

## Supplementary Information

### Aqueous Furfural Hydrogenation on Ni/TiO<sub>2</sub> Catalysts: Nature of Support Phase Steers the Product Selectivity

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## 26 **1. EXPERIMENTAL SECTION:**

27 **1.1. Materials.** Nickel(II) acetate tetrahydrate ( $\text{Ni}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ )-98%, from Central Drug  
28 House (P) Ltd., Furfural ( $\text{C}_5\text{H}_4\text{O}_2$ )-99% and Tetrahydrofurfuryl alcohol ( $\text{C}_5\text{H}_{10}\text{O}_2$ )-99% from  
29 Sigma Aldrich, Furfuryl alcohol ( $\text{C}_5\text{H}_6\text{O}_2$ )-98% from Avra synthesis Pvt. Ltd.,  
30 Cyclopentanone ( $\text{C}_5\text{H}_8\text{O}$ )-99% from Spectrochem Pvt. Ltd., Cyclopentanol ( $\text{C}_5\text{H}_{10}\text{O}$ )-  
31 99% from Alfa Aesar, Hydrochloric acid (HCl, 37%) from Merck Life Science Pvt. Ltd.,  
32 Titanium(IV) iso-propoxide ( $\text{C}_{12}\text{H}_{28}\text{O}_4\text{Ti}$ )-98% from Spectrochem Pvt. Ltd., Anatase  $\text{TiO}_2$   
33 (99.7% trace metals basis) from Sigma Aldrich, Hombikat UV-100~99% from Sachtleben  
34 Chemie GmbH, Anatase-rutile mixed phases  $\text{TiO}_2$  (99.9% trace metals basis) from Sigma  
35 Aldrich, Degussa P25 (AEROXIDE  $\text{TiO}_2$ , 99.5% trace metals basis) from EVONIK  
36 industries, and deionized water from Merck were used without further purification.

## 37 **1.2. Preparation of Supports.**

38 Anatase and mixed phases supports were used as received. Rutile  $\text{TiO}_2$  supports were  
39 synthesized from titanium iso-propoxide using sol-gel and hydrothermal methods as  
40 described below<sup>1,2</sup>.

41 **1.2.1. Sol-gel method.** In a typical sol-gel synthesis procedure, 42 mL of titanium iso-  
42 propoxide was hydrolyzed by the addition of 72 mL of 2 mol  $\text{L}^{-1}$  aqueous solution of  
43 hydrochloric acid under vigorous stirring. The hydrosol formed was then stirred at room  
44 temperature for 7 days. The resulting mixture was washed with water and methanol, followed  
45 by drying at 110°C in air oven for 24 h. This was then followed by calcination in air at 450°C  
46 for 4 h, at a heating rate of 2 °C/min. The obtained product is labelled as RS.

47 **1.2.2. Hydrothermal method.** The sol-gel method process is followed till the hydrolysis step  
48 of hydrothermal procedure except that the stirring was restricted to 2 h till solution became

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

### 54 **1.3. Preparation of catalysts**

55 **1.3.1. Synthesis of catalysts.** All Ni/TiO<sub>2</sub> were prepared by wetness impregnation method. In  
56 brief, 0.64 g Ni(CH<sub>3</sub>COO)<sub>2</sub>·4H<sub>2</sub>O was dissolved in 30 mL of deionized water in a beaker.  
57 The temperature was raised to 60 °C. 2.85 g TiO<sub>2</sub> support was added under stirring and water  
58 was allowed to evaporate. The sample was further dried at 100°C for overnight. The sample  
59 was then calcined in static air at 450°C for 6 h, followed by reduction in H<sub>2</sub> flow at 450°C for  
60 6 h (ramp rate: 5 °C/min). It was cooled to room temperature in H<sub>2</sub> flow for further catalytic  
61 evaluation. The optimum nickel loading on all catalysts was 5 wt%. The prepared catalysts  
62 were designated as three letter abbreviation. For example, those catalysts prepared from  
63 anatase titania supports obtained from Aldrich and Hombikat are labelled as ATA and ATH,  
64 mixed phase titania supports obtained from Aldrich and EVONIK are labelled as ART and  
65 P25, and rutile titania supports synthesized from hydrothermal and sol-gel method are  
66 labelled as RTH and RTS, respectively.

67 **1.3.2 Synthesis of RTH catalyst by hydrazine reduction method.** 10 mL of ethanolic  
68 solution of Ni(CH<sub>3</sub>COO)<sub>2</sub>·4H<sub>2</sub>O was taken in a round flask attached with condenser. The  
69 temperature was raised to 80 °C. 5 ml 1M ethanolic NaOH solution was added under stirring,  
70 followed by 4 ml of hydrazine hydrate. 0.95 g TiO<sub>2</sub> support was added once the solution turns  
71 black. The sample was further stirred for 1h. The resultant catalyst is obtained after washing  
72 with water till pH is neutral. The nickel loading calculated from AAS shows 4.9 wt%.

#### 73 **1.4. Experimental procedure**

74 Catalytic hydrogenation was carried out in 100 mL stainless steel autoclave batch reactor  
75 (Parr Instrument Company 4565). In a typical run, the autoclave was loaded with 5.2 mmol  
76 furfural in 50 mL water, and 100 mg catalyst. Before the reaction, the reactor was flushed and  
77 pressurized with hydrogen. The reactor was heated to the desired reaction temperature and  
78 then the reaction was initiated by switching on the stirrer at 500 rpm. The reaction was  
79 quenched after desired time by cooling reactor in a water-ice bath. The reaction solution was  
80 filtered and solid catalyst was separated to analyse products on Chemito GC 1000 gas  
81 chromatograph equipped with a Agilent HP-FFAP-19091F-413 capillary column (30 m x  
82 0.32 mm) and a flame ionization detector.

#### 83 **1.5. Characterization of catalysts**

84 Powder X-ray Diffraction (PXRD) patterns of samples were recorded using Bruker AXS D8  
85 advance diffractometer at room temperature using Cu K $\alpha$  radiation source ( $\lambda = 1.5406 \text{ \AA}$ ) and  
86 scanning in the  $2\theta$  range of 10-80° with a step of 0.03°. The diffractograms were analyzed by  
87 comparing with the JCPDS-ICDD data.

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

92 N<sub>2</sub>physisorption measurements on freshly prepared catalysts were carried out using a  
93 Micromeritics ASAP 2020 instrument at 77 K. Before measurements, catalysts were  
94 degassed under vacuum at 200°C for 8 h. Surface area was measured by BET method in the

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

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

99 BELCAT-II Chemisorption analyzer was used to perform both temperature programmed  
100 desorption of ammonia and temperature programmed reduction by hydrogen. In a typical  
101  $\text{NH}_3$ -TPD experiment, the reduced sample was pre-treated at 300 °C for 1 h under a He  
102 (99.9%) flow at a rate of 50 mL min<sup>-1</sup>. After pre-treatment, the sample was saturated with  
103 anhydrous ammonia (5%  $\text{NH}_3$  balance He) at 100 °C for 30 min and subsequently flushed  
104 with He at the same temperature to remove physisorbed ammonia. Then, the TPD analysis  
105 was carried out by heating the sample in He flow (30 mL min<sup>-1</sup>) upto 600 °C at a rate of 10  
106 °C min<sup>-1</sup>, and the desorbed  $\text{NH}_3$  was measured. The detector in  $\text{NH}_3$ -TPD is thermal  
107 conductivity detector (TCD). For  $\text{H}_2$ -TPR, the Ni impregnated sample calcined at 450 °C in  
108 air was taken. Prior to analysis, the sample was heated at 300 °C in high purity He gas (50  
109 mL min<sup>-1</sup>) for 1 h and then on cooling to 50 °C the gas was switched to Ar flow. After 15 min  
110 the flow was adjusted to 5 %  $\text{H}_2$  in Ar (30 mL min<sup>-1</sup>) at 50 °C and waited till baseline was  
111 stabilized. TPR of catalyst was recorded from 50 °C to 900 °C with a heating rate 10 °C min<sup>-1</sup>.  
112 X-ray photoelectron spectra (XPS) of the reduced catalysts were obtained  
113 from PHI5000VersaProbe III X-ray photoelectron spectroscopy using 1486.6 eV  
114 monochromatic Al- $K_\alpha$  radiation source. The binding energy of all catalyst atoms were  
115 calibrated with carbon 1s peak present at 284.8 eV.

## 116 **1.6. Computational details**

117 All electronic structure calculations were performed with Gaussian 16 program using density  
118 functional theory<sup>3</sup>. The geometry optimization of metal cluster and other molecules were

119 carried out using PBE functional, where metal atoms were treated with LANL2DZ basis set  
120 with effective core pseudopotential (ECP) and 6-31g\*\* basis set was employed to describe all  
121 other atoms type<sup>4,5,6</sup>. The Grimme's D3 dispersion correction was also included in  
122 calculations<sup>7</sup>. Lowest energy icosahedra Ni geometry is obtained with spin multiplicity 9 and  
123 8 for neutral and charged (-1) cluster. The Ni cluster was fixed at optimized coordinates for  
124 further catalytic studies. All calculations are done in aqueous medium using implicit solvent  
125 as conductor like polarizable continuum model (CPCM)<sup>8</sup>. The minima and transition states  
126 on potential energy surface were confirmed by the presence of all positive frequencies for  
127 minima and one negative frequency for the transition state geometry<sup>9</sup>. The transition states  
128 were connected to minima on potential energy surface by tracing intrinsic reaction  
129 coordinates<sup>10</sup>. The minima were characterized by all positive frequencies, whereas transition  
130 states exhibit one imaginary frequency. All structures were visualized using Chemcraft 1.8  
131 software<sup>11</sup>. The zero-point energy corrected adsorption energy ( $E_{ads}$ ) of a substrate on the  
132 metal cluster is given by,

$$133 \quad E_{ads} = E_{M-S} + \Delta ZPVE - E_M - E_S$$

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

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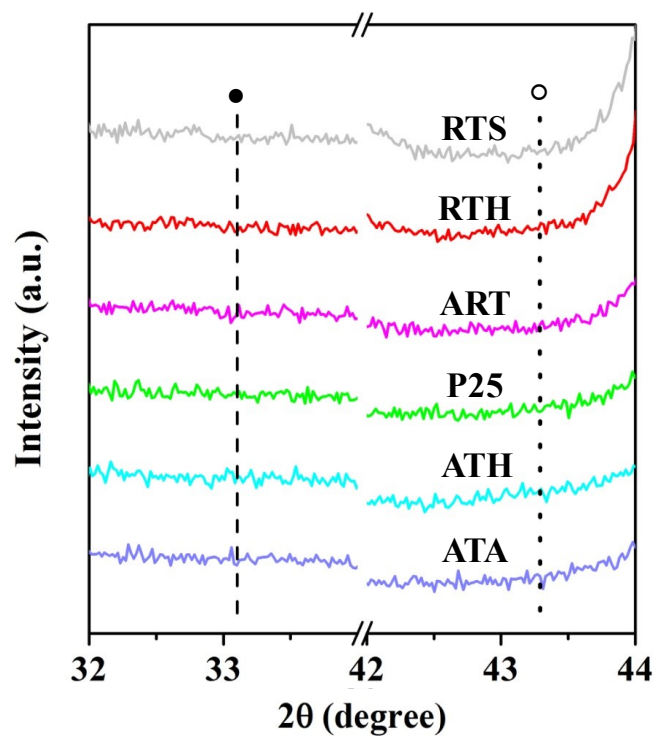
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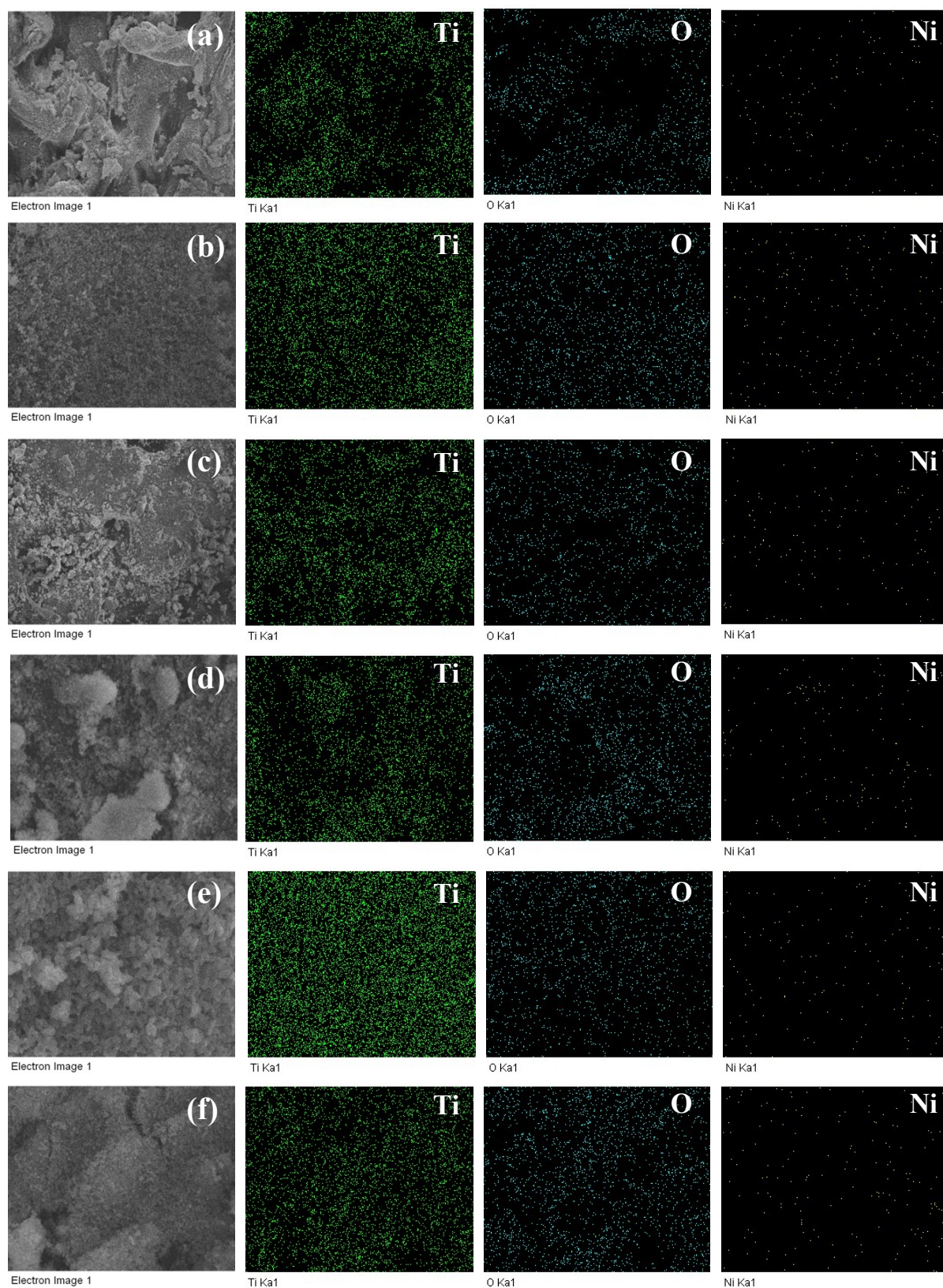
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168 **Figure S1.** XRD pattern Ni/TiO<sub>2</sub> catalysts: (a) ATA, (b) ATH, (c) P25, (d) ART, (e) RTH,  
 169 and (f) RTS showing (●) NiTiO<sub>3</sub> (104) and (○) NiO (200) region. (JCPDS No. for NiTiO<sub>3</sub>  
 170 and NiO is 33-0960 and 47-1049, respectively)

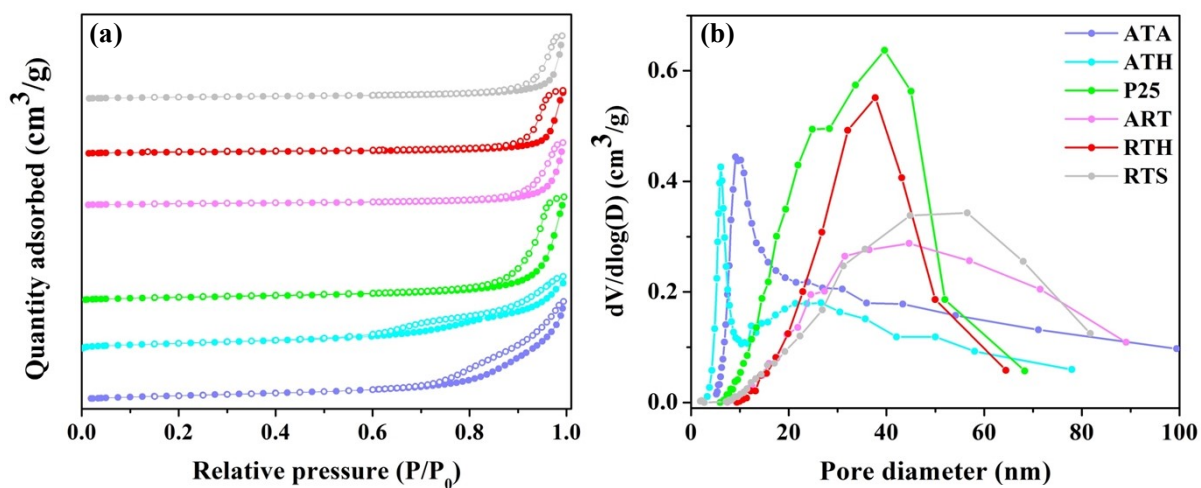




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172 **Figure S2.** SEM images with EDX elemental mapping of Ni/TiO<sub>2</sub> catalysts: (a) ATA, (b)  
 173 ATH, (c) P25, (d) ART, (e) RTH, and (f) RTS.

