

Supporting Information

Unraveling the reaction mechanism for nickel-catalyzed oxidative dehydrogenation of ethane by DFT: the C-H bond activation step and its following pathways

by

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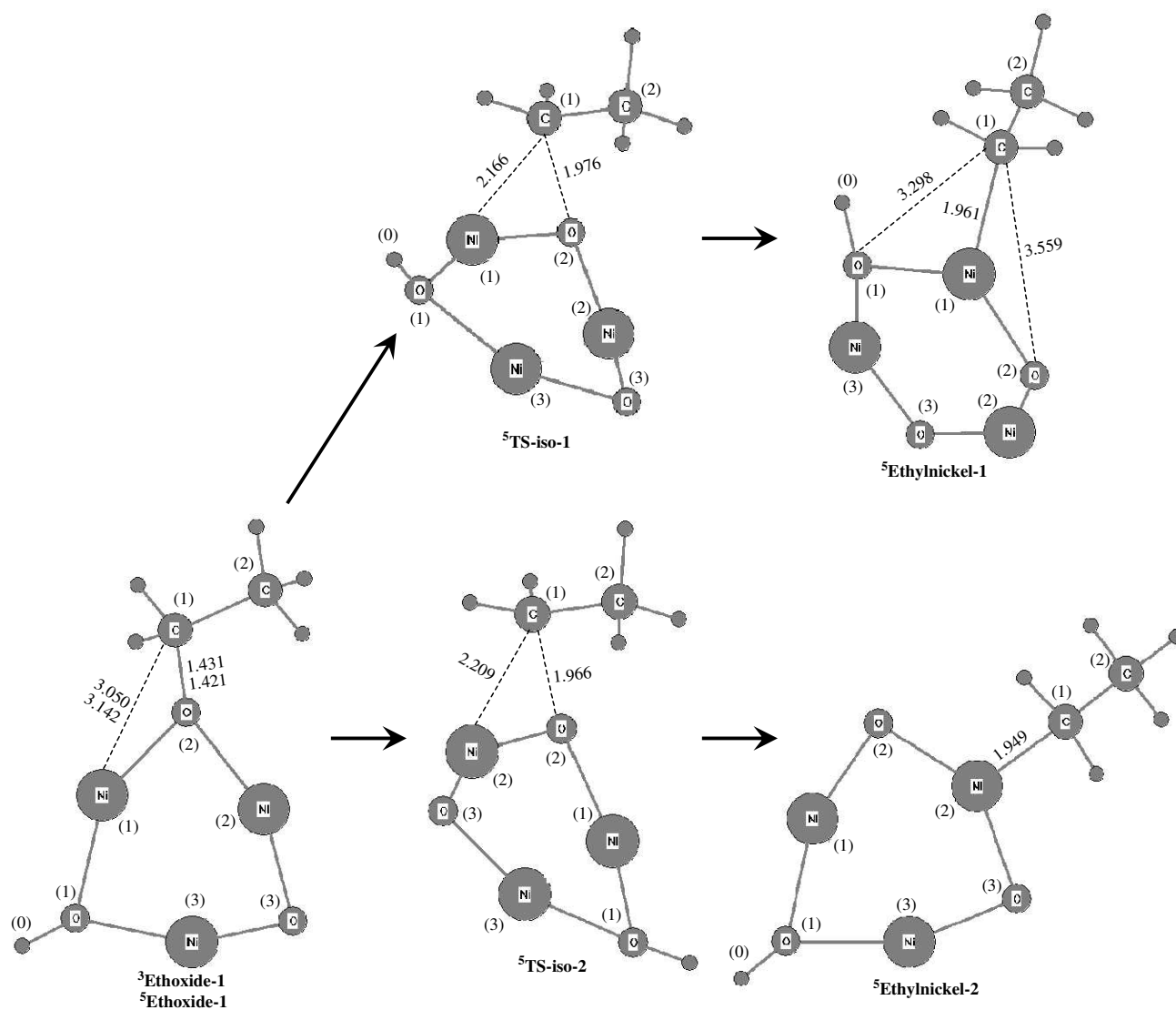


Figure 1S. Optimized geometries for the reactant, transition state and product for the isomerization of **Ethoxide-1** to **Ethynickel-2**. Key distances are indicated in Å. The upper-left number of the name of each structure is the spin multiplicity. See Scheme 1d as well.

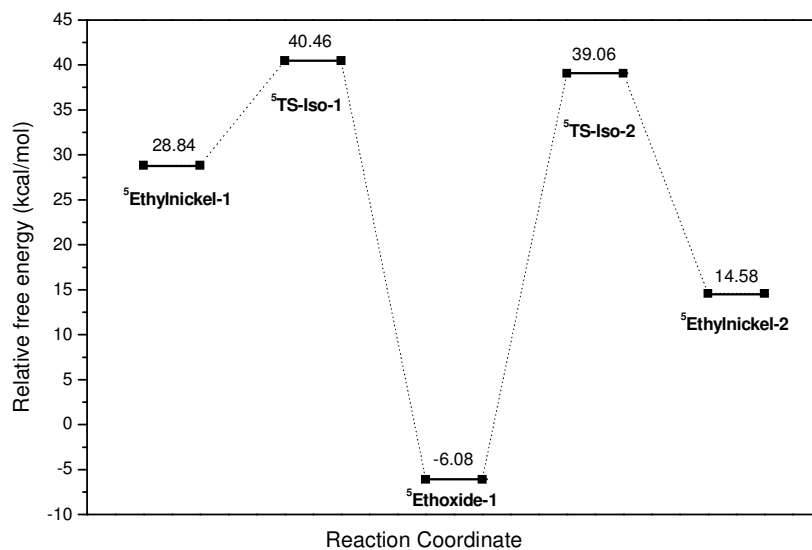


Figure 2S. Relative free energy (at 873.15 K) profiles for the isomerization of **Ethoxide-1** to **Ethylnickel-1** and **Ethylnickel-2**. The free energy of heptet Ni₃O₃ + C₂H₆ is the reference. See Figure 1S and Scheme 1d in the manuscript for detail

