450364000	-0.523184000	2.362658000
Ni	0.571216000	1.655786000	1.319304000
Ni	-0.908455000	2.249476000	-0.621789000
Ni	-0.756248000	0.411316000	-2.230344000
Ni	-1.706417000	-1.638790000	-1.313622000
Ni	-0.284611000	-2.288440000	0.597675000
Ni	1.554929000	-0.608846000	0.797279000
Ni	1.259451000	1.065455000	-1.000091000
Ni	0.754008000	-1.332741000	-1.415007000

Ni	-0.600266000	-0.005137000	0.091209000
Ni	-2.037214000	1.332326000	1.429087000
C	4.383256000	-0.824246000	-0.883213000
C	5.140739000	1.094690000	0.367671000
C	5.966655000	-0.117978000	0.869780000
C	5.335931000	-1.379062000	0.187878000
H	3.551702000	-1.508842000	-1.141502000
H	4.921851000	-0.567680000	-1.816556000
H	5.671484000	1.631131000	-0.441541000
H	4.909406000	1.831668000	1.155206000
H	7.030886000	-0.009447000	0.604317000
H	5.924405000	-0.208504000	1.968161000
H	6.097489000	-2.062611000	-0.221032000
H	4.749968000	-1.952572000	0.929504000
C	3.859761000	0.485012000	-0.251071000
O	3.132390000	1.338930000	-1.060232000
H	-0.130212000	3.036721000	0.687746000
H	3.240985000	0.154038000	0.685961000

e. TS2

E+ZPE=-2472.851883

G=-2472.899198

Ni	2.672731000	-0.594436000	-1.054575000
Ni	2.644417000	0.668931000	1.077626000
Ni	0.611143000	-0.013762000	2.419928000
Ni	-0.688670000	-1.777798000	0.977463000

Ni	0.653365000	-2.069746000	-1.127629000
Ni	0.668184000	0.089968000	-2.275251000
Ni	1.876810000	1.766639000	-0.981389000
Ni	0.600130000	2.112881000	1.098361000
Ni	-1.416903000	0.637802000	1.031794000
Ni	-1.372654000	-0.604785000	-1.114396000
Ni	-0.604661000	1.755357000	-1.011257000
Ni	0.630958000	-0.016703000	0.086920000
Ni	1.942464000	-1.767609000	1.010301000
C	-4.475430000	0.726456000	-0.920455000
C	-5.351865000	-1.028398000	0.505638000
C	-6.289489000	0.205107000	0.648188000
C	-5.544463000	1.392348000	-0.041146000
H	-3.613289000	1.373410000	-1.171477000
H	-4.911146000	0.344844000	-1.864417000
H	-5.754541000	-1.750427000	-0.227741000
H	-5.197913000	-1.575341000	1.451366000
H	-7.257497000	0.013664000	0.156736000
H	-6.512535000	0.435879000	1.702816000
H	-6.225373000	2.051666000	-0.603145000
H	-5.045339000	2.017224000	0.722540000
C	-4.029327000	-0.465882000	-0.058303000
O	-3.223815000	-1.419388000	-0.722811000
H	-2.196053000	-1.724672000	0.137556000
H	-3.437106000	-0.037590000	0.813629000

f. CPOL

E+ZPE=-2472.856557

G=-2472.905324

Ni	-2.499908000	0.804853000	-1.265029000
Ni	-2.837811000	-0.626028000	0.730382000
Ni	-0.984807000	-0.181158000	2.393946000
Ni	0.593158000	1.610023000	1.306975000
Ni	-0.419466000	2.154097000	-0.928781000
Ni	-0.378010000	0.098021000	-2.255219000
Ni	-1.841208000	-1.598475000	-1.293095000
Ni	-0.891427000	-2.191258000	0.907506000
Ni	1.185128000	-0.841636000	1.240009000
Ni	1.508303000	0.570832000	-0.763821000
Ni	0.616681000	-1.738528000	-0.980496000
Ni	-0.672518000	0.012229000	0.088343000
Ni	-2.012965000	1.759861000	0.976548000
C	4.557835000	-0.804396000	-0.765151000
C	5.690480000	1.038435000	0.312084000
C	6.459196000	-0.231319000	0.731465000
C	5.853878000	-1.383224000	-0.135620000
H	3.681770000	-1.478408000	-0.722617000
H	4.715566000	-0.531350000	-1.824625000
H	6.104184000	1.460617000	-0.622488000
H	5.694649000	1.830585000	1.079092000
H	7.547518000	-0.125749000	0.601071000