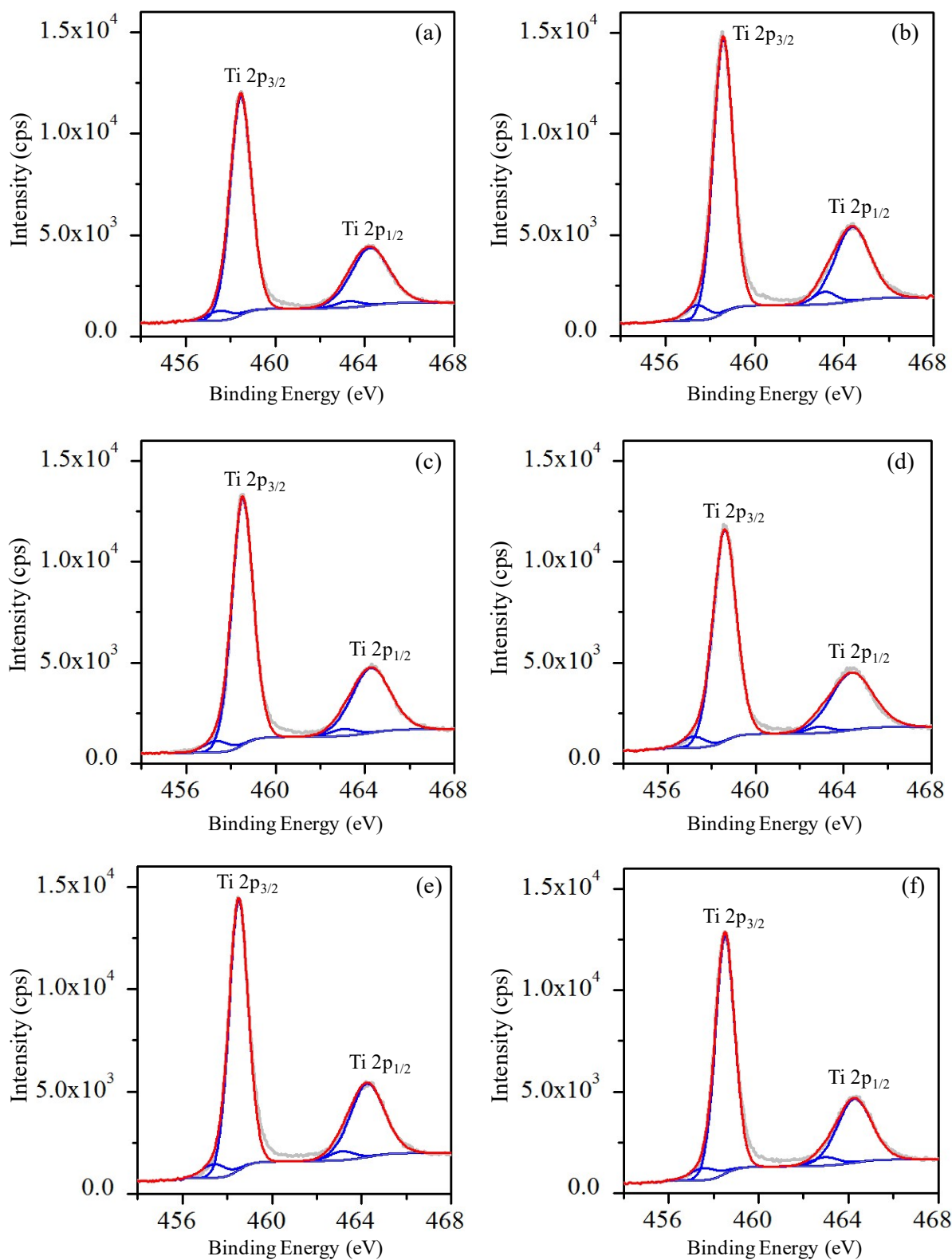
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176 **Figure S3.** Nitrogen sorption isotherms and BJH pore size distribution of Ni catalysts. The

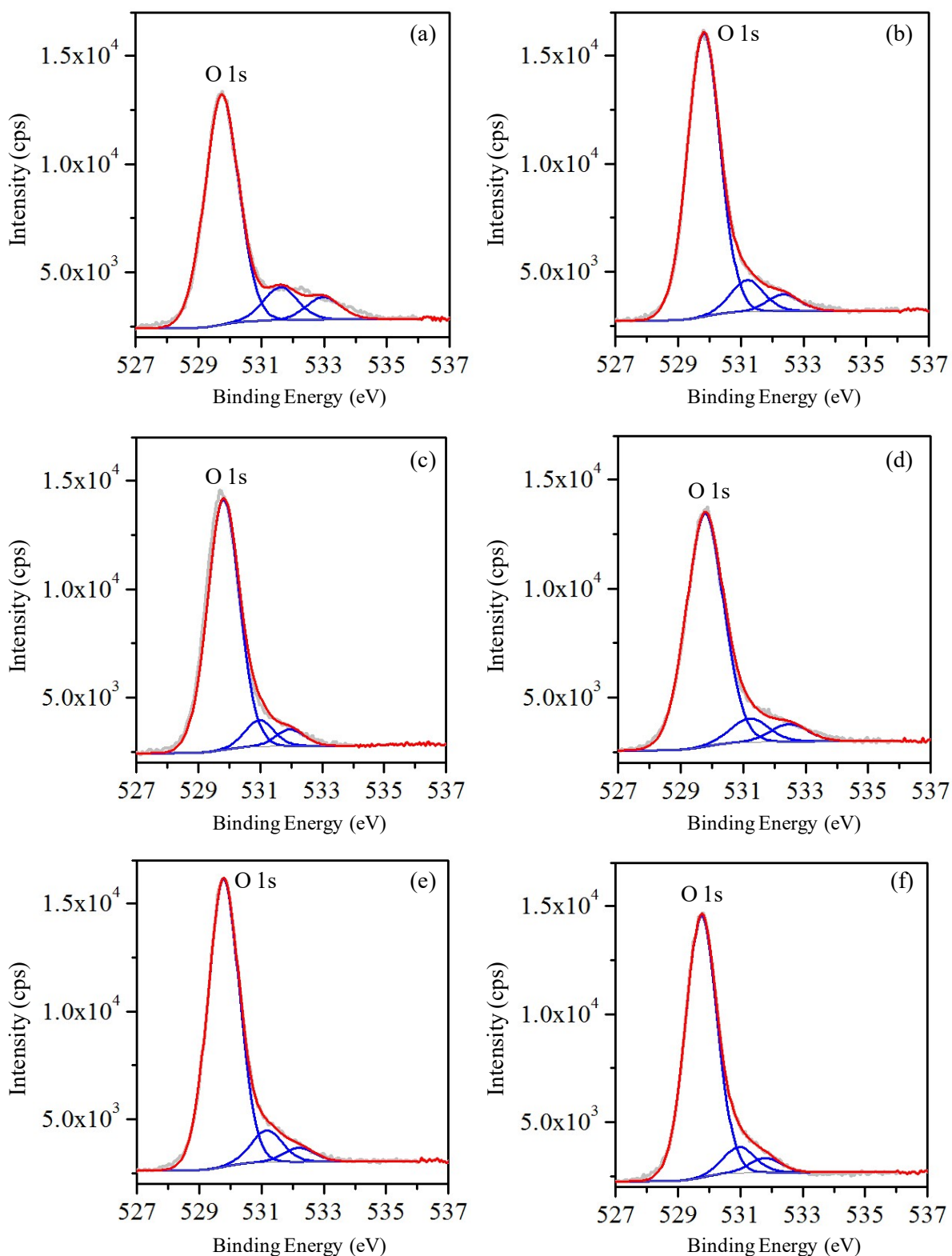
177 adsorption and desorption in isotherm are represented as closed and open circles respectively.



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



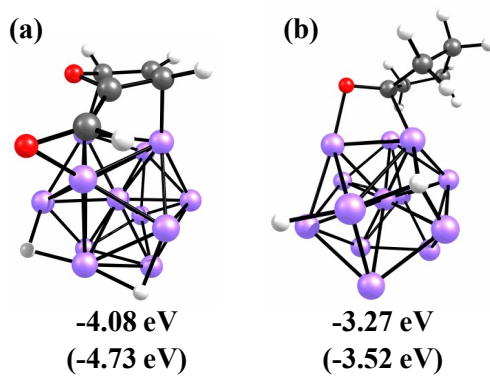


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183 **Figure S5.** O 1s core level XP spectra for the Ni catalysts supported on (a) ATA, (b) ATH,

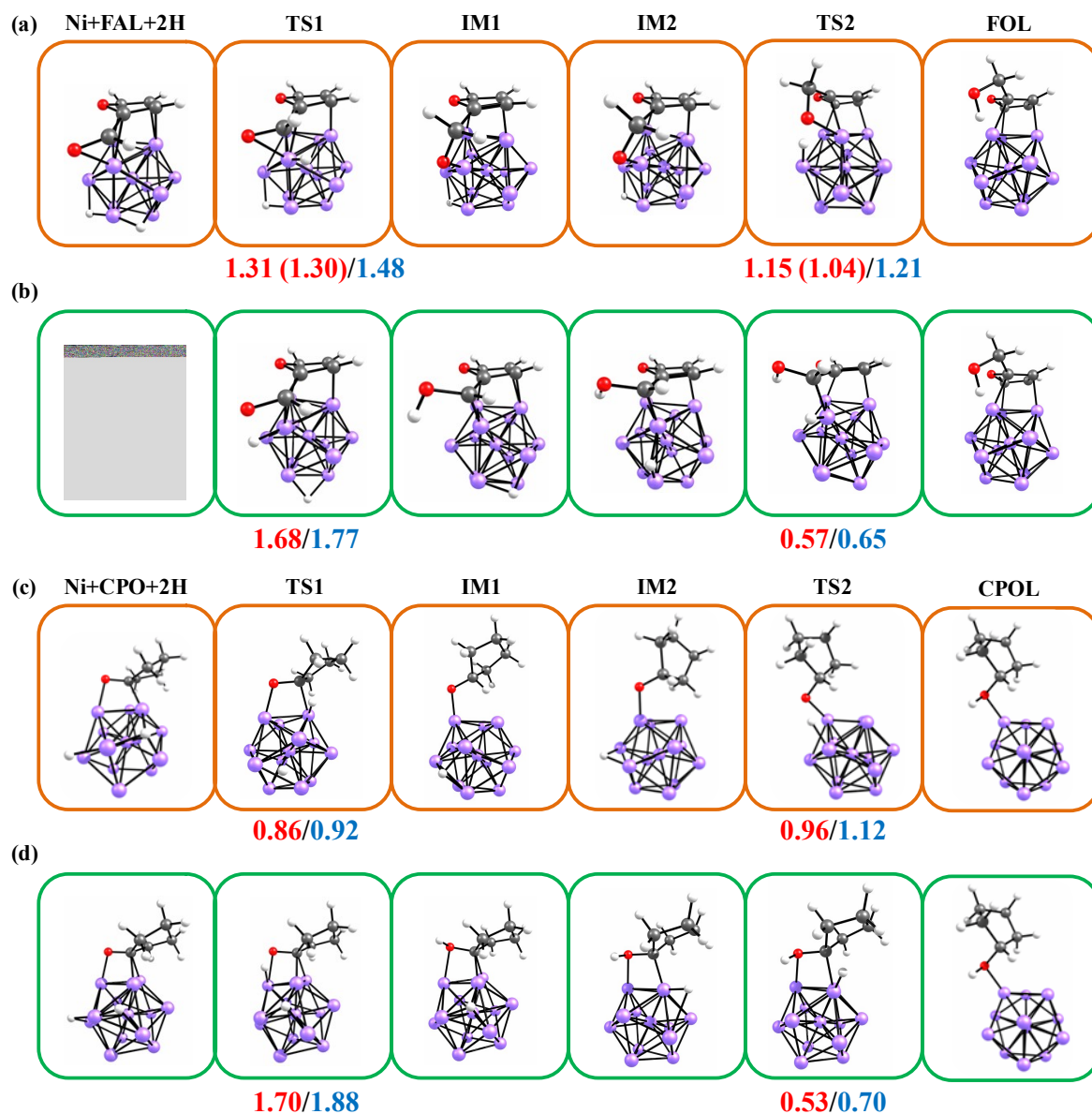
184 (c) P25, (d) ART, (e) RTH and, (f) RTS.

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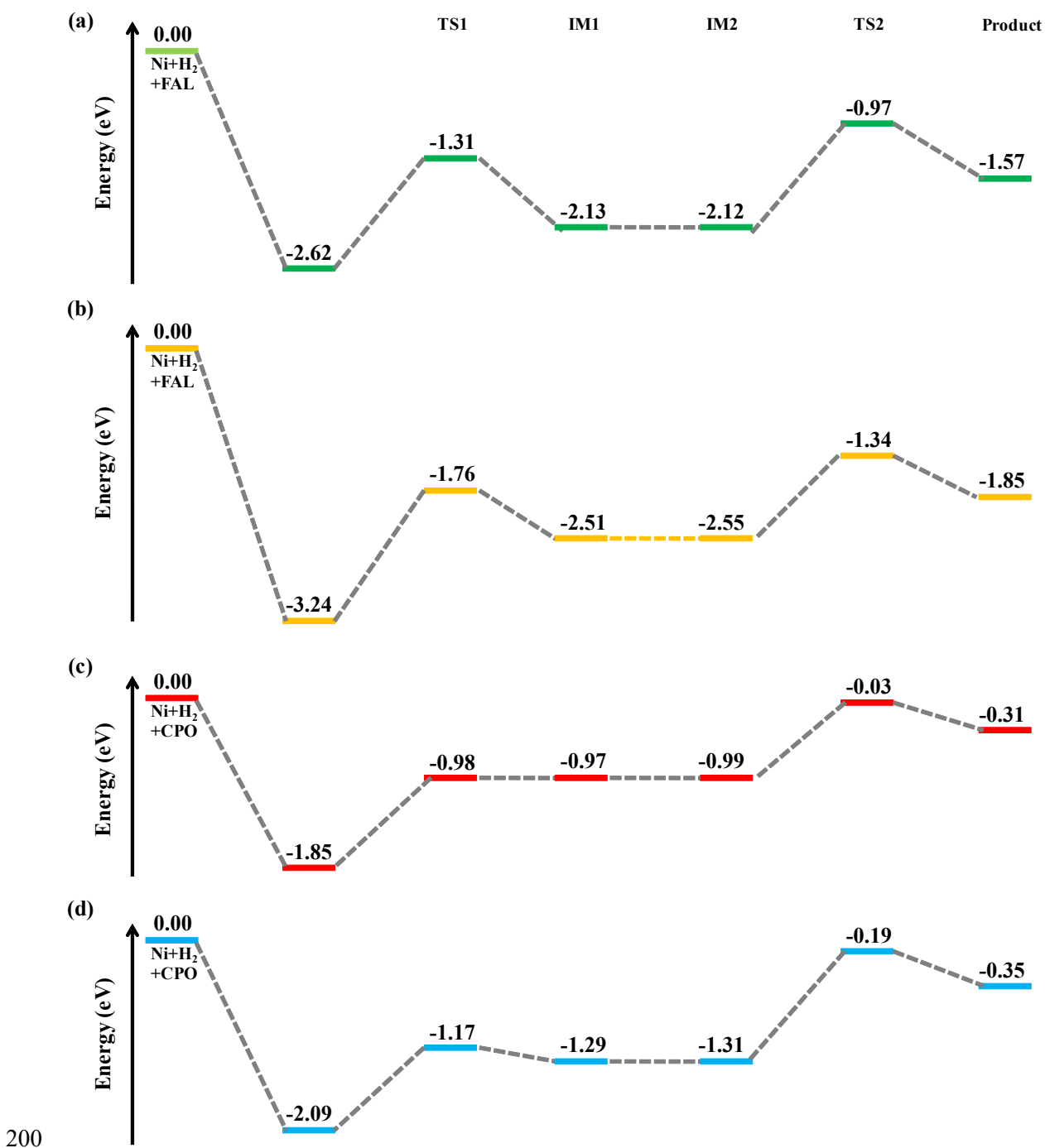
187 **Figure S6.** Co-adsorption of (a) FAL + 2H and, (b) CPO + 2H on Ni cluster. The adsorption  
188 energy on neutral Ni cluster is given below, where values in parentheses are for adsorption  
189 over charged (-1) cluster.



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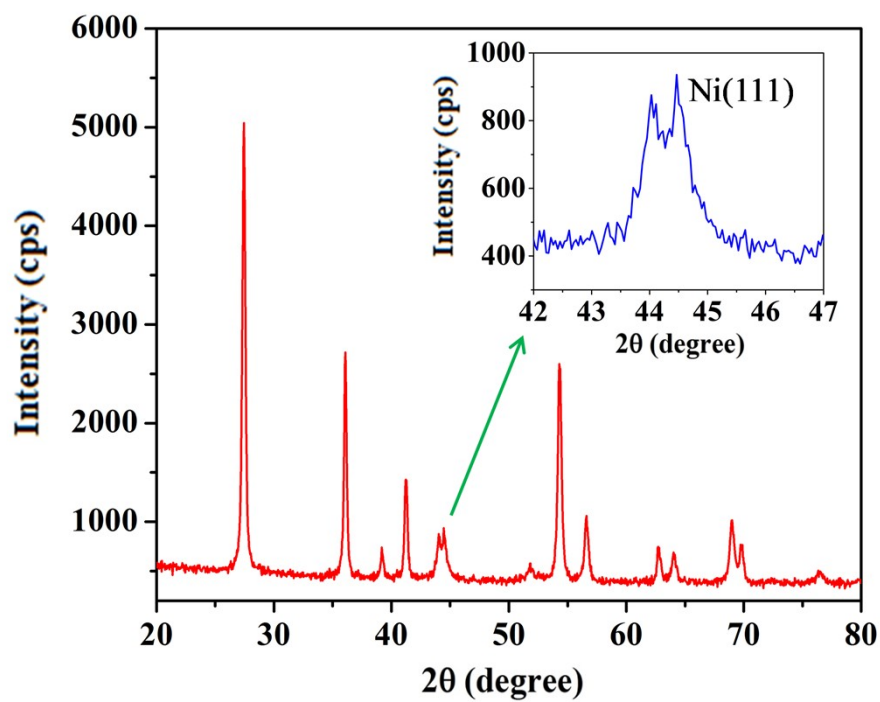
191 **Figure S7.** Initial, transition, intermediate and final state geometry during hydrogenation of  
 192 (a and b) FAL to FOL and (c and d) CPO to CPOL over Ni cluster. Colour code: Figures in  
 193 brown box (a and c) are corresponding to path a (addition of hydrogen first to carbon and  
 194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

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



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

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205 **Figure S9.** XRD pattern of RH support loaded with 10 wt% Ni content. The enlarged region

206 shows overlapped Rutile and Ni peak.