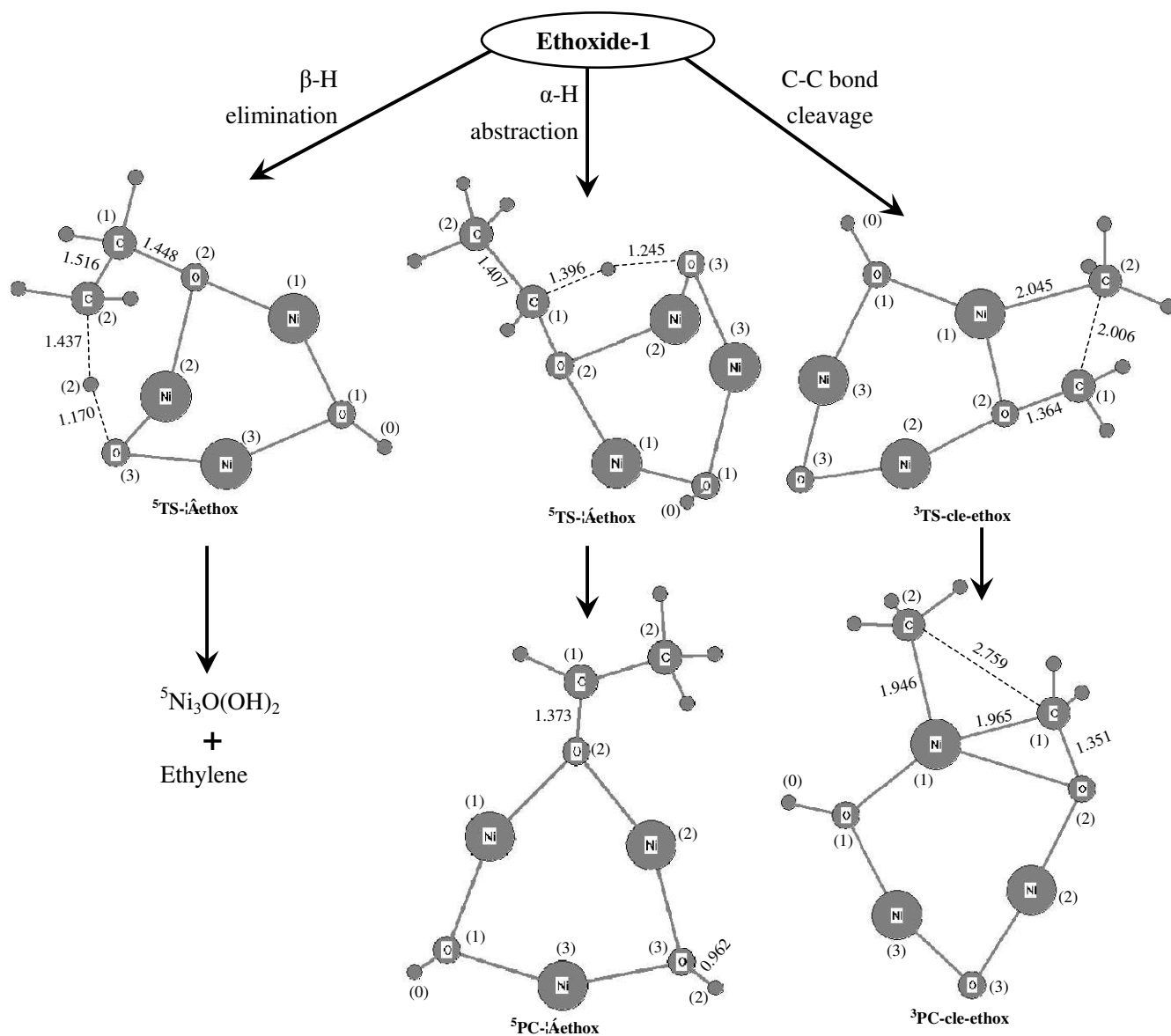


Figure 3S. Optimized geometries for the transition states and products for three reaction pathways of **Ethoxide-1** as indicated in the figure. Key distances are indicated in Å. The upper-left number of the name of each structure is the spin multiplicity. See the structure of $^5\text{Ni}_3\text{O}(\text{OH})_2$ in Figure 4.

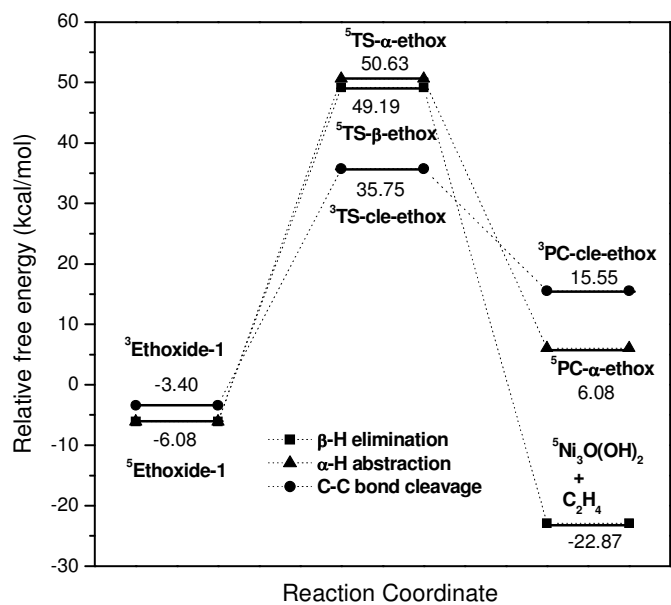


Figure 4S. Relative free energy (at 873.15 K) profiles for three reaction pathways of **Ethoxide-1** as indicated in the figure. The free energy of heptet $\text{Ni}_3\text{O}_3 + \text{C}_2\text{H}_6$ is the reference.

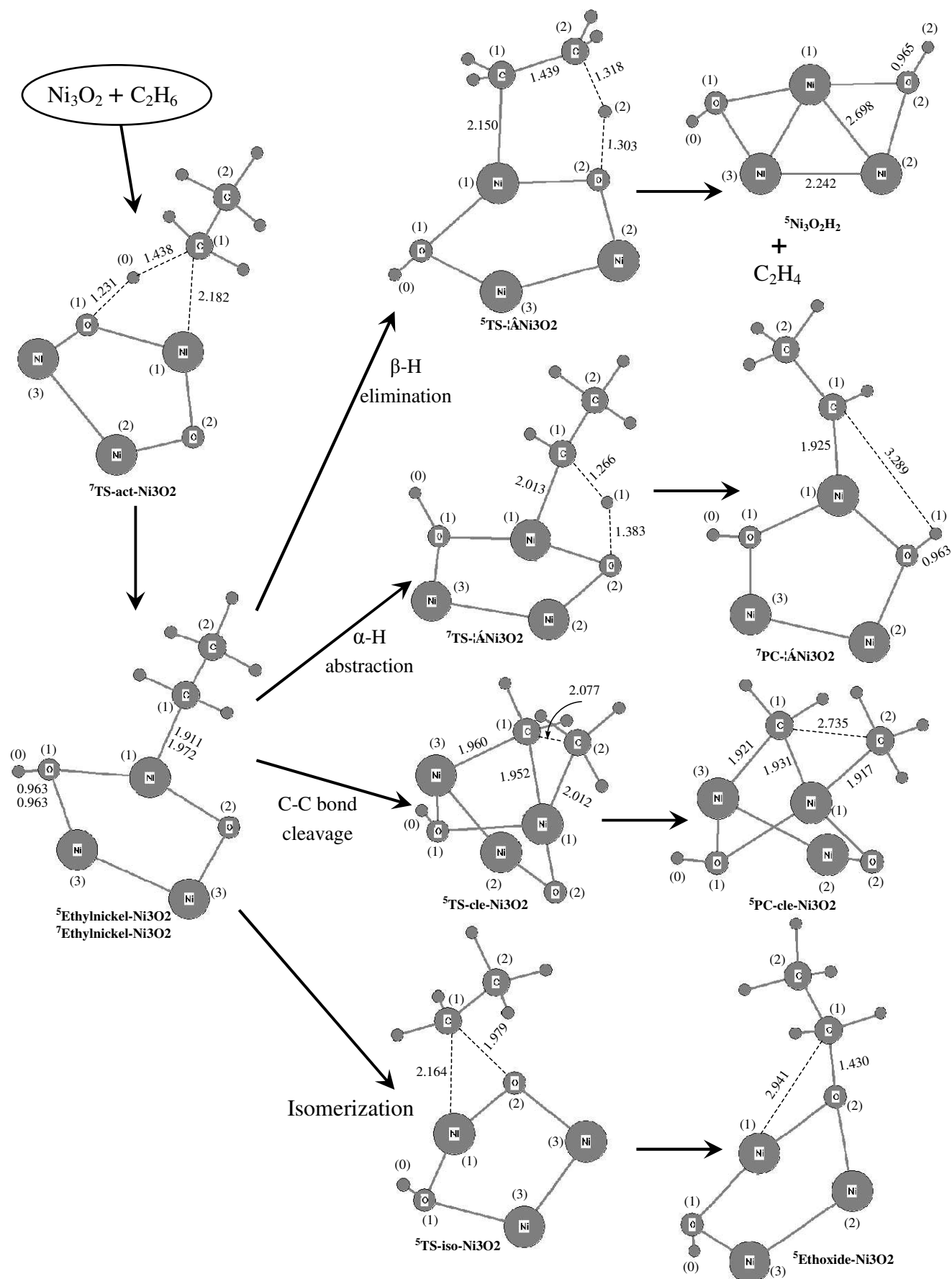


Figure 5S. Optimized geometries for the transition states, product complexes and separated products involved in the C-H bond activation step and the following four reaction pathways of **Ethylnickel-Ni₃O₂**, for C_2H_6 reacting with Ni_3O_2 . Key distances are indicated in Å.