H	6.282211000	-0.432112000	1.802391000
H	6.556439000	-1.710079000	-0.918582000
H	5.638005000	-2.268007000	0.485620000
C	4.294795000	0.482346000	0.021235000
O	3.440658000	1.372485000	-0.759117000
H	3.138837000	2.095556000	-0.159571000
H	3.754288000	0.248686000	0.965098000

8. CPO to CPOL on charged (-1) Ni cluster (path b)
   a. Ni + CPO+2H

      E+ZPE=-2472.936791

      G=-2472.981176

Ni	-2.534628000	-0.468215000	-1.114953000
Ni	-1.794569000	-1.823604000	0.823444000
Ni	-0.451414000	-0.362931000	2.390712000
Ni	-0.343851000	2.019050000	1.301713000
Ni	-1.652066000	1.856824000	-0.839505000
Ni	-0.495165000	0.240434000	-2.266022000
Ni	-0.576037000	-1.999682000	-1.301243000
Ni	0.707795000	-1.912267000	0.804869000
Ni	1.589203000	0.409762000	1.081628000
Ni	0.844875000	1.744715000	-0.867540000
Ni	1.489093000	-0.643337000	-1.152658000
Ni	-0.490813000	-0.007271000	0.087842000
Ni	-2.540112000	0.580203000	1.137741000
C	3.706211000	-0.492968000	-1.179801000

C	3.777081000	0.728746000	0.991974000
C	4.887701000	-0.341285000	0.929005000
C	4.396832000	-1.362146000	-0.117015000
H	3.012722000	-1.139792000	-1.854224000
H	4.409008000	-0.063845000	-1.918214000
H	4.135946000	1.750005000	1.193593000
H	3.109023000	0.482640000	1.918614000
H	5.814903000	0.139429000	0.568548000
H	5.108907000	-0.803037000	1.905282000
H	5.208506000	-1.986600000	-0.523552000
H	3.637638000	-2.028162000	0.336037000
C	3.062995000	0.670955000	-0.380421000
O	2.758471000	1.820842000	-1.021429000
H	-1.126878000	3.026858000	0.239516000
H	0.572812000	1.092906000	2.434571000

b. TS1

E+ZPE=-2472.867411

G=-2472.912192

Ni	-2.476017000	-0.605269000	-1.173761000
Ni	-1.727718000	-1.872274000	0.820749000
Ni	-0.524612000	-0.302368000	2.396801000
Ni	-0.515606000	2.057480000	1.253585000
Ni	-1.737159000	1.772376000	-0.925001000
Ni	-0.441212000	0.193835000	-2.272757000
Ni	-0.429203000	-2.023605000	-1.258343000

Ni	0.774296000	-1.816801000	0.887861000
Ni	1.510486000	0.560907000	1.135777000
Ni	0.761762000	1.803811000	-0.867962000
Ni	1.552090000	-0.552369000	-1.070579000
Ni	-0.504569000	-0.001232000	0.085205000
Ni	-2.619416000	0.491160000	1.051207000
C	3.761393000	-0.359066000	-1.242969000
C	3.796611000	0.591378000	1.054218000
C	4.810041000	-0.577141000	0.951012000
C	4.396070000	-1.392438000	-0.295034000
H	3.071907000	-0.870464000	-2.019928000
H	4.493615000	0.170752000	-1.881813000
H	4.280607000	1.563868000	1.243217000
H	3.113618000	0.429336000	1.968928000
H	5.816338000	-0.150296000	0.797784000
H	4.853239000	-1.197712000	1.860708000
H	5.240851000	-1.934781000	-0.750103000
H	3.618794000	-2.130154000	-0.020810000
C	3.060389000	0.634083000	-0.303491000
O	2.835097000	1.937088000	-0.816343000
H	1.921318000	2.325289000	0.121302000
H	0.514449000	1.158335000	2.471173000