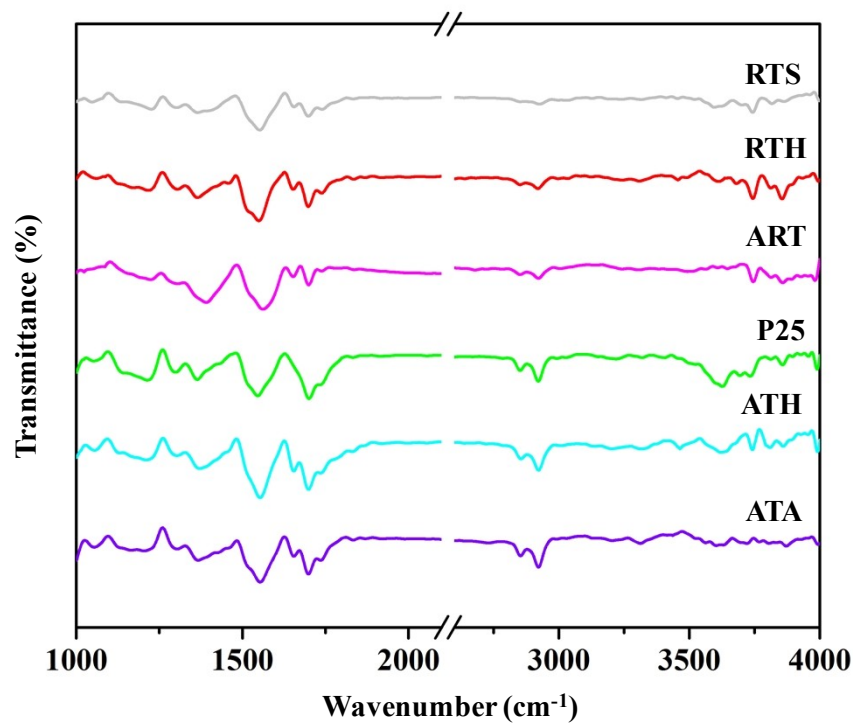
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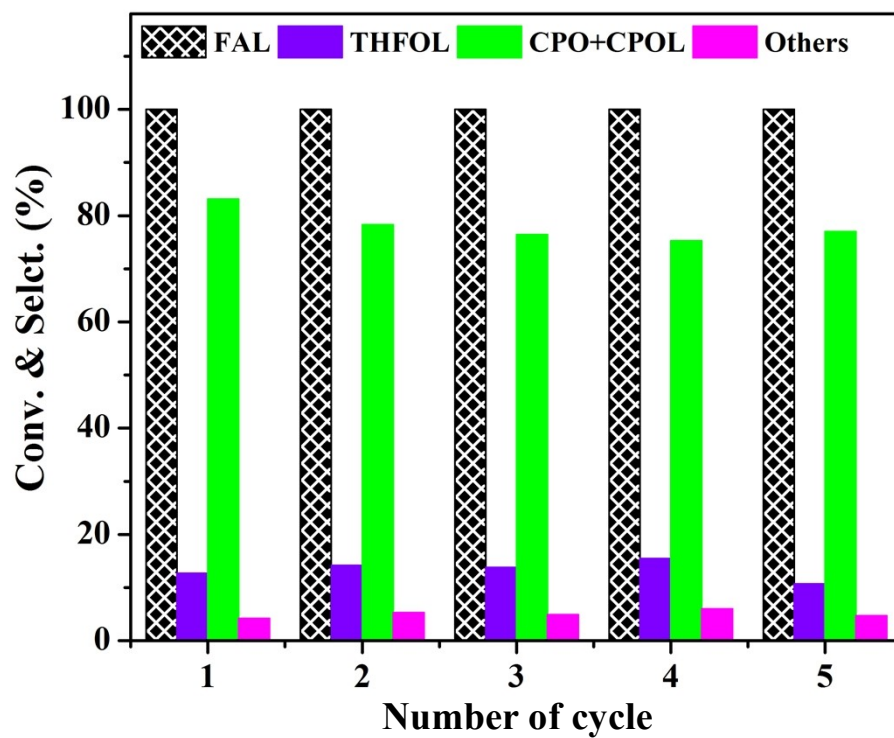
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212 **Figure S10.** FTIR spectra of dried Ni catalysts after reaction at 140°C.

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217 **Figure S11.** Recycling test over RTH catalyst. Reaction conditions: 5.2 mmol furfural, 50

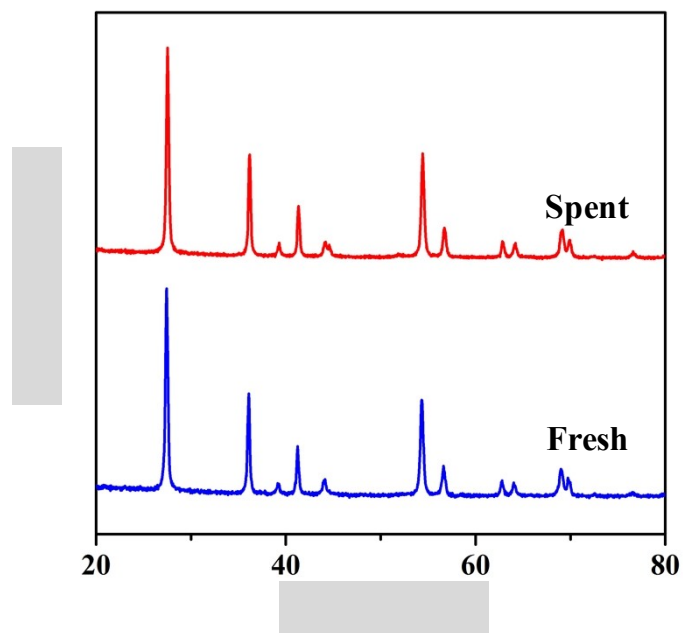
218 mL water, 50 bar H<sub>2</sub>, 140°C, 4h, 500 rpm.

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

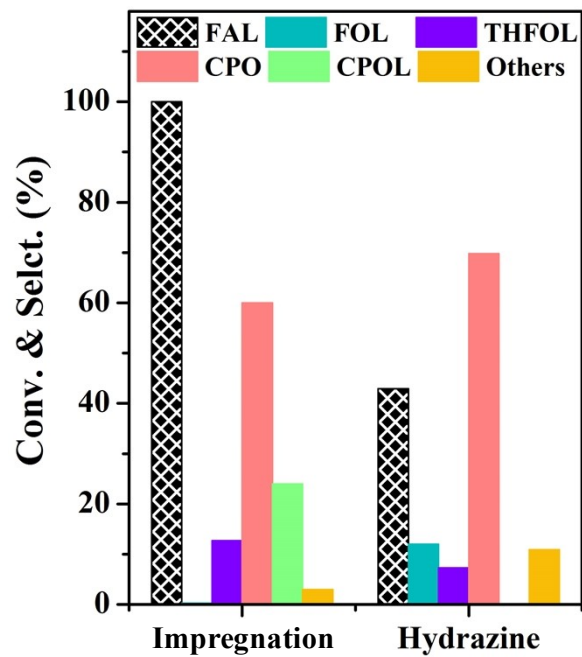
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231 **Figure S13.** Furfural hydrogenation over RTH catalysts prepared from impregnation method

232 and hydrazine reduction method. Reaction conditions: 5.2 mmol furfural, 50 mL water, 50

233 bar H<sub>2</sub>, 140°C, 4h, 500 rpm.

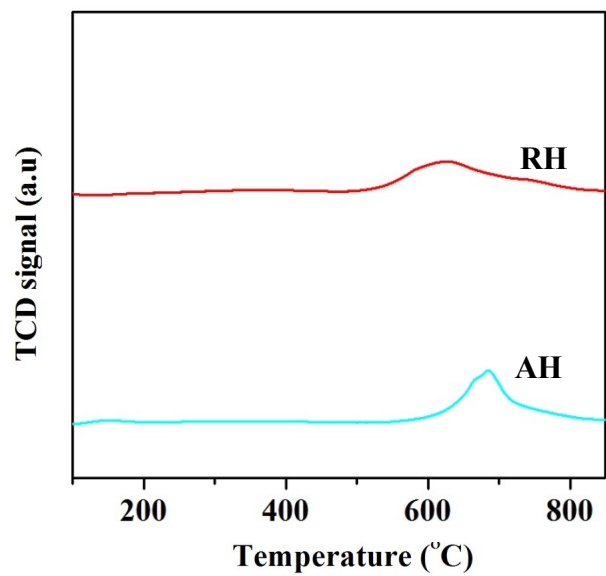
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240 **Figure S14.** H<sub>2</sub>-TPR profiles of bare anatase (AH) and rutile (RH) titania supports of ATH  
241 and RTH catalysts, respectively.

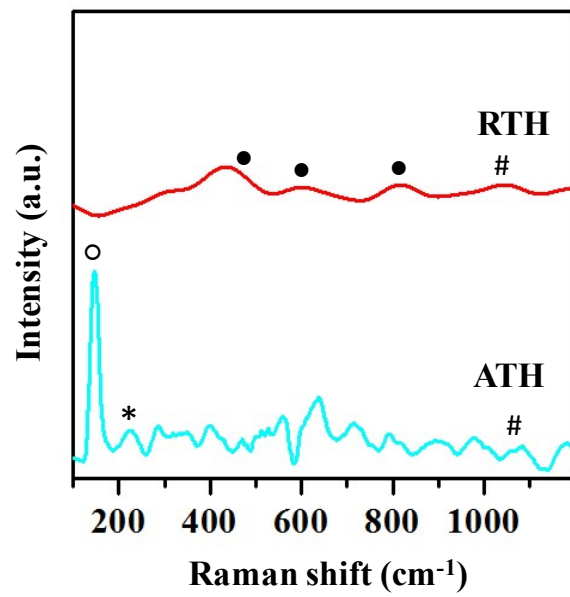
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248 **Figure S15.** Raman spectra of ATH and RTH catalysts showing presence of (○) anatase  
249 phase, (•) rutile phase, (\*) NiTiO<sub>3</sub> and (#) NiO.

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267 **Table S1.** Physico-chemical properties of catalysts support

Catalyst	A:R (%) <sup>a</sup>	D (nm) <sup>b</sup>	S <sub>BET</sub> (m <sup>2</sup> /g)	V <sub>p</sub> (cm <sup>3</sup> /g) <sup>c</sup>	D <sub>p</sub> (nm) <sup>c</sup>
<b>ATA</b>	100:0	19.4/-	62	0.28	16.1
<b>ATH</b>	100:0	15.9/-	66	0.21	11.1
<b>P25</b>	77:23	23.1/31.8	40	0.29	26.0
<b>ART</b>	48:52	47.7/54.4	23	0.17	34.6
<b>RTH</b>	0:100	-/29.9	22	0.17	31.4
<b>RTS</b>	0:100	-/22.5	23	0.17	33.8

268 <sup>a</sup>Percentage of anatase:rutile phases calculated using (101) and (110) XRD peaks intensities;<sup>b</sup>crystallite size of (101) and  
269 (110) plane of anatase and rutile phase calculated using Scherrer equation;<sup>c</sup>pore volume and diameter obtained from BJH  
270 analysis

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293 **Table S2.** Desorption temperature (°C) of NH<sub>3</sub> from titania catalysts based on their  
294 desorption strength

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

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

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

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

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

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355 **Cartesian coordinates**

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

358 1. FAL to FOL on neutral Ni cluster (path a)

359 a. Ni + FAL+2H

360 E+ZPE=-2545.619714

361 G=-2545.663595

362 Ni 1.506629000 -0.924052000 1.022357000

363 Ni -0.778447000 -1.281485000 1.987863000

364 Ni -2.425586000 -1.335050000 0.112106000

365 Ni -1.184186000 -1.017015000 -2.041289000

366 Ni 1.243532000 -0.746652000 -1.463221000

367 Ni 1.519886000 1.291373000 -0.034598000

368 Ni 0.263980000 0.994243000 2.058990000

369 Ni -2.133657000 0.685957000 1.455888000

370 Ni -2.426088000 0.904408000 -1.006852000

371 Ni -0.194546000 1.233535000 -1.990100000

372 Ni -0.746197000 2.332189000 0.190397000

373 Ni -0.431842000 0.018534000 -0.017420000

374 Ni -0.200267000 -2.313701000 -0.151042000

375 C 3.077821000 -1.510490000 -1.082253000

376 C 3.164867000 -1.999403000 0.288994000

377 C 3.532083000 -0.888866000 1.122329000

378 C 3.620845000 0.244666000 0.233128000

379 O 3.637645000 -0.179571000 -1.088068000

380	H	3.409316000	-2.098029000	-1.948913000
381	H	3.171786000	-3.056655000	0.556524000
382	H	3.857813000	-0.901035000	2.164207000
383	C	3.416403000	1.651966000	0.490125000
384	H	3.581644000	1.994235000	1.530743000
385	O	3.158087000	2.499521000	-0.474704000
386	H	-0.390936000	2.767376000	-1.365715000
387	H	-1.237474000	2.163352000	1.805178000
388	b. TS1			
389	E+ZPE=-2545.570702			
390	G=-2545.615413			
391	Ni	1.414998000	-1.189363000	0.886298000
392	Ni	-0.919928000	-1.608627000	1.701682000
393	Ni	-2.496093000	-1.218629000	-0.195700000
394	Ni	-1.161356000	-0.558967000	-2.210244000
395	Ni	1.248999000	-0.529085000	-1.523822000
396	Ni	1.562411000	1.184731000	0.281027000
397	Ni	0.220143000	0.555030000	2.239631000
398	Ni	-2.165669000	0.490212000	1.520761000
399	Ni	-2.354996000	1.189391000	-0.861668000
400	Ni	-0.071375000	1.590201000	-1.701083000
401	Ni	-0.660341000	2.275043000	0.635716000
402	Ni	-0.440084000	0.030788000	-0.003970000
403	Ni	-0.307612000	-2.241334000	-0.578251000
404	C	3.023296000	-1.523068000	-1.193877000

405	C	3.103549000	-2.102212000	0.137659000
406	C	3.440152000	-1.032342000	1.046453000
407	C	3.538838000	0.154414000	0.240303000
408	O	3.557722000	-0.183917000	-1.106320000
409	H	3.358432000	-2.037622000	-2.102606000
410	H	3.158555000	-3.174709000	0.332629000
411	H	3.750413000	-1.103297000	2.090598000
412	C	3.565309000	1.622483000	0.574022000
413	H	4.276015000	1.869687000	1.400318000
414	O	3.425461000	2.460015000	-0.439260000
415	H	-1.254118000	2.643203000	-0.988565000
416	H	2.483585000	1.735365000	1.474343000
417	c.	IM1		
418		E+ZPE=-2545.601080		
419		G=-2545.645537		
420	Ni	1.566324000	-0.689007000	1.023209000
421	Ni	-0.646426000	-0.987854000	2.166184000
422	Ni	-2.390352000	-1.357288000	0.417318000
423	Ni	-1.283284000	-1.297613000	-1.828954000
424	Ni	1.155303000	-0.867869000	-1.441297000
425	Ni	1.423361000	1.360257000	-0.320667000
426	Ni	0.301673000	1.310061000	1.864297000
427	Ni	-2.111427000	0.838645000	1.454475000
428	Ni	-2.547373000	0.703409000	-0.993563000
429	Ni	-0.385550000	0.973720000	-2.148213000

430	Ni	-0.867425000	2.340610000	-0.104837000
431	Ni	-0.465264000	0.033220000	-0.013419000
432	Ni	-0.142551000	-2.285508000	0.157245000
433	C	2.988588000	-1.606659000	-1.031453000
434	C	3.025673000	-1.990587000	0.377298000
435	C	3.630018000	-0.882470000	1.088083000
436	C	3.947793000	0.090810000	0.116274000
437	O	3.749497000	-0.393851000	-1.146710000
438	H	3.207322000	-2.305051000	-1.853345000
439	H	2.911000000	-3.017582000	0.727987000
440	H	3.918761000	-0.829392000	2.139883000
441	C	4.183817000	1.571633000	0.211306000
442	H	5.090824000	1.839515000	-0.375561000
443	O	3.065769000	2.293143000	-0.273570000
444	H	-1.708310000	2.129522000	-1.613156000
445	H	4.406722000	1.798335000	1.277575000
446	d. IM2			
447	E+ZPE=-2545.600857			
448	G=-2545.645250			
449	Ni	-1.579247000	-0.697186000	-1.006082000
450	Ni	0.628009000	-1.023779000	-2.147782000
451	Ni	2.381618000	-1.369972000	-0.410604000
452	Ni	1.291402000	-1.272003000	1.842747000
453	Ni	-1.151677000	-0.838670000	1.469483000
454	Ni	-1.420897000	1.367240000	0.316312000