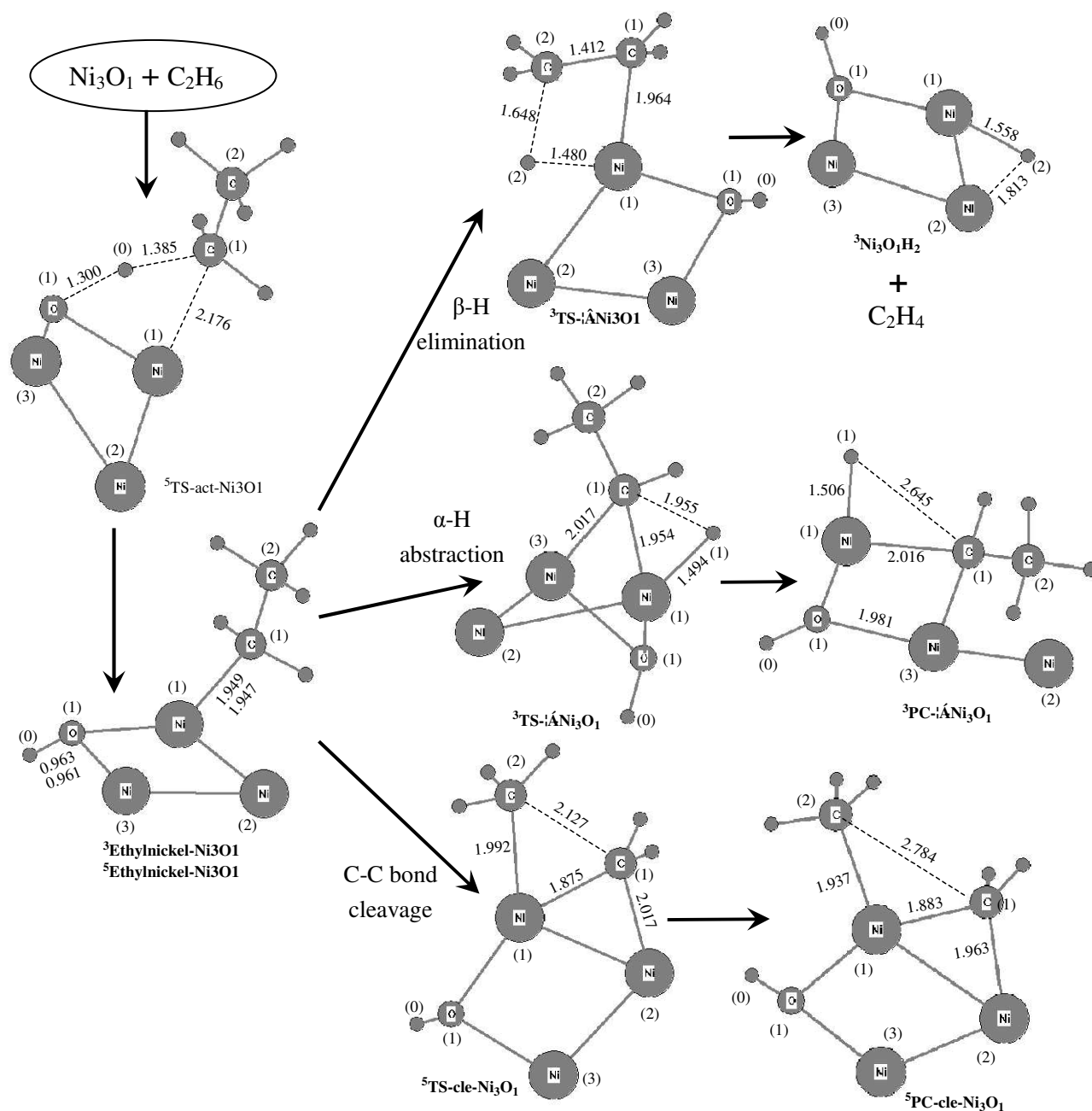


Figure 6S. Optimized geometries for the transition states, product complexes and separated products involved in the C-H bond activation step and the following three reaction pathways of **Ethylnickel-Ni₃O₁**, for C_2H_6 reacting with Ni_3O_1 . Key distances are indicated in Å.

Cartesian coordinates for all the optimized structures at the B3LYP/BS1 level of theory in the manuscript. See the manuscript for the detail basis set information. The order of the species listed here is the same as the order of species appearing in the manuscript. The number in the upper-left side of a species represents its spin multiplicity.

Ni₃O₃
in triplet

Ni	0.030438	1.594577	-0.000617
Ni	1.414068	-0.832355	-0.000419
Ni	-1.445611	-0.780852	-0.000268
O	1.666413	0.911780	0.002003
O	-1.628447	0.971840	0.001548
O	-0.034099	-1.818416	0.001014

in quintuplet

Ni	-0.822575	-1.296723	-0.022650
Ni	-0.822541	1.296739	-0.022652
Ni	1.700650	-0.000018	0.033620
O	-2.040931	0.000024	0.124245
O	0.923263	-1.581468	-0.041682
O	0.923302	1.581452	-0.041676

in heptet

Ni	0.000000	1.516798	0.000000
Ni	-1.382153	-0.689377	0.000000
Ni	1.413547	-0.856548	0.000000
O	-1.726635	1.071985	0.000000
O	1.686230	0.914147	0.000000
O	-0.069472	-1.884189	0.000000

Ni₃O₂
in triplet

Ni	-1.153767	-1.046485	-0.005662
Ni	1.297044	-0.866436	0.003804
Ni	-0.105066	1.465045	-0.004883
O	-1.700879	0.676383	0.02414
O	1.567140	0.891183	-0.000552

in quintuplet

Ni	-0.385951	1.439789	-0.000297
Ni	-1.416798	-0.675342	0.000292

Ni	1.397937	-0.614238	0.000004
O	1.387438	1.190551	0.000757
O	0.029401	-1.716284	-0.000755

in heptet

Ni	-1.213151	-0.951928	0.001330
Ni	-0.702259	1.351201	-0.002036
Ni	1.482472	-0.310591	-0.001675
O	0.403020	-1.742689	-0.000094
O	1.112266	1.432300	0.008428
O	-0.069472	-1.884189	0.000000