c. IM1

E+ZPE=-2472.881800

G=-2472.926366

Ni	-2.520226000	-0.469877000	-1.166326000
Ni	-1.777731000	-1.874580000	0.735994000
Ni	-0.496816000	-0.438222000	2.376727000
Ni	-0.432115000	1.983327000	1.372844000
Ni	-1.700849000	1.864898000	-0.794212000
Ni	-0.480632000	0.328724000	-2.256768000
Ni	-0.522005000	-1.943787000	-1.373524000
Ni	0.725552000	-1.901025000	0.757006000
Ni	1.542295000	0.433952000	1.128302000
Ni	0.798433000	1.815155000	-0.784598000
Ni	1.508692000	-0.548518000	-1.139428000
Ni	-0.508233000	-0.002557000	0.086673000
Ni	-2.588581000	0.497801000	1.121075000
C	3.723314000	-0.380179000	-1.221557000
C	3.827393000	0.542841000	1.077867000
C	4.853816000	-0.609606000	0.916039000
C	4.371297000	-1.426759000	-0.298895000
H	3.045002000	-0.888017000	-2.010945000
H	4.456989000	0.170477000	-1.840162000
H	4.314285000	1.511286000	1.288506000
H	3.170808000	0.348363000	1.997453000
H	5.842318000	-0.168679000	0.700013000
H	4.957185000	-1.222954000	1.825579000
H	5.181724000	-1.988682000	-0.790769000
H	3.588514000	-2.144050000	0.012211000

C	3.032023000	0.593538000	-0.251259000
O	2.956604000	1.954123000	-0.839873000
H	2.996835000	2.578167000	-0.082136000
H	0.608511000	0.983962000	2.500641000

d. IM2

E+ZPE=-2472.869646

G=-2472.915509

Ni	-2.837679000	0.280251000	-0.560853000
Ni	-2.087361000	-1.571080000	0.906514000
Ni	-0.063402000	-0.816431000	2.224143000
Ni	0.459015000	1.639633000	1.466876000
Ni	-1.295770000	2.222967000	-0.235510000
Ni	-1.001877000	0.693385000	-2.122892000
Ni	-1.488699000	-1.605830000	-1.475089000
Ni	0.214253000	-2.250213000	0.192437000
Ni	1.752020000	-0.313406000	0.514881000
Ni	0.990576000	1.526869000	-0.964275000
Ni	0.859935000	-0.841000000	-1.716004000
Ni	-0.535172000	-0.007556000	0.084177000
Ni	-2.031324000	0.829001000	1.724340000
C	4.095738000	-0.208770000	-1.213894000
C	4.488963000	0.640272000	0.980431000
C	5.103634000	-0.785828000	0.957448000
C	4.720161000	-1.383453000	-0.437125000
H	3.400412000	-0.530265000	-2.014305000

H	4.887830000	0.417326000	-1.685470000
H	5.257090000	1.392727000	0.687729000
H	4.099379000	0.930833000	1.971328000
H	6.196029000	-0.749813000	1.102647000
H	4.688999000	-1.405902000	1.769837000
H	5.580489000	-1.832946000	-0.960386000
H	3.950795000	-2.167344000	-0.309573000
C	3.403535000	0.574986000	-0.100608000
O	3.068330000	1.941949000	-0.625101000
H	2.825522000	2.461773000	0.175072000
H	1.528209000	-1.099702000	2.061509000

e. TS2

E+ZPE=-2472.843826

G=-2472.889929

Ni	-2.873121000	0.098833000	-0.606354000
Ni	-2.079205000	-1.426756000	1.178511000
Ni	-0.090920000	-0.379311000	2.340772000
Ni	0.362558000	1.911367000	1.146511000
Ni	-1.394336000	2.116283000	-0.639112000
Ni	-1.037377000	0.276165000	-2.212308000
Ni	-1.459040000	-1.879327000	-1.154366000
Ni	0.248215000	-2.152078000	0.608083000
Ni	1.723361000	-0.140977000	0.573911000
Ni	0.918378000	1.370687000	-1.221114000
Ni	0.866987000	-1.097501000	-1.524939000