455	Ni	-0.312080000	1.283968000	-1.878276000
456	Ni	2.101520000	0.810262000	-1.479584000
457	Ni	2.555033000	0.712747000	0.967237000
458	Ni	0.407526000	1.004543000	2.128727000
459	Ni	0.871864000	2.341805000	0.066185000
460	Ni	0.464636000	0.033730000	0.013202000
461	Ni	0.133648000	-2.286917000	-0.119083000
462	C	-2.988126000	-1.609101000	1.039142000
463	C	-3.043358000	-2.004262000	-0.363993000
464	C	-3.630948000	-0.892818000	-1.082208000
465	C	-3.906493000	0.102062000	-0.116950000
466	O	-3.724611000	-0.382241000	1.151587000
467	H	-3.206538000	-2.296563000	1.869618000
468	H	-2.937899000	-3.033606000	-0.709624000
469	H	-3.930976000	-0.845305000	-2.130947000
470	C	-4.154503000	1.580477000	-0.219519000
471	H	-5.071898000	1.838919000	0.356087000
472	O	-3.050701000	2.317938000	0.272836000
473	H	1.661774000	2.152136000	1.620351000
474	H	-4.369307000	1.799199000	-1.289224000
475	e.	TS2		
476		E+ZPE=-2545.558802		
477		G=-2545.603118		
478	Ni	0.992353000	-1.622992000	0.964485000
479	Ni	-1.456502000	-1.557831000	1.496695000

480	Ni	-2.684794000	-0.713425000	-0.501093000
481	Ni	-1.019306000	-0.246432000	-2.313155000
482	Ni	1.250577000	-0.793634000	-1.395861000
483	Ni	1.716581000	0.690340000	0.566533000
484	Ni	0.053658000	0.261596000	2.328196000
485	Ni	-2.192366000	0.771422000	1.377066000
486	Ni	-1.954435000	1.639357000	-0.945076000
487	Ni	0.436276000	1.569576000	-1.518858000
488	Ni	-0.246386000	2.227799000	0.796248000
489	Ni	-0.444144000	0.034113000	-0.005292000
490	Ni	-0.738428000	-2.171919000	-0.753344000
491	C	2.932371000	-1.777109000	-0.956500000
492	C	2.903432000	-2.006473000	0.488119000
493	C	3.350699000	-0.753327000	1.089238000
494	C	3.663507000	0.134053000	0.024081000
495	O	3.637408000	-0.542998000	-1.199221000
496	H	3.198490000	-2.546964000	-1.690382000
497	H	3.031882000	-2.998093000	0.943565000
498	H	3.612673000	-0.595394000	2.135558000
499	C	4.115228000	1.573746000	0.008473000
500	H	4.566700000	1.787696000	-0.982390000
501	O	2.996500000	2.422263000	0.296801000
502	H	1.864341000	2.090539000	-0.587202000
503	H	4.896876000	1.739588000	0.776550000
504	f. FOL			



505	E+ZPE=-2545.579669			
506	G=-2545.625067			
507	Ni	1.284067000	-0.976648000	1.245139000
508	Ni	-0.925894000	-0.438971000	2.297734000
509	Ni	-2.702585000	-0.667433000	0.557609000
510	Ni	-1.619044000	-1.355556000	-1.595107000
511	Ni	0.847035000	-1.527969000	-1.159732000
512	Ni	1.712518000	0.720009000	-0.475065000
513	Ni	0.615047000	1.413260000	1.613907000
514	Ni	-1.833554000	1.533639000	1.169151000
515	Ni	-2.287087000	1.036434000	-1.228393000
516	Ni	-0.137501000	0.480043000	-2.287390000
517	Ni	-0.222464000	2.305254000	-0.578264000
518	Ni	-0.470629000	0.039694000	-0.024850000
519	Ni	-0.795381000	-2.197340000	0.604676000
520	C	2.776851000	-1.871424000	-0.954041000
521	C	2.850427000	-2.169423000	0.475302000
522	C	3.311723000	-0.985574000	1.146218000
523	C	3.509591000	0.029979000	0.118396000
524	O	3.475830000	-0.617504000	-1.158404000
525	H	3.057560000	-2.599523000	-1.730897000
526	H	2.819767000	-3.182137000	0.880942000
527	H	3.727689000	-0.912791000	2.154983000
528	C	4.435527000	1.210826000	0.228622000
529	H	5.393601000	1.011653000	-0.284045000

530	O	3.908786000	2.413517000	-0.374400000
531	H	2.964380000	2.462712000	-0.054421000
532	H	4.648543000	1.362028000	1.305220000
533	2. FAL to FOL on neutral Ni cluster (path b)			
534	a. Ni + FAL+2H			
535	E+ZPE=-2545.619714			
536	G=-2545.663595			
537	Ni	1.506629000	-0.924052000	1.022357000
538	Ni	-0.778447000	-1.281485000	1.987863000
539	Ni	-2.425586000	-1.335050000	0.112106000
540	Ni	-1.184186000	-1.017015000	-2.041289000
541	Ni	1.243532000	-0.746652000	-1.463221000
542	Ni	1.519886000	1.291373000	-0.034598000
543	Ni	0.263980000	0.994243000	2.058990000
544	Ni	-2.133657000	0.685957000	1.455888000
545	Ni	-2.426088000	0.904408000	-1.006852000
546	Ni	-0.194546000	1.233535000	-1.990100000
547	Ni	-0.746197000	2.332189000	0.190397000
548	Ni	-0.431842000	0.018534000	-0.017420000
549	Ni	-0.200267000	-2.313701000	-0.151042000
550	C	3.077821000	-1.510490000	-1.082253000
551	C	3.164867000	-1.999403000	0.288994000
552	C	3.532083000	-0.888866000	1.122329000
553	C	3.620845000	0.244666000	0.233128000
554	O	3.637645000	-0.179571000	-1.088068000

555	H	3.409316000	-2.098029000	-1.948913000
556	H	3.171786000	-3.056655000	0.556524000
557	H	3.857813000	-0.901035000	2.164207000
558	C	3.416403000	1.651966000	0.490125000
559	H	3.581644000	1.994235000	1.530743000
560	O	3.158087000	2.499521000	-0.474704000
561	H	-0.390936000	2.767376000	-1.365715000
562	H	-1.237474000	2.163352000	1.805178000
563	b. TS1			
564	E+ZPE=-2545.557691			
565	G=-2545.601910			
566	Ni	1.476910000	-0.927495000	1.047966000
567	Ni	-0.802836000	-1.134634000	2.064684000
568	Ni	-2.480016000	-1.240469000	0.217901000
569	Ni	-1.261845000	-1.104541000	-1.967598000
570	Ni	1.183608000	-0.893149000	-1.440248000
571	Ni	1.558888000	1.217942000	-0.145193000
572	Ni	0.325476000	1.104408000	1.973450000
573	Ni	-2.091322000	0.846271000	1.429511000
574	Ni	-2.414526000	0.924124000	-1.037925000
575	Ni	-0.191528000	1.104911000	-2.071271000
576	Ni	-0.658502000	2.353899000	0.049930000
577	Ni	-0.439023000	0.024136000	-0.023227000
578	Ni	-0.297729000	-2.318801000	-0.013846000
579	C	2.989152000	-1.601700000	-1.025531000

580	C	3.099698000	-2.043674000	0.373340000
581	C	3.517043000	-0.925465000	1.160764000
582	C	3.632702000	0.185431000	0.222314000
583	O	3.635580000	-0.291740000	-1.084345000
584	H	3.342770000	-2.240152000	-1.849442000
585	H	3.094312000	-3.092773000	0.673693000
586	H	3.883778000	-0.921073000	2.188326000
587	C	3.484662000	1.576772000	0.456712000
588	H	3.614443000	1.951501000	1.482072000
589	O	3.300764000	2.460539000	-0.567282000
590	H	1.962078000	2.724893000	-0.499724000
591	H	-1.139168000	2.294214000	1.736769000
592	c.	IM1		
593		E+ZPE=-2545.586382		
594		G=-2545.631338		
595	Ni	1.229943000	-1.250464000	1.087542000
596	Ni	-1.149993000	-1.283457000	1.872540000
597	Ni	-2.636964000	-0.978398000	-0.110246000
598	Ni	-1.199941000	-0.758042000	-2.151010000
599	Ni	1.188804000	-0.910203000	-1.394690000
600	Ni	1.670893000	0.983304000	0.170734000
601	Ni	0.227617000	0.788720000	2.152961000
602	Ni	-2.135694000	0.899367000	1.371833000
603	Ni	-2.200844000	1.284388000	-1.087585000
604	Ni	0.123087000	1.298868000	-1.895781000

605	Ni	-0.413946000	2.363244000	0.305012000
606	Ni	-0.451703000	0.041668000	-0.021288000
607	Ni	-0.578864000	-2.288014000	-0.281315000
608	C	2.963349000	-1.717528000	-1.043788000
609	C	2.935972000	-2.176227000	0.345112000
610	C	3.252786000	-1.053304000	1.182999000
611	C	3.516424000	0.061368000	0.257960000
612	O	3.659227000	-0.434312000	-1.045378000
613	H	3.330527000	-2.359143000	-1.856211000
614	H	2.929163000	-3.230091000	0.632618000
615	H	3.608566000	-1.074565000	2.215469000
616	C	3.599796000	1.457215000	0.512096000
617	H	3.768837000	1.760824000	1.557210000
618	O	4.190915000	2.273994000	-0.473046000
619	H	3.720524000	3.127634000	-0.431185000
620	H	-0.595783000	2.281259000	1.979340000
621	d. IM2			
622	E+ZPE=-2545.588462			
623	G=-2545.633246			
624	Ni	-1.221244000	-1.409309000	-0.893637000
625	Ni	1.188513000	-1.677367000	-1.516610000
626	Ni	2.586782000	-0.989964000	0.437937000
627	Ni	1.059051000	-0.294721000	2.295738000
628	Ni	-1.295136000	-0.537862000	1.457139000
629	Ni	-1.624067000	0.980217000	-0.508295000

630	Ni	-0.087026000	0.327459000	-2.309124000
631	Ni	2.234585000	0.535574000	-1.438636000
632	Ni	2.189660000	1.442461000	0.882484000
633	Ni	-0.169100000	1.695111000	1.531608000
634	Ni	0.520773000	2.238433000	-0.814140000
635	Ni	0.451903000	0.049457000	0.010606000
636	Ni	0.472368000	-2.174830000	0.767072000
637	C	-2.956615000	-1.617620000	1.169226000
638	C	-2.948405000	-2.211269000	-0.159053000
639	C	-3.215154000	-1.153777000	-1.106072000
640	C	-3.466110000	0.046336000	-0.308590000
641	O	-3.571980000	-0.307739000	1.058655000
642	H	-3.300385000	-2.147794000	2.065622000
643	H	-2.999482000	-3.286904000	-0.343264000
644	H	-3.551457000	-1.259730000	-2.139884000
645	C	-3.591559000	1.422898000	-0.649458000
646	H	-3.903639000	1.694661000	-1.663336000
647	O	-4.060038000	2.342045000	0.302515000
648	H	-3.590734000	2.123081000	1.134600000
649	H	-1.128785000	2.512426000	-0.879423000
650	e.	TS2		
651		E+ZPE=-2545.567565		
652		G=-2545.612272		
653	Ni	1.188150000	-1.423600000	0.907210000
654	Ni	-1.214795000	-1.597545000	1.588458000

655	Ni	-2.634831000	-0.935589000	-0.358702000
656	Ni	-1.128845000	-0.350391000	-2.270832000
657	Ni	1.235883000	-0.634814000	-1.475086000
658	Ni	1.650457000	0.937322000	0.429515000
659	Ni	0.136612000	0.393339000	2.284503000
660	Ni	-2.196776000	0.641880000	1.455995000
661	Ni	-2.176407000	1.467374000	-0.895560000
662	Ni	0.174044000	1.626522000	-1.602698000
663	Ni	-0.447799000	2.270135000	0.737122000
664	Ni	-0.461545000	0.053238000	-0.012463000
665	Ni	-0.563814000	-2.194082000	-0.690793000
666	C	2.963339000	-1.620274000	-1.179727000
667	C	2.913930000	-2.217616000	0.152282000
668	C	3.217091000	-1.175087000	1.107094000
669	C	3.486196000	0.011349000	0.314975000
670	O	3.621586000	-0.328505000	-1.035193000
671	H	3.355504000	-2.162622000	-2.049506000
672	H	2.941371000	-3.295648000	0.330677000
673	H	3.517693000	-1.286896000	2.150868000
674	C	3.636257000	1.422534000	0.648378000
675	H	4.044829000	1.631876000	1.644474000
676	O	4.255845000	2.238601000	-0.314766000
677	H	3.837665000	2.002510000	-1.168535000
678	H	2.293240000	2.198447000	0.926960000

679 f. FOL

680	E+ZPE=-2545.579669			
681	G=-2545.625067			
682	Ni	1.284067000	-0.976648000	1.245139000
683	Ni	-0.925894000	-0.438971000	2.297734000
684	Ni	-2.702585000	-0.667433000	0.557609000
685	Ni	-1.619044000	-1.355556000	-1.595107000
686	Ni	0.847035000	-1.527969000	-1.159732000
687	Ni	1.712518000	0.720009000	-0.475065000
688	Ni	0.615047000	1.413260000	1.613907000
689	Ni	-1.833554000	1.533639000	1.169151000
690	Ni	-2.287087000	1.036434000	-1.228393000
691	Ni	-0.137501000	0.480043000	-2.287390000
692	Ni	-0.222464000	2.305254000	-0.578264000
693	Ni	-0.470629000	0.039694000	-0.024850000
694	Ni	-0.795381000	-2.197340000	0.604676000
695	C	2.776851000	-1.871424000	-0.954041000
696	C	2.850427000	-2.169423000	0.475302000
697	C	3.311723000	-0.985574000	1.146218000
698	C	3.509591000	0.029979000	0.118396000
699	O	3.475830000	-0.617504000	-1.158404000
700	H	3.057560000	-2.599523000	-1.730897000
701	H	2.819767000	-3.182137000	0.880942000
702	H	3.727689000	-0.912791000	2.154983000
703	C	4.435527000	1.210826000	0.228622000
704	H	5.393601000	1.011653000	-0.284045000



705	O	3.908786000	2.413517000	-0.374400000
706	H	2.964380000	2.462712000	-0.054421000
707	H	4.648543000	1.362028000	1.305220000
708	3. FAL to FOL on charged (-1) Ni cluster (path a)			
709	a. Ni + FAL+2H			
710	E+ZPE=-2545.733606			
711	G=-2545.777336			
712	Ni	-1.120644000	-1.073895000	-2.031095000
713	Ni	-0.185326000	1.223981000	-1.993234000
714	Ni	1.473951000	1.414373000	-0.098030000
715	Ni	1.507518000	-0.911105000	1.115389000
716	Ni	-0.108383000	-2.368227000	-0.142849000
717	Ni	-2.320787000	-1.347056000	0.082393000
718	Ni	-2.410126000	0.814893000	-1.041974000
719	Ni	-0.847346000	2.302899000	0.153385000
720	Ni	0.157172000	1.009659000	2.043567000
721	Ni	-0.793880000	-1.272878000	1.997042000
722	Ni	-2.204533000	0.693480000	1.427809000
723	Ni	-0.379177000	-0.002504000	-0.004746000
724	Ni	1.290478000	-0.782532000	-1.504048000
725	C	3.101464000	-1.474206000	-1.000072000
726	C	3.188157000	-1.927970000	0.389256000
727	C	3.510564000	-0.789489000	1.206535000
728	C	3.551514000	0.334200000	0.298334000
729	O	3.601790000	-0.110685000	-1.018731000

730	H	3.524456000	-2.063566000	-1.826838000
731	H	3.264755000	-2.979227000	0.671029000
732	H	3.863391000	-0.777377000	2.240146000
733	C	3.337799000	1.741534000	0.533461000
734	H	3.460606000	2.086760000	1.579050000
735	O	3.134924000	2.594571000	-0.446647000
736	H	-0.492543000	2.747844000	-1.400193000
737	H	-1.301045000	2.179602000	1.793750000
738	b. TS1			
739	E+ZPE=-2545.678789			
740	G=-2545.722791			
741	Ni	-1.097722000	-0.725542000	-2.178579000
742	Ni	-0.128794000	1.521090000	-1.766321000
743	Ni	1.486771000	1.386589000	0.170914000
744	Ni	1.455306000	-1.098123000	1.011780000
745	Ni	-0.151815000	-2.313708000	-0.490697000
746	Ni	-2.353069000	-1.297799000	-0.158747000
747	Ni	-2.381978000	1.012623000	-0.937997000
748	Ni	-0.826134000	2.269128000	0.506041000
749	Ni	0.112439000	0.682164000	2.195680000
750	Ni	-0.872305000	-1.547711000	1.777114000
751	Ni	-2.238399000	0.509013000	1.487375000
752	Ni	-0.389627000	0.007292000	0.004569000
753	Ni	1.303745000	-0.564597000	-1.560351000
754	C	3.047214000	-1.503493000	-1.075539000

755	C	3.131991000	-2.023271000	0.286558000
756	C	3.470047000	-0.913518000	1.149975000
757	C	3.535305000	0.241262000	0.305694000
758	O	3.542200000	-0.137939000	-1.028465000
759	H	3.458299000	-2.044152000	-1.939083000
760	H	3.232193000	-3.085785000	0.517144000
761	H	3.785161000	-0.941666000	2.195275000
762	C	3.466898000	1.714143000	0.597513000
763	H	4.151620000	2.028507000	1.421556000
764	O	3.310153000	2.522046000	-0.452786000
765	H	-1.437418000	2.547489000	-1.093499000
766	H	2.366856000	1.800329000	1.461513000
767	c.	IM1		
768		E+ZPE=-2545.706244		
769		G=-2545.750585		
770	Ni	-1.224009000	-1.291372000	-1.854163000
771	Ni	-0.333021000	1.008800000	-2.121689000
772	Ni	1.407969000	1.437810000	-0.342536000
773	Ni	1.542642000	-0.733114000	1.124126000
774	Ni	-0.101009000	-2.347060000	0.118211000
775	Ni	-2.320036000	-1.338094000	0.332062000
776	Ni	-2.503122000	0.679807000	-1.024622000
777	Ni	-0.916139000	2.316182000	-0.082083000
778	Ni	0.199566000	1.261896000	1.892232000
779	Ni	-0.708356000	-1.024166000	2.150440000