Ni₃O₁
in triplet

Ni	-0.506555	-1.294370	-0.033806
Ni	1.497399	-0.000312	0.025207
Ni	-0.505940	1.294538	-0.033812
O	-1.697163	0.000503	0.148434

in quintuplet

Ni	-0.363855	1.268447	-0.002592
Ni	1.541232	-0.135129	0.001850
Ni	-0.669172	-1.213161	-0.002231
O	-1.778716	0.279451	0.010405

in heptet

Ni	-1.381105	-0.469517	-0.001277
Ni	0.004305	1.416427	0.000979
Ni	1.378081	-0.476502	-0.001277
O	-0.004481	-1.646426	0.005515

C₂H₆

C	0.018746	-0.032470	0.013256
H	0.037021	-0.064122	1.106285
H	1.055355	-0.064122	-0.333858

H	-0.472147	-0.946026	-0.333858
C	-0.702283	1.216390	-0.496589
H	-0.720558	1.248042	-1.589618
H	-1.738892	1.248042	-0.149475
H	-0.211390	2.129946	-0.149475

Reactant complex of heptet Ni₃O₃ and C₂H₆

Ni	-1.736531	1.029005	-1.001574
Ni	-1.521831	-0.658127	0.923873
Ni	0.758796	-0.182606	-0.654538
O	-2.843647	0.289121	0.184272
O	-0.097459	1.083626	-1.642518
O	0.175211	-1.102858	0.816678
C	3.138979	0.278047	-0.034267
H	3.897199	0.826964	-0.597490
H	2.931105	-0.627873	-0.627101
C	3.573232	-0.092083	1.383850
H	4.464226	-0.723592	1.361225
H	3.810096	0.803667	1.962146
H	2.779442	-0.634402	1.899671
H	2.273517	0.971308	-0.001456

TS-activation-case1

In triplet

Ni	-1.385129	-0.145361	1.313629
Ni	-1.821148	0.371171	-1.286751
Ni	1.038882	0.195807	-0.357182
O	-2.731573	0.060601	0.233325
O	0.385225	-0.158725	1.412353
O	-0.143872	0.465226	-1.711135
C	2.876649	-0.038748	0.619023
H	3.150069	0.198190	1.656595
H	3.269152	0.810420	0.044235
C	3.496234	-1.373245	0.191558
H	4.582044	-1.378627	0.336328
H	3.083384	-2.202179	0.772396
H	3.313803	-1.592295	-0.864886
H	1.594576	-0.129981	1.221162

In quadruplet

Ni	-1.075034	1.328816	-0.400604
Ni	-2.104584	-0.989931	0.164462
Ni	0.987373	-0.575202	-0.009957
O	-2.711832	0.660177	-0.224958
O	0.724233	1.284788	-0.419720
O	-0.475335	-1.601079	0.300067
C	2.996368	0.015659	-0.161580
H	3.454625	0.716070	-0.872644
H	3.190242	-0.970528	-0.606288
C	3.625531	0.160526	1.227428
H	4.714782	0.051507	1.191443
H	3.406777	1.142571	1.654668

H	3.249929	-0.590634	1.928460
H	1.878446	0.839126	-0.350932

In heptet

Ni	-0.849123	1.468635	-0.275311
Ni	-1.547902	-0.842649	0.583236
Ni	1.041117	-0.769576	-0.713927
O	-2.282498	0.798562	0.511003
O	0.743699	1.171140	-1.008975
O	-0.139197	-1.810333	0.221877
C	2.992234	0.027653	-0.221363
H	3.574234	0.754885	-0.800206
H	3.351775	-0.945814	-0.588524
C	3.236083	0.172343	1.284402
H	4.299458	0.087586	1.532972
H	2.892270	1.145463	1.645627
H	2.703309	-0.592563	1.854609
H	1.846059	0.806532	-0.605574

Ethylnickel-1

In triplet

Ni	-1.363358	1.322372	0.153276
Ni	-1.387551	-1.360578	-0.035496
Ni	1.455723	-0.204446	-0.620370
O	-2.480099	0.023950	0.361745
O	0.405055	1.563203	-0.278444
O	0.218034	-1.601053	-0.563621
C	3.216275	0.122529	0.198680
H	3.652602	0.984931	-0.326545
H	3.848456	-0.741169	-0.038480
C	3.191562	0.366713	1.711196
H	4.194387	0.546120	2.120744
H	2.581513	1.236825	1.979968
H	2.774626	-0.491144	2.246961
H	0.948090	2.189538	0.212173

In quadruplet

Ni	-1.243181	1.286571	0.036217
Ni	-1.654782	-1.172336	0.225363
Ni	1.421933	-0.327244	-0.622953
O	-2.650551	0.318866	0.383521
O	0.494005	1.510113	-0.471793
O	-0.053163	-1.428915	-0.294648
C	3.272065	-0.198288	0.015590
H	3.777166	0.522498	-0.644259
H	3.744858	-1.172006	-0.163255
C	3.419955	0.215454	1.482354
H	4.471997	0.289912	1.788048
H	2.959008	1.188952	1.677710
H	2.941894	-0.506756	2.150725
H	0.959495	2.338134	-0.614834

In heptet

Ni	-1.558421	1.154659	0.039819
Ni	-1.548309	-1.308686	-0.139339
Ni	1.353491	-0.114776	-0.523518
O	-2.829509	-0.044350	0.115695
O	0.197757	1.573467	-0.196000
O	0.134006	-1.542148	-0.298314
C	3.166903	0.114574	0.197802
H	3.608660	0.979567	-0.317167
H	3.737530	-0.768527	-0.114073
C	3.222786	0.293084	1.716272
H	4.252180	0.408617	2.081069
H	2.666508	1.177862	2.042629
H	2.792084	-0.568045	2.235174
H	0.607408	2.433391	-0.065788

TS-activation-case2**In triplet**

Ni	1.302144	-1.096773	0.340715
Ni	1.156337	1.288390	-0.124071
Ni	-0.827848	-0.132818	-0.420808
O	2.318150	0.304639	0.838087
O	-0.279338	-1.782643	0.102377
O	-0.488497	1.644840	-0.566642
C	-2.776217	-0.232358	-0.322601
H	-3.107159	-1.228060	-0.608930
H	-3.214823	0.537278	-0.953639
C	-2.945573	0.047583	1.163849
H	-4.021532	0.026076	1.386906
H	-2.466877	-0.711765	1.784024
H	-2.572491	1.034067	1.443215
H	-1.484687	-0.408891	-1.631322

In quadruplet

Ni	1.307142	-1.170626	0.502773
Ni	1.149142	1.418195	-0.001926
Ni	-0.818569	-0.130224	-0.411756
O	2.366266	0.261097	0.598462
O	-0.275766	-1.774840	0.092161
O	-0.483864	1.634838	-0.572565
C	-2.769085	-0.233608	-0.331401
H	-3.098963	-1.229540	-0.618440
H	-3.206756	0.536424	-0.962739
C	-2.954395	0.044813	1.154673
H	-4.033265	0.019270	1.361412
H	-2.481573	-0.713958	1.779459
H	-2.588143	1.032053	1.439049
H	-1.520584	-0.404330	-1.598004

Ethynickel Hydride**In triplet**

Ni	-1.160348	1.413348	0.121659
Ni	-1.192819	-1.408162	0.120362
Ni	0.904745	0.005608	-0.495986
O	-2.217041	0.012495	0.389358
O	0.506247	1.750715	-0.320047
O	0.459871	-1.725354	-0.364093
C	2.795820	-0.028143	-0.146583
H	3.183531	0.875871	-0.610377
H	3.154244	-0.934791	-0.628457
C	2.886388	-0.043799	1.362693
H	3.950802	-0.066208	1.638420
H	2.453309	0.851813	1.811323
H	2.420202	-0.930655	1.795280
H	1.307884	0.030545	-1.833571