Ni	-0.568554000	0.007505000	0.087197000
Ni	-2.103852000	1.083249000	1.541402000
C	4.065765000	-0.535012000	-1.059101000
C	4.895047000	0.877864000	0.680494000
C	5.579410000	-0.491555000	0.899933000
C	5.030819000	-1.416132000	-0.238109000
H	3.238374000	-1.111684000	-1.522559000
H	4.599779000	-0.002858000	-1.872345000
H	5.496005000	1.510268000	-0.001040000
H	4.727404000	1.443750000	1.612544000
H	6.676607000	-0.399945000	0.875884000
H	5.311319000	-0.901992000	1.888140000
H	5.834096000	-1.833014000	-0.865746000
H	4.476123000	-2.266284000	0.195134000
C	3.585914000	0.514102000	-0.050142000
O	3.060232000	1.698974000	-0.765886000
H	2.770003000	2.323831000	-0.057078000
H	3.080058000	-0.117420000	1.166335000

f. CPOL

E+ZPE=-2472.856557

G=-2472.905324

Ni	-2.499908000	0.804853000	-1.265029000
Ni	-2.837811000	-0.626028000	0.730382000
Ni	-0.984807000	-0.181158000	2.393946000
Ni	0.593158000	1.610023000	1.306975000

Ni	-0.419466000	2.154097000	-0.928781000
Ni	-0.378010000	0.098021000	-2.255219000
Ni	-1.841208000	-1.598475000	-1.293095000
Ni	-0.891427000	-2.191258000	0.907506000
Ni	1.185128000	-0.841636000	1.240009000
Ni	1.508303000	0.570832000	-0.763821000
Ni	0.616681000	-1.738528000	-0.980496000
Ni	-0.672518000	0.012229000	0.088343000
Ni	-2.012965000	1.759861000	0.976548000
C	4.557835000	-0.804396000	-0.765151000
C	5.690480000	1.038435000	0.312084000
C	6.459196000	-0.231319000	0.731465000
C	5.853878000	-1.383224000	-0.135620000
H	3.681770000	-1.478408000	-0.722617000
H	4.715566000	-0.531350000	-1.824625000
H	6.104184000	1.460617000	-0.622488000
H	5.694649000	1.830585000	1.079092000
H	7.547518000	-0.125749000	0.601071000
H	6.282211000	-0.432112000	1.802391000
H	6.556439000	-1.710079000	-0.918582000
H	5.638005000	-2.268007000	0.485620000
C	4.294795000	0.482346000	0.021235000
O	3.440658000	1.372485000	-0.759117000
H	3.138837000	2.095556000	-0.159571000
H	3.754288000	0.248686000	0.965098000

9. FAL to FOL on neutral relaxed Ni cluster (path a)

   a. Ni + FAL+2H

      E+ZPE= -2545.614129

      G= -2545.677402

Ni	1.386831000	-0.962963000	1.173483000
Ni	-0.874489000	-0.999639000	2.131340000
Ni	-2.650299000	-1.070397000	0.145581000
Ni	-1.132338000	-1.234024000	-1.966784000
Ni	1.236284000	-1.266760000	-1.270262000
Ni	1.636333000	1.389175000	-0.069900000
Ni	0.134992000	1.238200000	1.864528000
Ni	-2.228561000	1.037671000	1.338460000
Ni	-2.225132000	0.862153000	-1.260402000
Ni	0.135346000	0.872953000	-2.095371000
Ni	-0.578642000	2.425498000	-0.199102000
Ni	-0.459955000	-0.013744000	-0.035707000
Ni	-0.433238000	-2.365692000	0.206041000
C	3.120590000	-1.685944000	-0.802430000
C	3.123079000	-1.993445000	0.623274000
C	3.414192000	-0.773958000	1.324519000
C	3.581601000	0.234546000	0.306794000
O	3.639477000	-0.351598000	-0.946923000
H	3.531108000	-2.365004000	-1.563701000
H	3.142919000	-3.007764000	1.024511000
H	3.680693000	-0.643598000	2.375335000