780	Ni	-2.181672000	0.844164000	1.430261000
781	Ni	-0.411069000	0.014979000	0.000028000
782	Ni	1.202517000	-0.908057000	-1.479463000
783	C	3.021568000	-1.573384000	-0.983460000
784	C	3.064464000	-1.943632000	0.432538000
785	C	3.597631000	-0.797052000	1.142476000
786	C	3.857779000	0.193963000	0.169182000
787	O	3.711503000	-0.310068000	-1.094697000
788	H	3.331461000	-2.265463000	-1.782619000
789	H	3.032420000	-2.976777000	0.783014000
790	H	3.894336000	-0.726331000	2.191900000
791	C	4.106878000	1.674062000	0.264486000
792	H	5.037375000	1.920268000	-0.297967000
793	O	3.019769000	2.424881000	-0.243296000
794	H	-1.667135000	2.102560000	-1.677074000
795	H	4.312160000	1.893811000	1.336800000
796	d. IM2			
797	E+ZPE=-2545.707166			
798	G=-2545.751857			
799	Ni	-1.227917000	-1.321859000	-1.830847000
800	Ni	-0.369807000	0.987581000	-2.135615000
801	Ni	1.383963000	1.459044000	-0.380178000
802	Ni	1.565831000	-0.692269000	1.108025000
803	Ni	-0.068436000	-2.340204000	0.139802000
804	Ni	-2.298631000	-1.359155000	0.367859000

805	Ni	-2.524477000	0.640703000	-1.008165000
806	Ni	-0.950748000	2.308767000	-0.101794000
807	Ni	0.203160000	1.291660000	1.870092000
808	Ni	-0.670162000	-1.003588000	2.163815000
809	Ni	-2.176433000	0.836796000	1.440829000
810	Ni	-0.411714000	0.015216000	-0.000791000
811	Ni	1.194947000	-0.903743000	-1.489588000
812	C	3.013136000	-1.557397000	-0.982500000
813	C	3.052729000	-1.929509000	0.436906000
814	C	3.611650000	-0.793568000	1.145444000
815	C	3.885431000	0.190936000	0.169189000
816	O	3.731338000	-0.308781000	-1.093738000
817	H	3.317468000	-2.258469000	-1.777165000
818	H	3.012368000	-2.964083000	0.783470000
819	H	3.915922000	-0.729459000	2.193098000
820	C	4.113100000	1.673807000	0.258862000
821	H	5.039894000	1.935511000	-0.301764000
822	O	3.014651000	2.401640000	-0.258223000
823	H	-1.806209000	2.131475000	-1.596005000
824	H	4.308207000	1.906029000	1.330198000
825	e.	TS2		
826		E+ZPE=-2545.663157		
827		G=-2545.707256		
828	Ni	-0.905444000	-0.288308000	-2.326913000
829	Ni	0.519380000	1.559987000	-1.492082000

830	Ni	1.706797000	0.804054000	0.610715000
831	Ni	0.914031000	-1.652749000	1.088089000
832	Ni	-0.677222000	-2.232739000	-0.770643000
833	Ni	-2.576950000	-0.699831000	-0.594112000
834	Ni	-1.895963000	1.598901000	-1.040436000
835	Ni	-0.335786000	2.240793000	0.761716000
836	Ni	-0.110802000	0.298176000	2.318031000
837	Ni	-1.544398000	-1.528956000	1.464355000
838	Ni	-2.282425000	0.835414000	1.289078000
839	Ni	-0.403126000	0.004941000	0.007332000
840	Ni	1.328450000	-0.840116000	-1.387692000
841	C	2.896925000	-1.872208000	-0.739394000
842	C	2.854410000	-1.975352000	0.718163000
843	C	3.282474000	-0.670326000	1.217540000
844	C	3.591230000	0.141438000	0.090718000
845	O	3.578112000	-0.639894000	-1.085562000
846	H	3.197336000	-2.697225000	-1.396613000
847	H	3.029773000	-2.920262000	1.252656000
848	H	3.557353000	-0.441264000	2.247716000
849	C	4.143743000	1.542047000	-0.022426000
850	H	4.583670000	1.658031000	-1.036202000
851	O	3.106515000	2.490475000	0.241312000
852	H	1.956546000	2.123166000	-0.580662000
853	H	4.962439000	1.691467000	0.711229000
854	f. FOL			

855	E+ZPE=-2545.680850			
856	G=-2545.726073			
857	Ni	-1.630469000	-1.342136000	-1.583820000
858	Ni	-0.103615000	0.480408000	-2.285811000
859	Ni	1.729645000	0.736937000	-0.562245000
860	Ni	1.249276000	-1.026020000	1.321688000
861	Ni	-0.824723000	-2.251220000	0.603550000
862	Ni	-2.637659000	-0.609546000	0.521263000
863	Ni	-2.245304000	1.046672000	-1.224577000
864	Ni	-0.221916000	2.301875000	-0.571771000
865	Ni	0.580214000	1.391196000	1.612361000
866	Ni	-0.961120000	-0.418514000	2.297529000
867	Ni	-1.828615000	1.610952000	1.155884000
868	Ni	-0.421108000	0.019098000	-0.006341000
869	Ni	0.808630000	-1.622591000	-1.202805000
870	C	2.735701000	-1.851710000	-0.925105000
871	C	2.823527000	-2.142819000	0.510911000
872	C	3.269791000	-0.954988000	1.187626000
873	C	3.463730000	0.074284000	0.168624000
874	O	3.413174000	-0.564796000	-1.120599000
875	H	3.105458000	-2.570892000	-1.676040000
876	H	2.846501000	-3.160859000	0.906373000
877	H	3.715674000	-0.895185000	2.185109000
878	C	4.433696000	1.219674000	0.285116000
879	H	5.405790000	0.966776000	-0.177707000

880	O	3.981144000	2.425374000	-0.364869000
881	H	2.994885000	2.444299000	-0.181982000
882	H	4.607902000	1.385483000	1.367615000
883	4. FAL to FOL on charged (-1) Ni cluster (path b)			
884	a. Ni + FAL+2H			
885	E+ZPE=-2545.733025			
886	G=-2545.776759			
887	Ni	-1.084290000	-1.217144000	-1.959602000
888	Ni	-0.328339000	1.141999000	-2.058880000
889	Ni	1.365964000	1.549329000	-0.214301000
890	Ni	1.593245000	-0.711417000	1.102384000
891	Ni	0.065021000	-2.342640000	-0.044629000
892	Ni	-2.213023000	-1.476739000	0.194605000
893	Ni	-2.489712000	0.616649000	-1.022283000
894	Ni	-1.022176000	2.256129000	0.073571000
895	Ni	0.131917000	1.147956000	1.974757000
896	Ni	-0.645564000	-1.199096000	2.066710000
897	Ni	-2.207172000	0.635318000	1.435417000
898	Ni	-0.377181000	-0.001226000	-0.010974000
899	Ni	1.309612000	-0.722666000	-1.517493000
900	C	3.069145000	-1.464350000	-0.982930000
901	C	3.183214000	-1.895167000	0.421085000
902	C	3.572375000	-0.762101000	1.214035000
903	C	3.547904000	0.354376000	0.294025000
904	O	3.595218000	-0.100983000	-1.022156000



905	H	3.511031000	-2.072987000	-1.787719000
906	H	3.236971000	-2.944171000	0.716569000
907	H	3.958486000	-0.748426000	2.235510000
908	C	3.257745000	1.750805000	0.506986000
909	H	3.338373000	2.107637000	1.552982000
910	O	3.090932000	2.599220000	-0.486346000
911	H	0.154943000	2.530921000	-1.135761000
912	H	-2.223704000	2.299094000	1.227328000
913	b.	TS1		
914		E+ZPE=-2545.668020		
915		G=-2545.711773		
916	Ni	-1.188986000	-1.166502000	-1.954551000
917	Ni	-0.233888000	1.118539000	-2.068841000
918	Ni	1.482420000	1.394320000	-0.220589000
919	Ni	1.511440000	-0.866542000	1.114831000
920	Ni	-0.146650000	-2.370617000	-0.026284000
921	Ni	-2.343198000	-1.311515000	0.196852000
922	Ni	-2.435848000	0.788029000	-1.037316000
923	Ni	-0.837393000	2.305289000	0.052048000
924	Ni	0.211058000	1.117638000	1.966378000
925	Ni	-0.764339000	-1.153805000	2.073126000
926	Ni	-2.161423000	0.802179000	1.421431000
927	Ni	-0.387349000	0.000055000	-0.012503000
928	Ni	1.236830000	-0.874811000	-1.506554000
929	C	3.023966000	-1.512706000	-0.976259000

930	C	3.121761000	-1.953937000	0.433918000
931	C	3.533185000	-0.835455000	1.230075000
932	C	3.624577000	0.282385000	0.294823000
933	O	3.661493000	-0.187748000	-1.010355000
934	H	3.455099000	-2.148717000	-1.768291000
935	H	3.158554000	-3.006843000	0.721688000
936	H	3.922710000	-0.839436000	2.249788000
937	C	3.417031000	1.662737000	0.518530000
938	H	3.490006000	2.047991000	1.544985000
939	O	3.273671000	2.545154000	-0.521159000
940	H	1.968905000	2.876055000	-0.484452000
941	H	-2.194594000	2.450353000	1.037088000
942	c.	IM1		
943		E+ZPE=-2545.694675		
944		G=-2545.739019		
945	Ni	1.036463000	-0.647495000	2.232653000
946	Ni	-0.267028000	1.410153000	1.771336000
947	Ni	-1.668911000	1.053715000	-0.310288000
948	Ni	-1.119455000	-1.360373000	-1.181479000
949	Ni	0.535162000	-2.325662000	0.447092000
950	Ni	2.546371000	-0.933346000	0.329280000
951	Ni	2.101530000	1.323413000	1.136942000
952	Ni	0.495164000	2.316507000	-0.438460000
953	Ni	-0.015762000	0.659849000	-2.208544000
954	Ni	1.302514000	-1.382627000	-1.742331000

955	Ni	2.245175000	0.878646000	-1.291615000
956	Ni	0.403960000	0.012929000	0.007402000
957	Ni	-1.293939000	-0.884512000	1.404843000
958	C	-3.017617000	-1.673146000	0.941800000
959	C	-2.896144000	-2.118244000	-0.455715000
960	C	-3.145281000	-0.979927000	-1.301196000
961	C	-3.484294000	0.124419000	-0.392250000
962	O	-3.713799000	-0.384268000	0.898592000
963	H	-3.480972000	-2.324488000	1.696802000
964	H	-2.944773000	-3.170914000	-0.750003000
965	H	-3.448314000	-0.996099000	-2.351454000
966	C	-3.587192000	1.534407000	-0.598915000
967	H	-3.811282000	1.904991000	-1.606611000
968	O	-4.187471000	2.351417000	0.387103000
969	H	-3.808913000	2.044549000	1.236481000
970	H	1.052729000	2.086212000	-2.064416000
971	d.	IM2		
972		E+ZPE=-2545.694190		
973		G=-2545.738020		
974	Ni	0.927743000	-0.289920000	2.326073000
975	Ni	-0.238822000	1.724614000	1.475313000
976	Ni	-1.591185000	1.098016000	-0.570948000
977	Ni	-1.176268000	-1.455263000	-0.998301000
978	Ni	0.374765000	-2.216546000	0.828058000
979	Ni	2.468256000	-0.979920000	0.555142000

980	Ni	2.140595000	1.402588000	0.955490000
981	Ni	0.632031000	2.220789000	-0.818839000
982	Ni	0.081028000	0.295539000	-2.312644000
983	Ni	1.261102000	-1.702083000	-1.451414000
984	Ni	2.338348000	0.535812000	-1.361354000
985	Ni	0.399567000	0.017589000	-0.004945000
986	Ni	-1.385605000	-0.534382000	1.458882000
987	C	-2.963062000	-1.654169000	1.011631000
988	C	-2.948382000	-2.179291000	-0.349768000
989	C	-3.152564000	-1.059880000	-1.240645000
990	C	-3.387961000	0.110456000	-0.394099000
991	O	-3.528833000	-0.313940000	0.960974000
992	H	-3.359675000	-2.219186000	1.864910000
993	H	-3.087129000	-3.237139000	-0.588261000
994	H	-3.481150000	-1.102576000	-2.281947000
995	C	-3.545902000	1.500926000	-0.678626000
996	H	-3.916388000	1.805104000	-1.664433000
997	O	-4.005355000	2.368157000	0.336303000
998	H	-3.415345000	2.191152000	1.101718000
999	H	-0.963150000	2.549352000	-1.155477000
1000	e.	TS2		
1001		E+ZPE=-2545.670093		
1002		G=-2545.714072		
1003	Ni	1.011228000	-0.369745000	2.296601000
1004	Ni	-0.212808000	1.656543000	1.562489000

1005	Ni	-1.614120000	1.089406000	-0.468260000
1006	Ni	-1.169375000	-1.436979000	-1.011584000
1007	Ni	0.446657000	-2.243820000	0.737401000
1008	Ni	2.510575000	-0.960189000	0.455723000
1009	Ni	2.155336000	1.398014000	0.962407000
1010	Ni	0.582252000	2.260363000	-0.733179000
1011	Ni	0.019888000	0.387653000	-2.288116000
1012	Ni	1.257440000	-1.621866000	-1.543345000
1013	Ni	2.299643000	0.629183000	-1.392652000
1014	Ni	0.410121000	0.022254000	-0.003657000
1015	Ni	-1.322023000	-0.620056000	1.486779000
1016	C	-2.962835000	-1.662909000	1.030358000
1017	C	-2.925430000	-2.192292000	-0.333808000
1018	C	-3.181284000	-1.087838000	-1.231944000
1019	C	-3.409113000	0.071411000	-0.390512000
1020	O	-3.558988000	-0.330871000	0.948854000
1021	H	-3.405293000	-2.231299000	1.859654000
1022	H	-3.035499000	-3.255227000	-0.565863000
1023	H	-3.486614000	-1.136187000	-2.279559000
1024	C	-3.597660000	1.493662000	-0.672036000
1025	H	-4.069868000	1.718572000	-1.637275000
1026	O	-4.198541000	2.262279000	0.348644000
1027	H	-3.658283000	2.085049000	1.148386000
1028	H	-2.321064000	2.294292000	-1.014668000
1029	f. FOL			

1030	E+ZPE=-2545.680850			
1031	G=-2545.726073			
1032	Ni	-1.630469000	-1.342136000	-1.583820000
1033	Ni	-0.103615000	0.480408000	-2.285811000
1034	Ni	1.729645000	0.736937000	-0.562245000
1035	Ni	1.249276000	-1.026020000	1.321688000
1036	Ni	-0.824723000	-2.251220000	0.603550000
1037	Ni	-2.637659000	-0.609546000	0.521263000
1038	Ni	-2.245304000	1.046672000	-1.224577000
1039	Ni	-0.221916000	2.301875000	-0.571771000
1040	Ni	0.580214000	1.391196000	1.612361000
1041	Ni	-0.961120000	-0.418514000	2.297529000
1042	Ni	-1.828615000	1.610952000	1.155884000
1043	Ni	-0.421108000	0.019098000	-0.006341000
1044	Ni	0.808630000	-1.622591000	-1.202805000
1045	C	2.735701000	-1.851710000	-0.925105000
1046	C	2.823527000	-2.142819000	0.510911000
1047	C	3.269791000	-0.954988000	1.187626000
1048	C	3.463730000	0.074284000	0.168624000
1049	O	3.413174000	-0.564796000	-1.120599000
1050	H	3.105458000	-2.570892000	-1.676040000
1051	H	2.846501000	-3.160859000	0.906373000
1052	H	3.715674000	-0.895185000	2.185109000
1053	C	4.433696000	1.219674000	0.285116000
1054	H	5.405790000	0.966776000	-0.177707000

1055	O	3.981144000	2.425374000	-0.364869000
1056	H	2.994885000	2.444299000	-0.181982000
1057	H	4.607902000	1.385483000	1.367615000
1058	5. CPO to CPOL on neutral Ni cluster (path a)			
1059	a. Ni + CPO+2H			
1060	E+ZPE=-2472.824296			
1061	G=-2472.869355			
1062	Ni	2.013125000	1.885071000	-0.091137000
1063	Ni	1.479338000	0.699183000	2.050948000
1064	Ni	1.040571000	-1.704674000	1.533619000
1065	Ni	1.306909000	-2.044028000	-0.934876000
1066	Ni	1.889228000	0.185329000	-1.932384000
1067	Ni	0.009761000	1.784446000	-1.507134000
1068	Ni	-0.275460000	2.081449000	0.918589000
1069	Ni	-0.802871000	-0.151755000	1.886412000
1070	Ni	-0.984419000	-1.843167000	0.071393000
1071	Ni	-0.441590000	-0.717491000	-2.046600000
1072	Ni	-1.784694000	0.494413000	-0.319514000
1073	Ni	0.500846000	0.036125000	-0.048724000
1074	Ni	2.765114000	-0.457706000	0.323579000
1075	C	-3.758584000	0.077351000	-1.224253000
1076	C	-4.208757000	-0.328636000	1.184462000
1077	C	-4.810381000	1.017993000	0.752965000
1078	C	-5.010476000	0.852955000	-0.769536000
1079	H	-2.947666000	0.872113000	-1.548900000

1080	H	-3.856143000	-0.536624000	-2.132670000
1081	H	-5.002538000	-1.091631000	1.321841000
1082	H	-3.617935000	-0.285534000	2.116640000
1083	H	-5.741437000	1.277116000	1.281444000
1084	H	-4.071569000	1.819915000	0.937296000
1085	H	-5.903259000	0.231461000	-0.965555000
1086	H	-5.144532000	1.812360000	-1.295820000
1087	C	-3.339588000	-0.750600000	-0.004543000
1088	O	-2.894182000	-1.999093000	-0.083232000
1089	H	-1.685522000	1.236199000	1.341501000
1090	H	-0.153214000	-1.478480000	2.658685000
1091	b. TS1			
1092	E+ZPE=-2472.791785			
1093	G=-2472.837718			
1094	Ni	2.071418000	1.825747000	0.348066000
1095	Ni	1.452755000	0.227164000	2.175922000
1096	Ni	0.990194000	-2.002784000	1.150270000
1097	Ni	1.321372000	-1.818266000	-1.325784000
1098	Ni	1.972493000	0.556215000	-1.813972000
1099	Ni	0.110069000	2.073392000	-1.108359000
1100	Ni	-0.242508000	1.858510000	1.317019000
1101	Ni	-0.844584000	-0.514239000	1.778965000
1102	Ni	-0.995657000	-1.781578000	-0.357812000
1103	Ni	-0.370297000	-0.248020000	-2.176224000
1104	Ni	-1.738356000	0.606675000	-0.267357000