In quadruplet

Ni	1.250323	-1.192374	0.426305
Ni	1.091928	1.402905	-0.079653
Ni	-0.885488	-0.151959	-0.502250
O	2.307104	0.242468	0.521466
O	-0.345001	-1.788227	0.018420
O	-0.552488	1.611424	-0.644352
C	-2.802396	-0.243932	-0.373896
H	-3.070461	-1.245785	-0.695273
H	-3.178601	0.525936	-1.040690
C	-3.035687	0.028158	1.094736
H	-4.118703	-0.001544	1.281450
H	-2.576225	-0.729157	1.731305
H	-2.682801	1.016901	1.390885
H	-1.161774	-0.430410	-1.844049

TS-activation-case3**In triplet**

Ni	-0.132191	-1.013241	0.615621
Ni	-2.514378	0.175569	0.054703
Ni	-0.055139	0.815189	-0.936598
O	-1.848985	-1.140818	1.044785
O	1.306265	-0.167002	-0.172391
O	-1.731659	1.357248	-1.034189
C	3.571458	0.500131	0.742310
C	4.594421	-0.323831	0.004425
H	3.600402	1.572239	0.543999
H	3.475273	0.286075	1.807371
H	2.389122	0.161139	0.276522
H	5.608151	-0.079765	0.351742
H	4.445586	-1.394042	0.167108
H	4.566631	-0.134897	-1.071473

In quadruplet

Ni	0.299206	-1.238933	-0.255989
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Ni	-2.079536	-0.275446	0.272772
Ni	-0.180467	1.450808	-0.191961
O	-1.374901	-1.853294	0.057694
O	1.256627	0.356423	-0.455646
O	-1.884815	1.536300	0.197035
C	3.618306	0.759498	0.372809
C	4.302963	-0.579636	0.359144
H	3.989907	1.488744	-0.347755
H	3.451497	1.194457	1.358650
H	2.374218	0.568188	-0.067404
H	5.339473	-0.483435	0.712565
H	3.807102	-1.296677	1.018778
H	4.345148	-1.003892	-0.647077

In heptet

Ni	-0.112602	-0.221480	1.260578
Ni	-2.354290	0.012283	-0.275768
Ni	0.239658	0.170508	-1.104229
O	-1.873963	-0.268144	1.444706
O	1.456794	-0.057055	0.334376
O	-1.453029	0.267449	-1.774197
C	3.947148	-0.134595	0.800471
C	4.674657	0.168780	-0.481081
H	4.036481	0.616156	1.585500
H	4.057504	-1.150503	1.179522
H	2.598851	-0.090932	0.539583
H	5.762635	0.144958	-0.323942
H	4.449171	-0.564278	-1.260095
H	4.429326	1.163533	-0.862292

Ni₃O₃H

In doublet

Ni	-0.156301	-0.953543	0.713775
Ni	-2.447464	0.122973	0.004099
Ni	-0.086860	0.833105	-0.871656
O	-1.909774	-1.173374	1.041460
O	1.360511	-0.189624	-0.231459
O	-1.733925	1.395923	-1.040442
H	2.193559	0.094052	0.152546

In quartet

Ni	0.758992	-1.166144	-0.028420
Ni	-1.726772	0.000104	0.041632
Ni	0.759273	1.166124	-0.028308
O	-0.953089	-1.592275	-0.038288
O	2.239857	-0.000358	0.087948
O	-0.952720	1.592385	-0.038554
H	3.165829	-0.000368	0.333865

In sextet

Ni	-0.635480	1.239249	0.058611
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Ni	1.416659	-0.014559	-0.139759
Ni	-0.659977	-1.226051	0.069319
O	1.037957	1.771680	-0.106349
O	-2.084395	0.021582	0.206589
O	1.002039	-1.792698	-0.095999
H	-3.038463	0.033593	0.297316

C₂H₅• radical

C	0.011399	0.000000	0.058277
H	0.169973	0.000000	1.130079
H	0.884903	0.000000	-0.580303
C	-1.366885	0.000000	-0.502517
H	-1.364831	0.000000	-1.594552
H	-1.943235	-0.876113	-0.171908
H	-1.943235	0.876113	-0.171908

TS-β-1

In triplet

Ni	0.285313	-0.869546	0.040917
Ni	-0.526735	1.319736	-0.958700
C	-2.170895	-1.197729	1.632799
C	-0.760096	-1.463874	1.744990
H	-0.163607	-0.887039	2.450044
H	-0.410007	-2.490816	1.585754
H	-2.584054	-0.484973	2.344877
H	-2.813234	-2.059097	1.456222
O	0.820090	2.502473	-1.103110
H	-2.135141	-0.588556	0.511963
O	-1.375804	-0.201175	-0.553800
Ni	1.790617	1.185011	-0.486123
O	2.205997	-0.546221	0.119553
H	3.001237	-1.080392	0.077169

In quindruplet

Ni	0.278583	-0.877928	-0.002249
Ni	-0.565978	1.336097	-0.910060
C	-2.146799	-1.185251	1.622477
C	-0.738132	-1.457088	1.750578
H	-0.136276	-0.862343	2.435149
H	-0.392818	-2.488765	1.625884
H	-2.555903	-0.437719	2.300682
H	-2.795262	-2.049183	1.483455
O	0.804066	2.509664	-1.070473
H	-2.118906	-0.620616	0.474014
O	-1.403709	-0.229681	-0.614132
Ni	1.753587	1.169320	-0.427279
O	2.193376	-0.569319	0.140617
H	2.987855	-1.099385	0.053891

In heptet

Ni	0.013381	-1.269850	0.151209
Ni	-0.872558	1.018814	-0.882814
C	-2.290826	-1.355573	1.743635
C	-0.920130	-1.879801	1.937106
H	-0.332761	-1.404341	2.723312
H	-0.825168	-2.967018	1.952958
H	-2.557460	-0.491770	2.354923
H	-3.090843	-2.098732	1.706035
O	0.378326	2.279566	-0.598891
H	-2.306006	-0.904689	0.584587
O	-1.641793	-0.623804	-0.613162
Ni	1.438829	0.881748	-0.368036
O	1.968530	-0.867683	-0.004746
H	2.704127	-1.161613	0.537432

TS- β -2 In triplet

Ni	-1.348936	0.595661	-0.364833
Ni	1.381660	0.950458	-0.110509
Ni	0.485180	-1.176230	-0.273866
O	-1.012468	-1.006178	-1.207638
O	-0.069733	1.900187	-0.202959
O	2.312715	-0.668032	0.188438
C	-0.666793	-1.061835	1.442013
H	0.134584	-0.718144	2.091467
H	-0.849700	-2.135852	1.457200
C	-1.867017	-0.229351	1.449394
H	-2.741902	0.872637	0.083932
H	-2.812201	-0.755043	1.398136
H	-1.866181	0.616759	2.128972
H	2.903674	-0.872309	0.916603