C	3.533252000	1.673412000	0.403041000
H	3.741142000	2.118103000	1.396627000
O	3.347100000	2.423132000	-0.657595000
H	-0.970785000	2.257802000	-1.812993000
H	-0.173670000	2.792485000	1.351790000

b. TS1

E+ZPE= -2545.565194

G= -2545.629545

Ni	1.393277000	-1.099247000	1.011299000
Ni	-0.899897000	-1.212141000	2.015948000
Ni	-2.568423000	-1.169018000	0.025168000
Ni	-1.156854000	-0.954665000	-2.068485000
Ni	1.247408000	-1.088041000	-1.432115000
Ni	1.577595000	1.434236000	0.073955000
Ni	0.175390000	0.979887000	2.027796000
Ni	-2.163194000	0.837688000	1.446251000
Ni	-2.310528000	0.984020000	-1.096704000
Ni	0.075465000	1.231011000	-1.979111000
Ni	-0.680490000	2.372785000	0.137221000
Ni	-0.422406000	0.031734000	-0.061707000
Ni	-0.449352000	-2.323620000	-0.076493000
C	3.109624000	-1.679028000	-0.929707000
C	3.118899000	-2.084155000	0.469894000
C	3.422186000	-0.910121000	1.252587000
C	3.575560000	0.160339000	0.317033000

O	3.606322000	-0.320373000	-0.968652000
H	3.546386000	-2.287288000	-1.734264000
H	3.159746000	-3.123533000	0.800973000
H	3.655559000	-0.847684000	2.317143000
C	3.566438000	1.650944000	0.487381000
H	4.236994000	2.012967000	1.300433000
O	3.436693000	2.378250000	-0.619734000
H	-1.032653000	2.419127000	-1.566146000
H	2.429868000	1.845932000	1.361169000

c. IM1

E+ZPE= -2545.592108

G= -2545.657251

Ni	1.497630000	-0.814391000	1.108393000
Ni	-0.763126000	-0.819081000	2.247030000
Ni	-2.539678000	-1.193592000	0.377470000
Ni	-1.271979000	-1.381168000	-1.788246000
Ni	1.184115000	-1.220051000	-1.281402000
Ni	1.515988000	1.417729000	-0.312396000
Ni	0.232647000	1.385112000	1.768415000
Ni	-2.173496000	1.137201000	1.366225000
Ni	-2.427109000	0.696004000	-1.192033000
Ni	-0.120455000	0.788454000	-2.189698000
Ni	-0.744448000	2.331316000	-0.330827000
Ni	-0.459012000	0.019968000	-0.021336000
Ni	-0.386394000	-2.270148000	0.360610000

C	3.065701000	-1.737511000	-0.849971000
C	3.077852000	-1.985280000	0.589318000
C	3.589316000	-0.774203000	1.203540000
C	3.894585000	0.117198000	0.153968000
O	3.745946000	-0.488474000	-1.062222000
H	3.362439000	-2.488464000	-1.598089000
H	3.041042000	-2.983235000	1.031031000
H	3.848772000	-0.602553000	2.250308000
C	4.225013000	1.583040000	0.137473000
H	5.103477000	1.743147000	-0.527460000
O	3.130218000	2.370622000	-0.301590000
H	-1.273146000	2.031325000	-1.960459000
H	4.542158000	1.857301000	1.167466000

d. IM2

E+ZPE= -2545.593656

G= -2545.658277

Ni	1.562147000	-0.688721000	1.007277000
Ni	-0.752653000	-0.903619000	2.194857000
Ni	-2.448025000	-1.330439000	0.481651000
Ni	-1.260071000	-1.305361000	-1.825280000
Ni	1.192413000	-1.080514000	-1.395280000
Ni	1.455142000	1.537208000	-0.249124000
Ni	0.240114000	1.323131000	1.813666000
Ni	-2.188049000	0.977398000	1.353846000
Ni	-2.535886000	0.661324000	-1.066089000