1105	Ni	0.525535000	0.044492000	-0.040443000
1106	Ni	2.768483000	-0.568987000	0.276205000
1107	C	-3.806524000	0.264169000	-1.152720000
1108	C	-4.662778000	-0.596940000	0.989473000
1109	C	-5.159373000	0.841381000	0.813357000
1110	C	-5.054690000	1.066579000	-0.712825000
1111	H	-2.979580000	0.987540000	-1.516444000
1112	H	-3.961261000	-0.376226000	-2.035668000
1113	H	-5.413060000	-1.318736000	0.611300000
1114	H	-4.410820000	-0.873877000	2.026339000
1115	H	-6.175992000	1.008661000	1.202409000
1116	H	-4.476080000	1.532281000	1.342750000
1117	H	-5.948928000	0.651214000	-1.209620000
1118	H	-4.994394000	2.133273000	-0.982857000
1119	C	-3.434633000	-0.670923000	0.050804000
1120	O	-2.913273000	-1.894233000	-0.217155000
1121	H	-2.612615000	-0.029324000	0.940626000
1122	H	0.401200000	-1.219585000	2.648010000
1123	c. IM1			
1124	E+ZPE=-2472.789316			
1125	G=-2472.837212			
1126	Ni	2.521497000	1.374801000	0.457590000
1127	Ni	2.009143000	-0.697368000	1.770037000
1128	Ni	0.865920000	-2.324955000	0.259315000
1129	Ni	0.659190000	-1.286315000	-2.010772000

1130	Ni	1.669559000	1.007179000	-1.873943000
1131	Ni	0.379602000	2.367710000	-0.216308000
1132	Ni	0.547623000	1.322753000	2.005110000
1133	Ni	-0.422000000	-0.965910000	1.830469000
1134	Ni	-1.317000000	-1.334572000	-0.463571000
1135	Ni	-0.810061000	0.673726000	-1.788557000
1136	Ni	-1.498015000	0.925865000	0.603254000
1137	Ni	0.587307000	0.055368000	-0.022729000
1138	Ni	2.661791000	-0.891225000	-0.577581000
1139	C	-4.387233000	0.434667000	-1.081621000
1140	C	-5.199395000	-0.850879000	0.782774000
1141	C	-5.979605000	0.486267000	0.808129000
1142	C	-5.384502000	1.354302000	-0.353813000
1143	H	-3.540805000	0.971207000	-1.555389000
1144	H	-4.888000000	-0.170741000	-1.861552000
1145	H	-5.741399000	-1.615972000	0.194523000
1146	H	-5.010846000	-1.273667000	1.783848000
1147	H	-7.062901000	0.324354000	0.687139000
1148	H	-5.844517000	1.000318000	1.775020000
1149	H	-6.163883000	1.749700000	-1.025154000
1150	H	-4.850233000	2.225911000	0.064827000
1151	C	-3.894770000	-0.526186000	0.020780000
1152	O	-3.164493000	-1.631671000	-0.401797000
1153	H	-3.278612000	0.118677000	0.759438000
1154	H	0.842632000	-2.023034000	2.109393000

1155	d. IM2			
1156	E+ZPE=-2472.789780			
1157	G=-2472.837783			
1158	Ni	-2.604223000	1.319424000	-0.113158000
1159	Ni	-2.649939000	-1.176898000	0.099095000
1160	Ni	-0.653385000	-1.893418000	1.417389000
1161	Ni	0.652297000	0.148766000	2.045548000
1162	Ni	-0.550294000	2.128844000	1.080093000
1163	Ni	-0.606858000	1.911785000	-1.412654000
1164	Ni	-1.853169000	-0.117963000	-2.027806000
1165	Ni	-0.664156000	-2.062229000	-1.019990000
1166	Ni	1.406122000	-1.285042000	0.127144000
1167	Ni	1.471416000	1.166082000	-0.040505000
1168	Ni	0.657331000	-0.174455000	-1.986745000
1169	Ni	-0.581554000	0.050048000	-0.010425000
1170	Ni	-1.838761000	0.174537000	1.967703000
1171	C	3.805862000	0.852860000	-0.157981000
1172	C	5.565530000	-0.851850000	-0.379907000
1173	C	6.012594000	0.272036000	0.575011000
1174	C	5.188643000	1.483111000	0.097256000
1175	H	3.207190000	1.448977000	-0.906520000
1176	H	3.262112000	0.785454000	0.821887000
1177	H	5.738946000	-1.866465000	0.014484000
1178	H	6.119098000	-0.765057000	-1.332944000
1179	H	5.729458000	0.023973000	1.615210000

1180	H	7.100144000	0.452501000	0.561625000
1181	H	5.154321000	2.311528000	0.824642000
1182	H	5.613033000	1.881240000	-0.843265000
1183	C	4.041472000	-0.622895000	-0.638481000
1184	O	3.242951000	-1.574067000	0.031702000
1185	H	3.838605000	-0.669269000	-1.734272000
1186	H	-0.566276000	-3.115352000	0.230845000
1187	e.	TS2		
1188		E+ZPE=-2472.752983		
1189		G=-2472.802588		
1190	Ni	-2.892752000	0.031029000	-0.827654000
1191	Ni	-1.714508000	-2.096019000	-0.223165000
1192	Ni	-0.135205000	-1.617805000	1.651701000
1193	Ni	-0.318300000	0.809568000	2.238419000
1194	Ni	-2.011474000	1.825348000	0.689228000
1195	Ni	-1.199209000	1.598167000	-1.667348000
1196	Ni	-0.979162000	-0.787123000	-2.228535000
1197	Ni	0.673381000	-1.779121000	-0.649162000
1198	Ni	1.597087000	-0.003794000	0.834035000
1199	Ni	0.444823000	2.096248000	0.283957000
1200	Ni	1.058843000	0.517546000	-1.553830000
1201	Ni	-0.645357000	0.050418000	-0.013969000
1202	Ni	-2.313351000	-0.510419000	1.538453000
1203	C	4.408932000	1.088550000	-0.223418000
1204	C	5.499481000	-1.105740000	-0.483661000

1205	C	6.407594000	-0.182876000	0.347359000
1206	C	5.946126000	1.220490000	-0.093611000
1207	H	3.988800000	1.697918000	-1.043617000
1208	H	3.890288000	1.406657000	0.700480000
1209	H	5.454859000	-2.148339000	-0.128755000
1210	H	5.853317000	-1.121109000	-1.532288000
1211	H	6.204543000	-0.327083000	1.424830000
1212	H	7.483905000	-0.358360000	0.184453000
1213	H	6.252867000	2.019792000	0.601375000
1214	H	6.391606000	1.455654000	-1.077745000
1215	C	4.106779000	-0.432223000	-0.421114000
1216	O	3.342019000	-0.963908000	0.668105000
1217	H	3.531303000	-0.600187000	-1.361524000
1218	H	2.184024000	-1.596130000	0.114994000
1219	f. CPOL			
1220	E+ZPE=-2472.764041			
1221	G=-2472.812995			
1222	Ni	2.981814000	0.395503000	0.473193000
1223	Ni	1.789724000	-1.668653000	1.245273000
1224	Ni	0.032415000	-2.239985000	-0.435073000
1225	Ni	0.116233000	-0.542026000	-2.273473000
1226	Ni	1.929673000	1.093815000	-1.695335000
1227	Ni	1.347460000	2.227968000	0.458601000
1228	Ni	1.223691000	0.552529000	2.255917000
1229	Ni	-0.552562000	-1.081579000	1.636044000

1230	Ni	-1.643467000	-0.378915000	-0.490238000
1231	Ni	-0.481854000	1.633675000	-1.290370000
1232	Ni	-0.891703000	1.347159000	1.158451000
1233	Ni	0.667806000	0.048093000	-0.014522000
1234	Ni	2.191524000	-1.334023000	-1.142781000
1235	C	-4.478349000	1.113274000	0.282652000
1236	C	-5.772286000	-0.920304000	0.673274000
1237	C	-6.464612000	-0.144120000	-0.461586000
1238	C	-5.913093000	1.290213000	-0.295218000
1239	H	-4.310091000	1.737623000	1.176017000
1240	H	-3.675443000	1.376280000	-0.432524000
1241	H	-5.813575000	-2.018057000	0.571309000
1242	H	-6.224943000	-0.659941000	1.647782000
1243	H	-6.153759000	-0.563575000	-1.434444000
1244	H	-7.563986000	-0.193096000	-0.412542000
1245	H	-5.919712000	1.857114000	-1.239984000
1246	H	-6.539620000	1.849183000	0.421005000
1247	C	-4.339226000	-0.377029000	0.650951000
1248	O	-3.583563000	-1.019299000	-0.446697000
1249	H	-3.767171000	-0.541789000	1.581937000
1250	H	-3.458962000	-1.961300000	-0.204649000

1251 6. CPO to CPO<sub>L</sub> on neutral Ni cluster (path b)

1252 a. Ni + CPO+2H

1253 E+ZPE=-2472.828914

1254 G=-2472.873489

1255	Ni	-1.792377000	1.991221000	0.375458000
1256	Ni	-2.487982000	0.197911000	-1.230834000
1257	Ni	-1.661034000	-1.996962000	-0.370391000
1258	Ni	-0.447033000	-1.593292000	1.783515000
1259	Ni	-0.518119000	0.876114000	2.227223000
1260	Ni	0.661949000	2.071779000	0.370904000
1261	Ni	-0.507395000	1.638982000	-1.750337000
1262	Ni	-0.459135000	-0.819412000	-2.144626000
1263	Ni	0.841702000	-1.939925000	-0.343587000
1264	Ni	1.521937000	-0.213377000	1.267984000
1265	Ni	1.546416000	0.312588000	-1.176565000
1266	Ni	-0.442322000	0.048351000	0.034804000
1267	Ni	-2.472372000	-0.275362000	1.167052000
1268	C	3.725032000	-0.292674000	1.204282000
1269	C	3.743301000	0.034074000	-1.268085000
1270	C	4.834696000	0.892821000	-0.592336000
1271	C	4.365475000	1.061922000	0.866500000
1272	H	3.048783000	-0.211006000	2.144661000
1273	H	4.456371000	-1.061736000	1.514034000
1274	H	4.117880000	-0.662684000	-2.033992000
1275	H	3.057212000	0.760065000	-1.876666000
1276	H	5.783173000	0.327053000	-0.612109000
1277	H	5.009904000	1.855914000	-1.098307000
1278	H	5.181509000	1.342069000	1.551362000
1279	H	3.582086000	1.840755000	0.921453000

1280	C	3.063576000	-0.750960000	-0.122832000
1281	O	2.756860000	-2.053913000	-0.298128000
1282	H	0.531936000	0.514690000	-2.637918000
1283	H	-1.174824000	-2.306106000	-1.909492000
1284	b. TS1			
1285	E+ZPE=-2472.766882			
1286	G=-2472.811192			
1287	Ni	1.738385000	-2.022772000	0.390399000
1288	Ni	2.555771000	-0.205961000	-1.129942000
1289	Ni	1.731843000	1.984810000	-0.256553000
1290	Ni	0.397893000	1.555118000	1.820046000
1291	Ni	0.392807000	-0.925598000	2.202058000
1292	Ni	-0.713277000	-2.047380000	0.256162000
1293	Ni	0.575017000	-1.588726000	-1.789444000
1294	Ni	0.599938000	0.879708000	-2.121105000
1295	Ni	-0.769485000	1.984082000	-0.360992000
1296	Ni	-1.570327000	0.232439000	1.166478000
1297	Ni	-1.477545000	-0.229089000	-1.288453000
1298	Ni	0.450160000	-0.041645000	0.030895000
1299	Ni	2.424243000	0.207225000	1.275474000
1300	C	-3.763737000	0.458768000	1.162425000
1301	C	-3.772247000	-0.199512000	-1.231614000
1302	C	-4.736479000	-1.116636000	-0.437488000
1303	C	-4.352314000	-0.960076000	1.053131000
1304	H	-3.086365000	0.564646000	2.096649000



1305	H	-4.518898000	1.249196000	1.333526000
1306	H	-4.292972000	0.449630000	-1.955211000
1307	H	-3.073542000	-0.836741000	-1.890030000
1308	H	-5.767694000	-0.758084000	-0.596685000
1309	H	-4.702349000	-2.167738000	-0.765450000
1310	H	-5.205211000	-1.124680000	1.731163000
1311	H	-3.561440000	-1.686495000	1.317067000
1312	C	-3.059947000	0.677285000	-0.183822000
1313	O	-2.830512000	2.018209000	-0.585258000
1314	H	-0.558484000	-0.587818000	-2.695890000
1315	H	-1.872447000	1.691565000	-1.529547000
1316	c.	IM1		
1317		E+ZPE=-2472.784056		
1318		G=-2472.828451		
1319	Ni	1.794608000	-1.964486000	0.484408000
1320	Ni	2.470940000	-0.301033000	-1.263278000
1321	Ni	1.682978000	1.958792000	-0.547616000
1322	Ni	0.513075000	1.727563000	1.654768000
1323	Ni	0.571865000	-0.703667000	2.276270000
1324	Ni	-0.659690000	-2.019079000	0.538137000
1325	Ni	0.466094000	-1.755788000	-1.633659000
1326	Ni	0.432106000	0.668505000	-2.205796000
1327	Ni	-0.818807000	1.932406000	-0.464991000
1328	Ni	-1.478980000	0.333306000	1.283513000
1329	Ni	-1.562814000	-0.366778000	-1.113747000

1330	Ni	0.455644000	-0.037108000	0.030408000
1331	Ni	2.512620000	0.346309000	1.093205000
1332	C	-3.741678000	0.314390000	1.206077000
1333	C	-3.782146000	-0.121057000	-1.228397000
1334	C	-4.715198000	-1.121978000	-0.501172000
1335	C	-4.262777000	-1.115370000	0.976691000
1336	H	-3.097858000	0.378081000	2.157702000
1337	H	-4.549439000	1.047586000	1.391211000
1338	H	-4.338427000	0.584700000	-1.873397000
1339	H	-3.101966000	-0.650652000	-1.999612000
1340	H	-5.753765000	-0.756765000	-0.575477000
1341	H	-4.685784000	-2.129979000	-0.943821000
1342	H	-5.067231000	-1.395962000	1.674805000
1343	H	-3.419333000	-1.817821000	1.117666000
1344	C	-3.030708000	0.642312000	-0.114454000
1345	O	-2.940786000	2.101388000	-0.354345000
1346	H	-0.696112000	-0.846856000	-2.543446000
1347	H	-3.198674000	2.256375000	-1.288727000
1348	d. IM2			
1349	E+ZPE=-2472.768054			
1350	G=-2472.814057			
1351	Ni	-2.030948000	1.899766000	0.002096000
1352	Ni	-1.867326000	0.329289000	-1.943267000
1353	Ni	-1.322151000	-1.947901000	-1.074292000
1354	Ni	-1.146186000	-1.820027000	1.421386000

1355	Ni	-1.568341000	0.565822000	2.075856000
1356	Ni	0.190410000	2.017064000	1.041946000
1357	Ni	0.043275000	1.855784000	-1.409503000
1358	Ni	0.423654000	-0.527162000	-2.026992000
1359	Ni	0.932137000	-1.863782000	0.011489000
1360	Ni	0.757025000	-0.353752000	1.946591000
1361	Ni	1.758739000	0.500872000	-0.175858000
1362	Ni	-0.528181000	0.030637000	0.035120000
1363	Ni	-2.817990000	-0.462690000	0.164564000
1364	C	4.136171000	-0.364230000	1.170575000
1365	C	4.463681000	-0.118503000	-1.201649000
1366	C	5.179322000	1.087763000	-0.549640000
1367	C	4.953582000	0.934687000	0.990946000
1368	H	3.443674000	-0.329648000	2.033440000
1369	H	4.808091000	-1.237035000	1.320750000
1370	H	5.178446000	-0.960436000	-1.336325000
1371	H	4.028400000	0.113104000	-2.188937000
1372	H	6.248702000	1.110891000	-0.815230000
1373	H	4.727460000	2.028394000	-0.902802000
1374	H	5.901873000	0.896569000	1.551407000
1375	H	4.378460000	1.794383000	1.373002000
1376	C	3.414256000	-0.519252000	-0.166453000
1377	O	3.004687000	-1.946702000	-0.333226000
1378	H	2.354176000	1.854680000	-0.465519000
1379	H	2.935848000	-2.089850000	-1.302489000

1380	e.	TS2		
1381		E+ZPE=-2472.748401		
1382		G=-2472.794421		
1383	Ni	2.054586000	-1.851547000	-0.424579000
1384	Ni	1.979812000	0.171767000	-1.900450000
1385	Ni	1.391956000	2.151129000	-0.495290000
1386	Ni	1.100102000	1.381730000	1.870833000
1387	Ni	1.494256000	-1.096682000	1.901382000
1388	Ni	-0.212652000	-2.210501000	0.447391000
1389	Ni	0.048288000	-1.420035000	-1.868728000
1390	Ni	-0.305841000	1.045551000	-1.862461000
1391	Ni	-0.910426000	1.812660000	0.428131000
1392	Ni	-0.823697000	-0.149744000	1.910284000
1393	Ni	-1.724342000	-0.413126000	-0.404477000
1394	Ni	0.549609000	-0.038776000	0.024832000
1395	Ni	2.830295000	0.379021000	0.381585000
1396	C	-4.054201000	-0.014866000	1.178587000
1397	C	-4.871419000	0.478274000	-1.017207000
1398	C	-5.568975000	-0.836602000	-0.604368000
1399	C	-5.053975000	-1.143468000	0.840637000
1400	H	-3.232185000	-0.349768000	1.842848000
1401	H	-4.558219000	0.837707000	1.675297000
1402	H	-5.465684000	1.354330000	-0.693316000
1403	H	-4.697695000	0.565174000	-2.103064000
1404	H	-6.664896000	-0.741131000	-0.650719000