In quindruplet

Ni	-1.423541	0.504696	-0.277544
Ni	1.238569	1.094191	0.110333
Ni	0.566628	-1.093371	-0.378746
O	-0.860600	-0.856557	-1.356487
O	-0.289779	1.934677	0.055211
O	2.298708	-0.458755	0.251241
C	-0.507060	-1.365020	1.224069
H	0.187987	-1.072920	2.010403
H	-0.607505	-2.449914	1.126248
C	-1.823397	-0.668488	1.314015
H	-2.840031	0.511559	0.189866
H	-2.686868	-1.306105	1.162785
H	-1.941312	0.000526	2.161847
H	2.954972	-0.743937	0.889947

In heptet

Ni	-1.427795	1.087384	-0.830216
Ni	1.165202	1.276467	-0.714313
Ni	0.463698	-1.274912	-0.067080
O	-0.045754	-0.159312	-1.418123
O	-0.189889	2.429067	-0.483006

O	2.050506	-0.180110	0.261066
C	-0.798831	-1.925781	1.503328
H	-0.057677	-1.746793	2.280852
H	-0.923849	-2.960761	1.186821
C	-1.926863	-1.114883	1.504052
H	-2.307448	0.200787	0.152969
H	-2.865724	-1.471018	1.103627
H	-1.983802	-0.243674	2.141676
H	2.434629	-0.033244	1.129102

TS- β -3 In triplet

C	-0.263208	-1.230547	1.670413
Ni	0.695663	-1.098610	-0.209877
Ni	0.831023	1.279132	-0.237528
Ni	-1.506530	0.136988	-1.357776
O	2.217871	0.104683	0.240079
O	-1.005869	1.435917	-0.155959
O	-0.712584	-1.391440	-1.378391
H	2.620174	0.198100	1.108666
C	-1.147539	-0.134338	1.953453
H	-2.211204	-0.374289	1.962031
H	-0.847409	0.524634	2.768689
H	-1.142148	0.746783	0.920866
H	0.657886	-1.303102	2.248232
H	-0.711387	-2.189806	1.413382

In quindruplet

C	1.738856	0.073197	-1.001966
Ni	-0.047557	1.079430	-0.750165
Ni	-0.299046	0.409820	1.519109
Ni	-0.900279	-1.431003	-0.555269
O	0.287113	2.086854	0.911762
O	-0.299298	-1.395711	1.233463
O	-1.049731	-0.072015	-1.717815
H	1.117558	2.461732	1.218319
C	1.633577	-1.325365	-0.588341
H	1.492585	-2.027865	-1.411300
H	2.441566	-1.670343	0.064914
H	0.750064	-1.467166	0.439197
H	2.408927	0.700136	-0.416317
H	1.769874	0.273944	-2.072307

In heptet

C	-0.159269	-0.760032	1.783776
Ni	0.778270	-1.392884	-0.231506
Ni	1.014502	0.839109	0.761503
Ni	-1.421325	0.258609	-0.621396
O	2.389534	-0.332888	0.123706
O	-0.517872	1.745261	0.286230
O	-0.612928	-1.228303	-1.328822
H	2.998412	-0.089148	-0.580808
C	-1.594588	-0.258427	1.541015
H	-2.256479	-1.055992	1.191939

H	-2.072706	0.176571	2.425280
H	-1.260962	1.009922	0.991867
H	0.281219	-0.356850	2.705441
H	-0.091070	-1.850841	1.898054
TS-β-5			
In triplet			
Ni	-0.778405	-0.734555	-0.191937
Ni	1.860208	-0.906734	0.230062
Ni	0.501427	1.460292	-0.080962
O	-1.230935	2.112844	-0.373799
O	0.476715	-1.967568	0.037207
C	-2.461019	-0.049574	0.443412
H	-2.524351	0.236327	1.498625
H	-1.887907	1.114899	-0.120870
C	-3.730070	-0.690930	-0.037684
H	-4.577127	0.000798	0.085234
H	-3.697407	-0.991685	-1.086611
H	-3.980106	-1.572469	0.567524
O	2.134861	0.822440	0.079025
H	-1.562130	2.981325	-0.118303
In quadruplet			
Ni	-0.782236	-0.744186	-0.132937
Ni	1.893608	-0.875093	0.038704
Ni	0.469441	1.500832	0.012127
O	-1.302257	2.104937	-0.096661
O	0.516033	-1.959791	-0.034200
C	-2.441799	-0.194417	0.497320
H	-2.564248	0.105251	1.542274
H	-1.875371	1.017863	-0.036531
C	-3.688429	-0.815132	-0.066033
H	-4.527157	-0.104839	-0.008195
H	-3.588615	-1.130831	-1.106330
H	-3.993040	-1.684594	0.530046
O	2.126113	0.900467	0.061729
H	-1.652090	2.806084	-0.656971
In heptet			
Ni	0.711062	-0.967695	-0.235032
Ni	-2.002528	-0.578986	0.170085
Ni	-0.313629	1.484599	-0.104469
O	1.505604	1.902532	-0.124007
O	-0.779351	-1.850845	0.230919
C	2.602516	-0.456184	-0.296601
H	3.053964	-0.480180	-1.294748
H	2.049229	0.847470	-0.134667
C	3.569319	-0.878680	0.776829
H	4.495255	-0.286663	0.742122
H	3.151919	-0.795501	1.782949
H	3.880980	-1.922624	0.633530
O	-2.060196	1.167125	-0.129642
H	1.951865	2.634477	0.314918

TS-β-6
In triplet

Ni	1.093832	1.581644	-0.591167
Ni	1.967551	-0.589977	0.283953
Ni	-1.140885	-0.683852	-0.041548
O	-0.697200	1.282250	-0.741280
O	2.700571	0.991574	-0.248567
O	0.496881	-1.445100	0.387584
C	-3.267060	-0.423066	0.162089
H	-3.845850	-1.333306	0.052169
H	-3.636987	0.405466	-0.431228
C	-2.614993	-0.163613	1.380952
H	-2.379957	0.852231	1.670517
H	-2.589568	-0.917841	2.158134
H	-1.171672	1.534812	-1.539090
H	-2.286248	-0.928281	-1.090179
In quintuplet			
Ni	0.672265	1.365197	0.066518
Ni	1.645628	-0.969872	0.061214
Ni	-1.020261	-0.443612	-0.262606
O	-0.933677	1.500100	-0.883199
O	2.178623	0.591760	0.667842
O	0.166491	-1.768246	-0.538236
C	-3.165146	-0.502836	0.357932
H	-3.433451	-1.516822	0.631774
H	-3.741609	-0.050489	-0.440776
C	-2.432296	0.286117	1.215755
H	-2.385821	1.356897	1.073435
H	-2.045380	-0.116647	2.145477
H	-0.815714	1.689940	-1.819610
H	-2.061238	-1.258548	-0.863183
In heptet			
Ni	1.319335	1.297966	0.036947
Ni	1.553324	-1.186201	0.018947
Ni	-1.457704	-0.323352	-0.297073
O	-0.471369	1.543491	-0.158062
O	2.698160	0.224832	0.075435
O	-0.093790	-1.630203	-0.079901
C	-3.496029	0.342404	-0.043248
H	-4.236494	-0.274347	-0.540361
H	-3.614039	1.402960	-0.235965
C	-2.959511	-0.082508	1.186126
H	-2.552705	0.636281	1.885442
H	-3.183246	-1.070925	1.568241
H	-0.840946	2.259492	-0.683136
H	-2.509449	0.176042	-1.370145
Ni₃O(OH)₂			
In triplet			