Ni	-0.156741000	0.928962000	-2.160942000
Ni	-0.893120000	2.309765000	-0.283105000
Ni	-0.463056000	0.000468000	-0.008079000
Ni	-0.234696000	-2.293471000	0.180379000
C	3.048895000	-1.689948000	-0.917545000
C	3.033562000	-2.034957000	0.499924000
C	3.597870000	-0.906965000	1.209464000
C	3.921775000	0.054961000	0.227320000
O	3.776595000	-0.454276000	-1.031432000
H	3.329701000	-2.399840000	-1.711004000
H	2.901201000	-3.051041000	0.874265000
H	3.855479000	-0.830381000	2.267674000
C	4.223208000	1.523390000	0.314360000
H	5.156456000	1.737868000	-0.253059000
O	3.159483000	2.303038000	-0.199619000
H	-0.606866000	2.514449000	-1.939751000
H	4.433011000	1.748279000	1.383384000

e. TS2

E+ZPE= -2545.555410

G= -2545.620061

Ni	-1.045430000	-1.496577000	-1.091655000
Ni	1.455077000	-1.417265000	-1.632940000
Ni	2.699510000	-0.730748000	0.488588000
Ni	1.035774000	-0.453490000	2.227789000
Ni	-1.227007000	-1.139089000	1.300230000

Ni	-1.771648000	0.850910000	-0.537024000
Ni	0.065545000	0.524481000	-2.254000000
Ni	2.240302000	0.936297000	-1.303871000
Ni	1.922400000	1.574048000	1.178941000
Ni	-0.565100000	1.401233000	1.560576000
Ni	0.325988000	2.304945000	-0.514755000
Ni	0.475602000	-0.017276000	-0.011700000
Ni	0.753297000	-2.300857000	0.527930000
C	-2.977791000	-1.861596000	0.730215000
C	-2.956123000	-1.911606000	-0.735217000
C	-3.378208000	-0.589544000	-1.185341000
C	-3.671642000	0.174228000	-0.020981000
O	-3.639211000	-0.636094000	1.114500000
H	-3.305581000	-2.703910000	1.354137000
H	-3.106481000	-2.837080000	-1.307954000
H	-3.655575000	-0.313069000	-2.203045000
C	-4.167343000	1.587988000	0.159526000
H	-4.632538000	1.672731000	1.163313000
O	-3.069997000	2.495076000	-0.014135000
H	-1.974882000	2.065194000	0.827981000
H	-4.945308000	1.822291000	-0.593624000

f. FOL

E+ZPE= -2545.577764

G= -2545.642560

Ni	0.749962000	-1.645203000	1.133498000

Ni	-1.691897000	-1.197428000	1.612748000
Ni	-2.825117000	-0.422693000	-0.545551000
Ni	-0.923915000	-0.444160000	-2.315508000
Ni	1.123444000	-1.347975000	-1.206143000
Ni	1.758002000	0.572387000	0.657948000
Ni	-0.153062000	0.551632000	2.243704000
Ni	-2.244734000	1.261431000	1.167526000
Ni	-1.697438000	1.636868000	-1.208130000
Ni	0.789639000	1.189014000	-1.604855000
Ni	0.035327000	2.266814000	0.519897000
Ni	-0.489003000	0.051603000	-0.059981000
Ni	-1.085939000	-2.204086000	-0.463517000
C	2.913082000	-1.914075000	-0.627650000
C	2.726019000	-1.967350000	0.827751000
C	3.232105000	-0.685734000	1.334552000
C	3.678488000	0.069998000	0.200862000
O	3.694867000	-0.757172000	-0.943571000
H	3.229610000	-2.782277000	-1.224764000
H	2.780331000	-2.911786000	1.393210000
H	3.485761000	-0.476672000	2.376167000
C	4.544606000	1.290653000	0.137191000
H	5.499666000	1.069470000	-0.374014000
O	3.934566000	2.376787000	-0.592135000
H	2.959756000	2.286287000	-0.387067000
H	4.776075000	1.587371000	1.180064000