1405	H	-5.286639000	-1.652253000	-1.291272000
1406	H	-5.872061000	-1.187699000	1.576536000
1407	H	-4.539944000	-2.119239000	0.864429000
1408	C	-3.568486000	0.469283000	-0.192873000
1409	O	-3.032823000	1.846772000	-0.085878000
1410	H	-3.064625000	-0.654818000	-0.987749000
1411	H	-2.867639000	2.137309000	-1.011320000
1412	f.	CPOL		
1413		E+ZPE=-2472.764041		
1414		G=-2472.812995		
1415	Ni	2.981814000	0.395503000	0.473193000
1416	Ni	1.789724000	-1.668653000	1.245273000
1417	Ni	0.032415000	-2.239985000	-0.435073000
1418	Ni	0.116233000	-0.542026000	-2.273473000
1419	Ni	1.929673000	1.093815000	-1.695335000
1420	Ni	1.347460000	2.227968000	0.458601000
1421	Ni	1.223691000	0.552529000	2.255917000
1422	Ni	-0.552562000	-1.081579000	1.636044000
1423	Ni	-1.643467000	-0.378915000	-0.490238000
1424	Ni	-0.481854000	1.633675000	-1.290370000
1425	Ni	-0.891703000	1.347159000	1.158451000
1426	Ni	0.667806000	0.048093000	-0.014522000
1427	Ni	2.191524000	-1.334023000	-1.142781000
1428	C	-4.478349000	1.113274000	0.282652000
1429	C	-5.772286000	-0.920304000	0.673274000

1430	C	-6.464612000	-0.144120000	-0.461586000
1431	C	-5.913093000	1.290213000	-0.295218000
1432	H	-4.310091000	1.737623000	1.176017000
1433	H	-3.675443000	1.376280000	-0.432524000
1434	H	-5.813575000	-2.018057000	0.571309000
1435	H	-6.224943000	-0.659941000	1.647782000
1436	H	-6.153759000	-0.563575000	-1.434444000
1437	H	-7.563986000	-0.193096000	-0.412542000
1438	H	-5.919712000	1.857114000	-1.239984000
1439	H	-6.539620000	1.849183000	0.421005000
1440	C	-4.339226000	-0.377029000	0.650951000
1441	O	-3.583563000	-1.019299000	-0.446697000
1442	H	-3.767171000	-0.541789000	1.581937000
1443	H	-3.458962000	-1.961300000	-0.204649000

1444 7. CPO to CPO<sub>L</sub> on charged (-1) Ni cluster (path a)

1445 a. Ni + CPO+2H

1446 E+ZPE=-2472.923643

1447 G=-2472.969288

1448	Ni	2.797154000	-0.678930000	-0.180844000
1449	Ni	2.141102000	1.267033000	1.206956000
1450	Ni	-0.173190000	0.872588000	2.148385000
1451	Ni	-0.975008000	-1.450869000	1.229902000
1452	Ni	0.908798000	-2.323684000	-0.178475000
1453	Ni	1.205899000	-0.757030000	-2.035805000
1454	Ni	1.964170000	1.418483000	-1.238209000

1455	Ni	0.142676000	2.342851000	0.148999000
1456	Ni	-1.737638000	0.694722000	0.149958000
1457	Ni	-1.066492000	-1.229020000	-1.247459000
1458	Ni	-0.406883000	1.079184000	-1.886474000
1459	Ni	0.505461000	0.012604000	0.086748000
1460	Ni	1.537277000	-1.090830000	1.920888000
1461	C	-3.773917000	1.111317000	-0.551003000
1462	C	-4.167112000	-1.117500000	0.500355000
1463	C	-5.400728000	-0.214139000	0.705973000
1464	C	-4.852488000	1.221311000	0.549587000
1465	H	-2.920514000	1.889471000	-0.354409000
1466	H	-4.104743000	1.398358000	-1.563622000
1467	H	-4.409379000	-2.122527000	0.117960000
1468	H	-3.606967000	-1.240081000	1.447440000
1469	H	-6.138420000	-0.415517000	-0.092248000
1470	H	-5.907269000	-0.373018000	1.672598000
1471	H	-5.637595000	1.954523000	0.301531000
1472	H	-4.376273000	1.547419000	1.491382000
1473	C	-3.311680000	-0.359486000	-0.535718000
1474	O	-2.936068000	-0.995258000	-1.648452000
1475	H	-0.376463000	-2.915981000	0.724024000
1476	H	-1.611390000	-0.008483000	1.939815000
1477	b. TS1			
1478	E+ZPE=-2472.890367			
1479	G=-2472.935441			

1480	Ni	2.820951000	-0.643892000	-0.340073000
1481	Ni	2.208905000	1.079424000	1.332777000
1482	Ni	-0.083242000	0.554177000	2.264542000
1483	Ni	-0.918497000	-1.610071000	1.037377000
1484	Ni	0.925165000	-2.268874000	-0.530637000
1485	Ni	1.184081000	-0.447954000	-2.145674000
1486	Ni	1.972144000	1.586652000	-1.058809000
1487	Ni	0.190187000	2.300373000	0.493953000
1488	Ni	-1.697657000	0.675525000	0.301922000
1489	Ni	-1.070299000	-1.029546000	-1.377935000
1490	Ni	-0.416059000	1.347568000	-1.690023000
1491	Ni	0.539529000	0.002574000	0.083372000
1492	Ni	1.611535000	-1.356650000	1.710083000
1493	C	-3.832888000	1.049601000	-0.418167000
1494	C	-4.679377000	-1.085421000	0.542286000
1495	C	-5.832168000	-0.086289000	0.332165000
1496	C	-5.122515000	1.279957000	0.390513000
1497	H	-3.042658000	1.839840000	-0.145753000
1498	H	-3.981559000	1.179644000	-1.503311000
1499	H	-4.865799000	-2.089723000	0.129905000
1500	H	-4.471050000	-1.196546000	1.621332000
1501	H	-6.282721000	-0.227729000	-0.667268000
1502	H	-6.637594000	-0.189847000	1.077682000
1503	H	-5.729878000	2.108784000	-0.008935000
1504	H	-4.865773000	1.525444000	1.437376000



1505	C	-3.450923000	-0.457641000	-0.192966000
1506	O	-2.991614000	-1.148113000	-1.270344000
1507	H	0.398560000	-2.656874000	1.164373000
1508	H	-2.550218000	-0.609903000	0.869840000
1509	c. IM1			
1510	E+ZPE=-2472.892005			
1511	G=-2472.939916			
1512	Ni	2.755282000	-0.566996000	-0.812259000
1513	Ni	2.460126000	1.116234000	0.982905000
1514	Ni	0.429023000	0.510571000	2.362919000
1515	Ni	-0.585260000	-1.663561000	1.297955000
1516	Ni	0.906571000	-2.246624000	-0.632564000
1517	Ni	0.772027000	-0.399015000	-2.232325000
1518	Ni	1.714368000	1.645198000	-1.296768000
1519	Ni	0.277992000	2.285266000	0.606795000
1520	Ni	-1.563159000	0.604946000	0.783166000
1521	Ni	-1.255167000	-1.057767000	-1.021565000
1522	Ni	-0.745606000	1.341332000	-1.419530000
1523	Ni	0.596293000	0.003988000	0.090342000
1524	Ni	2.021619000	-1.341404000	1.431774000
1525	C	-4.384661000	0.834342000	-0.872307000
1526	C	-5.120109000	-1.108689000	0.356461000
1527	C	-5.939229000	0.094315000	0.892178000
1528	C	-5.316709000	1.368183000	0.227058000
1529	H	-3.559738000	1.525603000	-1.132374000

1530	H	-4.941804000	0.593597000	-1.798994000
1531	H	-5.662730000	-1.632510000	-0.453074000
1532	H	-4.874144000	-1.858200000	1.127522000
1533	H	-7.006505000	-0.008926000	0.637145000
1534	H	-5.883655000	0.163575000	1.991486000
1535	H	-6.082907000	2.063094000	-0.152987000
1536	H	-4.714710000	1.922860000	0.970357000
1537	C	-3.849951000	-0.486964000	-0.273554000
1538	O	-3.133405000	-1.322491000	-1.108281000
1539	H	0.722580000	-2.722579000	1.087562000
1540	H	-3.220252000	-0.174401000	0.666883000
1541	d. IM2			
1542	E+ZPE=-2472.891813			
1543	G=-2472.940473			
1544	Ni	-2.752375000	0.569988000	-0.824983000
1545	Ni	-2.470266000	-1.123132000	0.963101000
1546	Ni	-0.450364000	-0.523184000	2.362658000
1547	Ni	0.571216000	1.655786000	1.319304000
1548	Ni	-0.908455000	2.249476000	-0.621789000
1549	Ni	-0.756248000	0.411316000	-2.230344000
1550	Ni	-1.706417000	-1.638790000	-1.313622000
1551	Ni	-0.284611000	-2.288440000	0.597675000
1552	Ni	1.554929000	-0.608846000	0.797279000
1553	Ni	1.259451000	1.065455000	-1.000091000
1554	Ni	0.754008000	-1.332741000	-1.415007000

1555	Ni	-0.600266000	-0.005137000	0.091209000
1556	Ni	-2.037214000	1.332326000	1.429087000
1557	C	4.383256000	-0.824246000	-0.883213000
1558	C	5.140739000	1.094690000	0.367671000
1559	C	5.966655000	-0.117978000	0.869780000
1560	C	5.335931000	-1.379062000	0.187878000
1561	H	3.551702000	-1.508842000	-1.141502000
1562	H	4.921851000	-0.567680000	-1.816556000
1563	H	5.671484000	1.631131000	-0.441541000
1564	H	4.909406000	1.831668000	1.155206000
1565	H	7.030886000	-0.009447000	0.604317000
1566	H	5.924405000	-0.208504000	1.968161000
1567	H	6.097489000	-2.062611000	-0.221032000
1568	H	4.749968000	-1.952572000	0.929504000
1569	C	3.859761000	0.485012000	-0.251071000
1570	O	3.132390000	1.338930000	-1.060232000
1571	H	-0.130212000	3.036721000	0.687746000
1572	H	3.240985000	0.154038000	0.685961000
1573	e.	TS2		
1574		E+ZPE=-2472.851883		
1575		G=-2472.899198		
1576	Ni	2.672731000	-0.594436000	-1.054575000
1577	Ni	2.644417000	0.668931000	1.077626000
1578	Ni	0.611143000	-0.013762000	2.419928000
1579	Ni	-0.688670000	-1.777798000	0.977463000

1580	Ni	0.653365000	-2.069746000	-1.127629000
1581	Ni	0.668184000	0.089968000	-2.275251000
1582	Ni	1.876810000	1.766639000	-0.981389000
1583	Ni	0.600130000	2.112881000	1.098361000
1584	Ni	-1.416903000	0.637802000	1.031794000
1585	Ni	-1.372654000	-0.604785000	-1.114396000
1586	Ni	-0.604661000	1.755357000	-1.011257000
1587	Ni	0.630958000	-0.016703000	0.086920000
1588	Ni	1.942464000	-1.767609000	1.010301000
1589	C	-4.475430000	0.726456000	-0.920455000
1590	C	-5.351865000	-1.028398000	0.505638000
1591	C	-6.289489000	0.205107000	0.648188000
1592	C	-5.544463000	1.392348000	-0.041146000
1593	H	-3.613289000	1.373410000	-1.171477000
1594	H	-4.911146000	0.344844000	-1.864417000
1595	H	-5.754541000	-1.750427000	-0.227741000
1596	H	-5.197913000	-1.575341000	1.451366000
1597	H	-7.257497000	0.013664000	0.156736000
1598	H	-6.512535000	0.435879000	1.702816000
1599	H	-6.225373000	2.051666000	-0.603145000
1600	H	-5.045339000	2.017224000	0.722540000
1601	C	-4.029327000	-0.465882000	-0.058303000
1602	O	-3.223815000	-1.419388000	-0.722811000
1603	H	-2.196053000	-1.724672000	0.137556000
1604	H	-3.437106000	-0.037590000	0.813629000

1605	f. CPOL			
1606	E+ZPE=-2472.856557			
1607	G=-2472.905324			
1608	Ni	-2.499908000	0.804853000	-1.265029000
1609	Ni	-2.837811000	-0.626028000	0.730382000
1610	Ni	-0.984807000	-0.181158000	2.393946000
1611	Ni	0.593158000	1.610023000	1.306975000
1612	Ni	-0.419466000	2.154097000	-0.928781000
1613	Ni	-0.378010000	0.098021000	-2.255219000
1614	Ni	-1.841208000	-1.598475000	-1.293095000
1615	Ni	-0.891427000	-2.191258000	0.907506000
1616	Ni	1.185128000	-0.841636000	1.240009000
1617	Ni	1.508303000	0.570832000	-0.763821000
1618	Ni	0.616681000	-1.738528000	-0.980496000
1619	Ni	-0.672518000	0.012229000	0.088343000
1620	Ni	-2.012965000	1.759861000	0.976548000
1621	C	4.557835000	-0.804396000	-0.765151000
1622	C	5.690480000	1.038435000	0.312084000
1623	C	6.459196000	-0.231319000	0.731465000
1624	C	5.853878000	-1.383224000	-0.135620000
1625	H	3.681770000	-1.478408000	-0.722617000
1626	H	4.715566000	-0.531350000	-1.824625000
1627	H	6.104184000	1.460617000	-0.622488000
1628	H	5.694649000	1.830585000	1.079092000
1629	H	7.547518000	-0.125749000	0.601071000

1630	H	6.282211000	-0.432112000	1.802391000
1631	H	6.556439000	-1.710079000	-0.918582000
1632	H	5.638005000	-2.268007000	0.485620000
1633	C	4.294795000	0.482346000	0.021235000
1634	O	3.440658000	1.372485000	-0.759117000
1635	H	3.138837000	2.095556000	-0.159571000
1636	H	3.754288000	0.248686000	0.965098000
1637	8. CPO to CPOL on charged (-1) Ni cluster (path b)			
1638	a. Ni + CPO+2H			
1639	E+ZPE=-2472.936791			
1640	G=-2472.981176			
1641	Ni	-2.534628000	-0.468215000	-1.114953000
1642	Ni	-1.794569000	-1.823604000	0.823444000
1643	Ni	-0.451414000	-0.362931000	2.390712000
1644	Ni	-0.343851000	2.019050000	1.301713000
1645	Ni	-1.652066000	1.856824000	-0.839505000
1646	Ni	-0.495165000	0.240434000	-2.266022000
1647	Ni	-0.576037000	-1.999682000	-1.301243000
1648	Ni	0.707795000	-1.912267000	0.804869000
1649	Ni	1.589203000	0.409762000	1.081628000
1650	Ni	0.844875000	1.744715000	-0.867540000
1651	Ni	1.489093000	-0.643337000	-1.152658000
1652	Ni	-0.490813000	-0.007271000	0.087842000
1653	Ni	-2.540112000	0.580203000	1.137741000
1654	C	3.706211000	-0.492968000	-1.179801000

1655	C	3.777081000	0.728746000	0.991974000
1656	C	4.887701000	-0.341285000	0.929005000
1657	C	4.396832000	-1.362146000	-0.117015000
1658	H	3.012722000	-1.139792000	-1.854224000
1659	H	4.409008000	-0.063845000	-1.918214000
1660	H	4.135946000	1.750005000	1.193593000
1661	H	3.109023000	0.482640000	1.918614000
1662	H	5.814903000	0.139429000	0.568548000
1663	H	5.108907000	-0.803037000	1.905282000
1664	H	5.208506000	-1.986600000	-0.523552000
1665	H	3.637638000	-2.028162000	0.336037000
1666	C	3.062995000	0.670955000	-0.380421000
1667	O	2.758471000	1.820842000	-1.021429000
1668	H	-1.126878000	3.026858000	0.239516000
1669	H	0.572812000	1.092906000	2.434571000
1670	b. TS1			
1671	E+ZPE=-2472.867411			
1672	G=-2472.912192			
1673	Ni	-2.476017000	-0.605269000	-1.173761000
1674	Ni	-1.727718000	-1.872274000	0.820749000
1675	Ni	-0.524612000	-0.302368000	2.396801000
1676	Ni	-0.515606000	2.057480000	1.253585000
1677	Ni	-1.737159000	1.772376000	-0.925001000
1678	Ni	-0.441212000	0.193835000	-2.272757000
1679	Ni	-0.429203000	-2.023605000	-1.258343000

1680	Ni	0.774296000	-1.816801000	0.887861000
1681	Ni	1.510486000	0.560907000	1.135777000
1682	Ni	0.761762000	1.803811000	-0.867962000
1683	Ni	1.552090000	-0.552369000	-1.070579000
1684	Ni	-0.504569000	-0.001232000	0.085205000
1685	Ni	-2.619416000	0.491160000	1.051207000
1686	C	3.761393000	-0.359066000	-1.242969000
1687	C	3.796611000	0.591378000	1.054218000
1688	C	4.810041000	-0.577141000	0.951012000
1689	C	4.396070000	-1.392438000	-0.295034000
1690	H	3.071907000	-0.870464000	-2.019928000
1691	H	4.493615000	0.170752000	-1.881813000
1692	H	4.280607000	1.563868000	1.243217000
1693	H	3.113618000	0.429336000	1.968928000
1694	H	5.816338000	-0.150296000	0.797784000
1695	H	4.853239000	-1.197712000	1.860708000
1696	H	5.240851000	-1.934781000	-0.750103000
1697	H	3.618794000	-2.130154000	-0.020810000
1698	C	3.060389000	0.634083000	-0.303491000
1699	O	2.835097000	1.937088000	-0.816343000
1700	H	1.921318000	2.325289000	0.121302000
1701	H	0.514449000	1.158335000	2.471173000
1702	c.	IM1		
1703		E+ZPE=-2472.881800		
1704		G=-2472.926366		