Ni	1.337040	-0.190003	-0.012046
Ni	-0.733177	1.481053	-0.059312
Ni	-0.782555	-1.179298	-0.082619
O	1.153861	1.701007	0.071193
O	-2.117872	0.173965	-0.037754
O	0.830790	-1.889373	0.215151
H	-2.842215	0.175745	0.594283
H	1.582087	2.240742	0.741606

In quintuplet

Ni	1.124867	-0.845249	-0.039093
Ni	0.113563	1.454480	0.014507
Ni	-1.245167	-0.661971	-0.033111
O	1.956059	0.834009	-0.065279
O	-1.801220	1.124403	-0.071788
O	-0.161234	-2.069499	0.136315
H	-2.506081	1.512551	0.451624
H	2.694958	1.099211	0.487423

In heptet

Ni	-0.025756	1.161913	-0.689323
Ni	0.271010	0.022862	1.721810
Ni	-0.172944	-1.237049	-0.614819
O	0.296796	1.974094	0.915841
O	0.052789	-1.963418	1.048854
O	-0.310057	-0.064909	-1.947533
H	0.138303	-2.858040	1.394308
H	0.360711	2.892828	1.197402

Ni₂O₂OH-NiH-para

In triplet

O	0.960044	1.752294	0.033364
Ni	1.425002	0.022242	-0.012190
Ni	-0.660191	-1.231825	-0.015845
O	-2.134083	-0.045951	0.018598
Ni	-0.721088	1.204496	-0.011117
O	1.048186	-1.689666	0.045546
H	-3.072111	-0.094729	0.211633
H	2.854695	0.103717	0.104564

In quintuplet

O	1.013474	-1.724285	0.056218
Ni	1.432225	0.005131	-0.040220
Ni	-0.698546	1.207037	0.006830
O	-2.147044	-0.010888	-0.030835
Ni	-0.687411	-1.213868	0.006840
O	0.997771	1.731398	0.054092
H	-3.105468	-0.016819	-0.016863
H	2.855643	0.006714	0.160753

In heptet

O	0.839066	1.609841	0.045474
Ni	1.786768	0.056255	0.026198
Ni	-0.782061	-1.184316	0.076364
O	-2.298737	-0.065187	0.067861
Ni	-0.853666	1.144977	0.020230
O	0.934376	-1.550489	0.013056
H	-3.256205	-0.093548	0.087552
H	3.330913	0.103044	0.037817

Ni₂O₂OH-NiH-ortho

In triplet

O	-0.821899	-1.666828	0.033165
Ni	-1.685881	-0.097544	0.005527
Ni	0.658206	1.294507	-0.042368
O	2.159389	0.123941	0.055823
Ni	0.801181	-1.116590	-0.046370
O	-1.088325	1.548430	0.092235
H	2.961645	0.095178	0.583009
H	1.386877	-2.389944	0.297124

In quintuplet

O	-0.849873	-1.833460	0.006493
Ni	-1.349684	-0.048455	-0.064828
Ni	0.559248	1.322999	0.096006
O	2.046644	0.144592	0.229630
Ni	0.748560	-1.202990	0.129340
O	-1.152032	1.749461	-0.010429
H	2.995338	0.166144	0.367032
H	1.372992	-2.507143	0.224901

In heptet

O	-0.888907	-1.443190	-0.103511
Ni	-1.551294	0.132835	-0.043453
Ni	0.568535	1.431322	0.131855
O	1.821636	0.112914	0.007148
Ni	0.964755	-1.753402	-0.176233
O	-1.117740	1.886570	0.187377
H	2.710993	0.144540	0.372920
H	1.863214	-2.720441	0.602043

Ni₃O₂-H₂O

In triplet

Ni	-1.529932	-0.291474	0.001475
Ni	0.877568	-1.187073	0.004207
Ni	0.416504	1.524910	0.000739
O	-0.765777	-1.877635	0.002984
O	2.228237	0.426115	0.001662
O	-1.366751	1.451223	0.000863
H	2.785248	0.527388	0.790206
H	2.783625	0.523952	-0.788468

In quindruplet

Ni	-1.520568	-0.000120	0.000031
Ni	0.646966	-1.351459	-0.000059
Ni	0.646717	1.351548	0.000002
O	-1.105464	-1.705670	0.000070
O	2.291194	0.000230	0.000081
O	-1.105772	1.705499	-0.000093
H	2.856481	0.000140	0.788506
H	2.856607	0.000254	-0.788256

In heptet

Ni	0.825130	1.384260	0.016736
Ni	-1.168006	-0.482631	-0.452904
Ni	0.967953	-1.363117	0.087080
O	-0.885496	1.392244	-0.394743
O	-2.605345	0.014659	1.018737
O	2.004433	0.087860	0.380654
H	-2.313661	0.940827	0.863310
H	-3.550703	-0.026220	0.833131

C₂H₄

C	0.000000	0.000000	0.003974
C	0.000000	0.000000	1.331026
H	0.922461	0.000000	-0.566784
H	0.922461	0.000000	1.901784
H	-0.922461	0.000000	1.901784
H	-0.922461	0.000000	-0.566784

⁷TS-*α*-1

Ni	0.878264	-0.128959	-0.105976
Ni	-1.190198	1.239097	-0.981650
Ni	-1.529896	-0.440910	0.625751
O	0.015237	-1.221714	1.228413
O	0.657191	1.406939	-1.286690
H	1.198104	2.184627	-1.439696
C	2.554137	-0.811944	0.957357
H	3.043150	-0.079901	1.602754
H	1.301181	-1.131876	1.340923
C	3.396034	-2.003522	0.628722
H	3.758112	-2.507157	1.537141
H	2.866134	-2.744475	0.025934
H	4.297204	-1.698354	0.077650
O	-2.662945	0.735176	-0.135235

⁷TS-*α*-5

Ni	0.711062	-0.967695	-0.235032
Ni	-2.002528	-0.578986	0.170085
Ni	-0.313629	1.484599	-0.104469
O	1.505604	1.902532	-0.124007

O	-0.779351	-1.850845	0.230919
C	2.602516	-0.456184	-0.296601
H	3.053964	-0.480180	-1.294748
H	2.049229	0.847470	-0.134667
C	3.569319	-0.878680	0.776829
H	4.495255	-0.286663	0.742122
H	3.151919	-0.795501	1.782949
H	3.880980	-1.922624	0.633530
O	-2.060196	1.167125	-0.129642
H	1.951865	2.634477	0.314918

⁵TS-*α*-6

Ni	0.518265	0.642547	1.018726
Ni	-1.540840	-0.921500	0.527262
Ni	0.361516	0.270701	-1.402426
O	-0.556421	-0.571476	1.917921
O	0.547557	1.804167	-0.283487
O	-1.470281	-0.737901	-1.315139
C	1.567233	-0.543462	-0.229549
H	1.326927	-1.560260	0.080513
H	1.167708	-0.804321	-2.061525
C	3.034048	-0.214663	-0.224174
H	3.574622	-0.899768	-0.888870
H	3.226691	0.808801	-0.543097
H	3.450075	-0.350384	0.781345
H	-1.552859	-1.510018	-1.883252

⁷PC-*α*-1

Ni	-1.566918	1.024160	0.023487
Ni	-1.231818	-1.267151	0.010104
Ni	1.200138	0.256284	-0.041613
O	-2.738034	-0.317484	-0.004590
O	0.049766	1.910146	-0.002134
O	0.572383	-1.658556	-0.024317
C	3.094301	0.555250	-0.030162
H	3.463432	1.576436	-0.157359
H	1.035285	-2.479036	-0.203829
C	4.163467	-0.482963	0.117620
H	4.820306	-0.270116	0.974859
H	3.762490	-1.490806	0.261714
H	4.822477	-0.517326	-0.763984
H	0.275976	2.842158	-0.008610