1705	Ni	-2.520226000	-0.469877000	-1.166326000
1706	Ni	-1.777731000	-1.874580000	0.735994000
1707	Ni	-0.496816000	-0.438222000	2.376727000
1708	Ni	-0.432115000	1.983327000	1.372844000
1709	Ni	-1.700849000	1.864898000	-0.794212000
1710	Ni	-0.480632000	0.328724000	-2.256768000
1711	Ni	-0.522005000	-1.943787000	-1.373524000
1712	Ni	0.725552000	-1.901025000	0.757006000
1713	Ni	1.542295000	0.433952000	1.128302000
1714	Ni	0.798433000	1.815155000	-0.784598000
1715	Ni	1.508692000	-0.548518000	-1.139428000
1716	Ni	-0.508233000	-0.002557000	0.086673000
1717	Ni	-2.588581000	0.497801000	1.121075000
1718	C	3.723314000	-0.380179000	-1.221557000
1719	C	3.827393000	0.542841000	1.077867000
1720	C	4.853816000	-0.609606000	0.916039000
1721	C	4.371297000	-1.426759000	-0.298895000
1722	H	3.045002000	-0.888017000	-2.010945000
1723	H	4.456989000	0.170477000	-1.840162000
1724	H	4.314285000	1.511286000	1.288506000
1725	H	3.170808000	0.348363000	1.997453000
1726	H	5.842318000	-0.168679000	0.700013000
1727	H	4.957185000	-1.222954000	1.825579000
1728	H	5.181724000	-1.988682000	-0.790769000
1729	H	3.588514000	-2.144050000	0.012211000

1730	C	3.032023000	0.593538000	-0.251259000
1731	O	2.956604000	1.954123000	-0.839873000
1732	H	2.996835000	2.578167000	-0.082136000
1733	H	0.608511000	0.983962000	2.500641000
1734	d. IM2			
1735	E+ZPE=-2472.869646			
1736	G=-2472.915509			
1737	Ni	-2.837679000	0.280251000	-0.560853000
1738	Ni	-2.087361000	-1.571080000	0.906514000
1739	Ni	-0.063402000	-0.816431000	2.224143000
1740	Ni	0.459015000	1.639633000	1.466876000
1741	Ni	-1.295770000	2.222967000	-0.235510000
1742	Ni	-1.001877000	0.693385000	-2.122892000
1743	Ni	-1.488699000	-1.605830000	-1.475089000
1744	Ni	0.214253000	-2.250213000	0.192437000
1745	Ni	1.752020000	-0.313406000	0.514881000
1746	Ni	0.990576000	1.526869000	-0.964275000
1747	Ni	0.859935000	-0.841000000	-1.716004000
1748	Ni	-0.535172000	-0.007556000	0.084177000
1749	Ni	-2.031324000	0.829001000	1.724340000
1750	C	4.095738000	-0.208770000	-1.213894000
1751	C	4.488963000	0.640272000	0.980431000
1752	C	5.103634000	-0.785828000	0.957448000
1753	C	4.720161000	-1.383453000	-0.437125000
1754	H	3.400412000	-0.530265000	-2.014305000

1755	H	4.887830000	0.417326000	-1.685470000
1756	H	5.257090000	1.392727000	0.687729000
1757	H	4.099379000	0.930833000	1.971328000
1758	H	6.196029000	-0.749813000	1.102647000
1759	H	4.688999000	-1.405902000	1.769837000
1760	H	5.580489000	-1.832946000	-0.960386000
1761	H	3.950795000	-2.167344000	-0.309573000
1762	C	3.403535000	0.574986000	-0.100608000
1763	O	3.068330000	1.941949000	-0.625101000
1764	H	2.825522000	2.461773000	0.175072000
1765	H	1.528209000	-1.099702000	2.061509000
1766	e.	TS2		
1767		E+ZPE=-2472.843826		
1768		G=-2472.889929		
1769	Ni	-2.873121000	0.098833000	-0.606354000
1770	Ni	-2.079205000	-1.426756000	1.178511000
1771	Ni	-0.090920000	-0.379311000	2.340772000
1772	Ni	0.362558000	1.911367000	1.146511000
1773	Ni	-1.394336000	2.116283000	-0.639112000
1774	Ni	-1.037377000	0.276165000	-2.212308000
1775	Ni	-1.459040000	-1.879327000	-1.154366000
1776	Ni	0.248215000	-2.152078000	0.608083000
1777	Ni	1.723361000	-0.140977000	0.573911000
1778	Ni	0.918378000	1.370687000	-1.221114000
1779	Ni	0.866987000	-1.097501000	-1.524939000

1780	Ni	-0.568554000	0.007505000	0.087197000
1781	Ni	-2.103852000	1.083249000	1.541402000
1782	C	4.065765000	-0.535012000	-1.059101000
1783	C	4.895047000	0.877864000	0.680494000
1784	C	5.579410000	-0.491555000	0.899933000
1785	C	5.030819000	-1.416132000	-0.238109000
1786	H	3.238374000	-1.111684000	-1.522559000
1787	H	4.599779000	-0.002858000	-1.872345000
1788	H	5.496005000	1.510268000	-0.001040000
1789	H	4.727404000	1.443750000	1.612544000
1790	H	6.676607000	-0.399945000	0.875884000
1791	H	5.311319000	-0.901992000	1.888140000
1792	H	5.834096000	-1.833014000	-0.865746000
1793	H	4.476123000	-2.266284000	0.195134000
1794	C	3.585914000	0.514102000	-0.050142000
1795	O	3.060232000	1.698974000	-0.765886000
1796	H	2.770003000	2.323831000	-0.057078000
1797	H	3.080058000	-0.117420000	1.166335000
1798	f. CPOL			
1799	E+ZPE=-2472.856557			
1800	G=-2472.905324			
1801	Ni	-2.499908000	0.804853000	-1.265029000
1802	Ni	-2.837811000	-0.626028000	0.730382000
1803	Ni	-0.984807000	-0.181158000	2.393946000
1804	Ni	0.593158000	1.610023000	1.306975000

1805	Ni	-0.419466000	2.154097000	-0.928781000
1806	Ni	-0.378010000	0.098021000	-2.255219000
1807	Ni	-1.841208000	-1.598475000	-1.293095000
1808	Ni	-0.891427000	-2.191258000	0.907506000
1809	Ni	1.185128000	-0.841636000	1.240009000
1810	Ni	1.508303000	0.570832000	-0.763821000
1811	Ni	0.616681000	-1.738528000	-0.980496000
1812	Ni	-0.672518000	0.012229000	0.088343000
1813	Ni	-2.012965000	1.759861000	0.976548000
1814	C	4.557835000	-0.804396000	-0.765151000
1815	C	5.690480000	1.038435000	0.312084000
1816	C	6.459196000	-0.231319000	0.731465000
1817	C	5.853878000	-1.383224000	-0.135620000
1818	H	3.681770000	-1.478408000	-0.722617000
1819	H	4.715566000	-0.531350000	-1.824625000
1820	H	6.104184000	1.460617000	-0.622488000
1821	H	5.694649000	1.830585000	1.079092000
1822	H	7.547518000	-0.125749000	0.601071000
1823	H	6.282211000	-0.432112000	1.802391000
1824	H	6.556439000	-1.710079000	-0.918582000
1825	H	5.638005000	-2.268007000	0.485620000
1826	C	4.294795000	0.482346000	0.021235000
1827	O	3.440658000	1.372485000	-0.759117000
1828	H	3.138837000	2.095556000	-0.159571000
1829	H	3.754288000	0.248686000	0.965098000

1830 9. FAL to FOL on neutral relaxed Ni cluster (path a)

1831 a. Ni + FAL+2H

1832 E+ZPE= -2545.614129

1833 G= -2545.677402

1834	Ni	1.386831000	-0.962963000	1.173483000
1835	Ni	-0.874489000	-0.999639000	2.131340000
1836	Ni	-2.650299000	-1.070397000	0.145581000
1837	Ni	-1.132338000	-1.234024000	-1.966784000
1838	Ni	1.236284000	-1.266760000	-1.270262000
1839	Ni	1.636333000	1.389175000	-0.069900000
1840	Ni	0.134992000	1.238200000	1.864528000
1841	Ni	-2.228561000	1.037671000	1.338460000
1842	Ni	-2.225132000	0.862153000	-1.260402000
1843	Ni	0.135346000	0.872953000	-2.095371000
1844	Ni	-0.578642000	2.425498000	-0.199102000
1845	Ni	-0.459955000	-0.013744000	-0.035707000
1846	Ni	-0.433238000	-2.365692000	0.206041000
1847	C	3.120590000	-1.685944000	-0.802430000
1848	C	3.123079000	-1.993445000	0.623274000
1849	C	3.414192000	-0.773958000	1.324519000
1850	C	3.581601000	0.234546000	0.306794000
1851	O	3.639477000	-0.351598000	-0.946923000
1852	H	3.531108000	-2.365004000	-1.563701000
1853	H	3.142919000	-3.007764000	1.024511000
1854	H	3.680693000	-0.643598000	2.375335000

1855	C	3.533252000	1.673412000	0.403041000
1856	H	3.741142000	2.118103000	1.396627000
1857	O	3.347100000	2.423132000	-0.657595000
1858	H	-0.970785000	2.257802000	-1.812993000
1859	H	-0.173670000	2.792485000	1.351790000
1860	b. TS1			
1861	E+ZPE=	-2545.565194		
1862	G=	-2545.629545		
1863	Ni	1.393277000	-1.099247000	1.011299000
1864	Ni	-0.899897000	-1.212141000	2.015948000
1865	Ni	-2.568423000	-1.169018000	0.025168000
1866	Ni	-1.156854000	-0.954665000	-2.068485000
1867	Ni	1.247408000	-1.088041000	-1.432115000
1868	Ni	1.577595000	1.434236000	0.073955000
1869	Ni	0.175390000	0.979887000	2.027796000
1870	Ni	-2.163194000	0.837688000	1.446251000
1871	Ni	-2.310528000	0.984020000	-1.096704000
1872	Ni	0.075465000	1.231011000	-1.979111000
1873	Ni	-0.680490000	2.372785000	0.137221000
1874	Ni	-0.422406000	0.031734000	-0.061707000
1875	Ni	-0.449352000	-2.323620000	-0.076493000
1876	C	3.109624000	-1.679028000	-0.929707000
1877	C	3.118899000	-2.084155000	0.469894000
1878	C	3.422186000	-0.910121000	1.252587000
1879	C	3.575560000	0.160339000	0.317033000

1880	O	3.606322000	-0.320373000	-0.968652000
1881	H	3.546386000	-2.287288000	-1.734264000
1882	H	3.159746000	-3.123533000	0.800973000
1883	H	3.655559000	-0.847684000	2.317143000
1884	C	3.566438000	1.650944000	0.487381000
1885	H	4.236994000	2.012967000	1.300433000
1886	O	3.436693000	2.378250000	-0.619734000
1887	H	-1.032653000	2.419127000	-1.566146000
1888	H	2.429868000	1.845932000	1.361169000
1889	c. IM1			
1890	E+ZPE=	-2545.592108		
1891	G=	-2545.657251		
1892	Ni	1.497630000	-0.814391000	1.108393000
1893	Ni	-0.763126000	-0.819081000	2.247030000
1894	Ni	-2.539678000	-1.193592000	0.377470000
1895	Ni	-1.271979000	-1.381168000	-1.788246000
1896	Ni	1.184115000	-1.220051000	-1.281402000
1897	Ni	1.515988000	1.417729000	-0.312396000
1898	Ni	0.232647000	1.385112000	1.768415000
1899	Ni	-2.173496000	1.137201000	1.366225000
1900	Ni	-2.427109000	0.696004000	-1.192033000
1901	Ni	-0.120455000	0.788454000	-2.189698000
1902	Ni	-0.744448000	2.331316000	-0.330827000
1903	Ni	-0.459012000	0.019968000	-0.021336000
1904	Ni	-0.386394000	-2.270148000	0.360610000



1905	C	3.065701000	-1.737511000	-0.849971000
1906	C	3.077852000	-1.985280000	0.589318000
1907	C	3.589316000	-0.774203000	1.203540000
1908	C	3.894585000	0.117198000	0.153968000
1909	O	3.745946000	-0.488474000	-1.062222000
1910	H	3.362439000	-2.488464000	-1.598089000
1911	H	3.041042000	-2.983235000	1.031031000
1912	H	3.848772000	-0.602553000	2.250308000
1913	C	4.225013000	1.583040000	0.137473000
1914	H	5.103477000	1.743147000	-0.527460000
1915	O	3.130218000	2.370622000	-0.301590000
1916	H	-1.273146000	2.031325000	-1.960459000
1917	H	4.542158000	1.857301000	1.167466000
1918	d. IM2			
1919	E+ZPE=	-2545.593656		
1920	G=	-2545.658277		
1921	Ni	1.562147000	-0.688721000	1.007277000
1922	Ni	-0.752653000	-0.903619000	2.194857000
1923	Ni	-2.448025000	-1.330439000	0.481651000
1924	Ni	-1.260071000	-1.305361000	-1.825280000
1925	Ni	1.192413000	-1.080514000	-1.395280000
1926	Ni	1.455142000	1.537208000	-0.249124000
1927	Ni	0.240114000	1.323131000	1.813666000
1928	Ni	-2.188049000	0.977398000	1.353846000
1929	Ni	-2.535886000	0.661324000	-1.066089000

1930	Ni	-0.156741000	0.928962000	-2.160942000
1931	Ni	-0.893120000	2.309765000	-0.283105000
1932	Ni	-0.463056000	0.000468000	-0.008079000
1933	Ni	-0.234696000	-2.293471000	0.180379000
1934	C	3.048895000	-1.689948000	-0.917545000
1935	C	3.033562000	-2.034957000	0.499924000
1936	C	3.597870000	-0.906965000	1.209464000
1937	C	3.921775000	0.054961000	0.227320000
1938	O	3.776595000	-0.454276000	-1.031432000
1939	H	3.329701000	-2.399840000	-1.711004000
1940	H	2.901201000	-3.051041000	0.874265000
1941	H	3.855479000	-0.830381000	2.267674000
1942	C	4.223208000	1.523390000	0.314360000
1943	H	5.156456000	1.737868000	-0.253059000
1944	O	3.159483000	2.303038000	-0.199619000
1945	H	-0.606866000	2.514449000	-1.939751000
1946	H	4.433011000	1.748279000	1.383384000
1947	e.	TS2		
1948		E+ZPE=	-2545.555410	
1949		G=	-2545.620061	
1950	Ni	-1.045430000	-1.496577000	-1.091655000
1951	Ni	1.455077000	-1.417265000	-1.632940000
1952	Ni	2.699510000	-0.730748000	0.488588000
1953	Ni	1.035774000	-0.453490000	2.227789000
1954	Ni	-1.227007000	-1.139089000	1.300230000

1955	Ni	-1.771648000	0.850910000	-0.537024000
1956	Ni	0.065545000	0.524481000	-2.254000000
1957	Ni	2.240302000	0.936297000	-1.303871000
1958	Ni	1.922400000	1.574048000	1.178941000
1959	Ni	-0.565100000	1.401233000	1.560576000
1960	Ni	0.325988000	2.304945000	-0.514755000
1961	Ni	0.475602000	-0.017276000	-0.011700000
1962	Ni	0.753297000	-2.300857000	0.527930000
1963	C	-2.977791000	-1.861596000	0.730215000
1964	C	-2.956123000	-1.911606000	-0.735217000
1965	C	-3.378208000	-0.589544000	-1.185341000
1966	C	-3.671642000	0.174228000	-0.020981000
1967	O	-3.639211000	-0.636094000	1.114500000
1968	H	-3.305581000	-2.703910000	1.354137000
1969	H	-3.106481000	-2.837080000	-1.307954000
1970	H	-3.655575000	-0.313069000	-2.203045000
1971	C	-4.167343000	1.587988000	0.159526000
1972	H	-4.632538000	1.672731000	1.163313000
1973	O	-3.069997000	2.495076000	-0.014135000
1974	H	-1.974882000	2.065194000	0.827981000
1975	H	-4.945308000	1.822291000	-0.593624000
1976	f. FOL			
1977	E+ZPE=	-2545.577764		
1978	G=	-2545.642560		
1979	Ni	0.749962000	-1.645203000	1.133498000

1980	Ni	-1.691897000	-1.197428000	1.612748000
1981	Ni	-2.825117000	-0.422693000	-0.545551000
1982	Ni	-0.923915000	-0.444160000	-2.315508000
1983	Ni	1.123444000	-1.347975000	-1.206143000
1984	Ni	1.758002000	0.572387000	0.657948000
1985	Ni	-0.153062000	0.551632000	2.243704000
1986	Ni	-2.244734000	1.261431000	1.167526000
1987	Ni	-1.697438000	1.636868000	-1.208130000
1988	Ni	0.789639000	1.189014000	-1.604855000
1989	Ni	0.035327000	2.266814000	0.519897000
1990	Ni	-0.489003000	0.051603000	-0.059981000
1991	Ni	-1.085939000	-2.204086000	-0.463517000
1992	C	2.913082000	-1.914075000	-0.627650000
1993	C	2.726019000	-1.967350000	0.827751000
1994	C	3.232105000	-0.685734000	1.334552000
1995	C	3.678488000	0.069998000	0.200862000
1996	O	3.694867000	-0.757172000	-0.943571000
1997	H	3.229610000	-2.782277000	-1.224764000
1998	H	2.780331000	-2.911786000	1.393210000
1999	H	3.485761000	-0.476672000	2.376167000
2000	C	4.544606000	1.290653000	0.137191000
2001	H	5.499666000	1.069470000	-0.374014000
2002	O	3.934566000	2.376787000	-0.592135000
2003	H	2.959756000	2.286287000	-0.387067000
2004	H	4.776075000	1.587371000	1.180064000