⁷PC-*α*-5

Ni	0.788199	-0.907287	-0.356567
Ni	-1.883525	-0.796425	0.168064
Ni	-0.476337	1.476061	-0.016985
O	1.301128	2.207004	0.011638
O	-0.579622	-1.960300	0.208726
C	2.592636	-0.238169	-0.345097
H	3.048814	0.052690	-1.299254
H	1.910617	1.389642	-0.027737
C	3.613887	-0.634564	0.687612

H	4.427133	0.099004	0.779899
H	3.179253	-0.789784	1.678259
H	4.099616	-1.580402	0.401798
O	-2.161901	0.950465	-0.029704
H	1.625135	2.862130	0.640345

⁵PC- α -6

Ni	0.449769	0.683331	1.030957
Ni	-1.609599	-0.882069	0.535055
Ni	0.304778	0.306293	-1.413109
O	-0.620825	-0.529957	1.923691
O	0.475914	1.833213	-0.273073
O	-1.543386	-0.687116	-1.300633
C	1.493686	-0.479451	-0.190551
H	1.249956	-1.506591	0.079717
H	0.941238	-0.695877	-2.300163
C	2.961071	-0.170856	-0.218606
H	3.468115	-0.852305	-0.911110
H	3.163710	0.855007	-0.521982
H	3.404503	-0.336122	0.771113
H	-1.592448	-1.458411	-1.872030

⁵TS-cle-1

Ni	-1.245225	1.491923	0.028766
Ni	1.256538	-0.092337	-0.387952
O	0.472741	1.903030	-0.518311
Ni	-0.888041	-1.180404	0.009383
O	-2.110880	0.091932	0.580988
C	0.678464	-0.768331	1.243051
H	1.054735	-1.737074	1.556883
H	0.280371	-0.154452	2.045825
C	2.572381	0.276231	1.071123
H	2.955649	-0.427141	1.804661
H	3.324253	0.369454	0.269871
H	2.365819	1.247625	1.512796
O	0.337936	-1.510990	-1.200424
H	0.595486	2.392655	-1.338273

⁵PC-cle-1

Ni	-1.384859	1.240322	0.050862
Ni	1.440831	-0.025165	-0.277658
O	0.265749	1.724274	-0.627162
Ni	-0.777635	-1.336531	-0.019867
O	-2.104920	-0.233532	0.635553
C	0.678923	-0.939449	1.190228
H	1.224888	-1.842669	1.460220
H	0.322724	-0.360496	2.039320
C	2.769151	0.834319	0.826589
H	3.368240	0.153517	1.431926
H	3.399688	1.289526	0.047823
H	2.334193	1.617921	1.445640
O	0.414714	-1.341977	-1.266213

H	0.264060	1.981302	-1.556667
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⁵TS-cle-2

Ni	-1.416374	1.187913	-0.303986
Ni	1.189040	0.336507	-0.272604
O	0.103552	1.721886	-0.955158
Ni	-0.734948	-1.254939	0.151799
O	-2.123190	-0.239740	0.544257
C	0.660658	-0.523190	1.319499
H	0.985765	-1.478598	1.734495
H	0.301128	0.161004	2.084465
C	2.746175	-0.125885	0.906450
H	3.113594	-1.138609	0.759083
H	3.322916	0.585862	0.296018
H	2.832191	0.174260	1.948200
O	0.625254	-1.538688	-1.113272
H	1.229681	-2.273462	-0.960902

⁵PC-cle-2

Ni	1.341729	-1.248815	-0.062264
Ni	-1.014052	-0.285103	-0.195531
O	-0.307847	-1.848028	0.244692
Ni	0.656440	1.524264	0.145385
O	2.036390	0.350566	-0.279000
C	-0.625126	0.719436	1.426700
H	-1.523301	1.278918	1.699003
H	-0.360123	-0.003980	2.195414
C	-2.846118	-0.682901	0.091436
H	-3.392664	0.245871	0.245170
H	-3.102860	-1.160763	-0.857303
H	-2.922602	-1.369208	0.929102
O	-0.950301	1.378015	-1.118520
H	-1.652195	2.015849	-0.950107

⁵TS-iso-1

Ni	0.805833	0.846240	-0.554593
Ni	-1.401522	-0.233418	-0.051559
O	-0.543241	0.350837	-1.625493
O	-1.581108	-0.892942	1.624446
Ni	-0.027102	-0.044947	1.809956
O	1.607783	0.738274	1.188899
C	1.174030	-0.294340	-2.359201
H	2.188642	-0.027596	-2.028049
H	0.913077	0.232238	-3.266841
C	0.922788	-1.772016	-2.352417
H	1.637019	-2.262117	-3.028436
H	1.063072	-2.206135	-1.359868
H	-0.086457	-1.998147	-2.695288
H	2.492898	0.445933	1.418973

³Ethoxide-1

Ni	0.984414	1.258288	-0.077165
Ni	-0.384081	-0.978234	0.160727
O	0.519073	-0.139906	-1.279356
O	-0.711783	-1.399568	1.867751
Ni	-0.044683	0.239666	2.128643
O	1.016691	1.772332	1.753585
C	1.205486	-0.706321	-2.400039
H	2.195192	-1.056195	-2.083043
H	1.355001	0.085633	-3.141344
C	0.410135	-1.849459	-3.010609
H	0.930887	-2.256579	-3.882551
H	0.278581	-2.663954	-2.290552
H	-0.576766	-1.505175	-3.329961
H	1.804963	2.027539	2.240289

⁵Ethoxide-1

Ni	-0.248811	1.406086	0.111590
Ni	0.355316	-1.026860	0.266937
O	1.438396	0.477944	0.309256
O	-1.127275	-2.020631	0.214994
Ni	-1.927076	-0.449293	-0.056734
O	-2.173931	1.406456	-0.168441
C	2.798167	0.792729	0.573716
H	2.859882	1.341208	1.522286
H	3.160915	1.460607	-0.217259
C	3.661831	-0.457794	0.636891
H	4.705662	-0.196390	0.834568
H	3.324479	-1.122741	1.438010
H	3.622559	-1.003675	-0.310146
H	-2.836133	1.905672	0.315464

⁵TS-iso-2

Ni	0.848817	0.876521	-0.517114
Ni	-1.320415	-0.435627	-0.108067
O	-0.489037	0.259534	-1.576557
O	-1.607457	-0.848502	1.708952
Ni	0.149373	-0.122651	1.755882
O	1.595173	0.644769	1.142920
C	1.231714	-0.264507	-2.368951
H	2.200048	0.162521	-2.075851
H	0.871014	0.175746	-3.288386
C	1.182391	-1.758127	-2.273783
H	1.913306	-2.190417	-2.971038
H	1.441874	-2.107793	-1.272412
H	0.195264	-2.137348	-2.541296
H	-2.356779	-0.987130	2.289684

⁵Ethylnickel-2

Ni	-1.132190	-1.198422	0.016571
Ni	-1.131254	1.198473	-0.002139
O	-2.565117	0.002999	0.321457

O	0.534223	1.713170	-0.277196
Ni	0.993944	-0.005455	-0.590320
O	0.532995	-1.718551	-0.250009
C	2.927972	-0.004456	-0.344836
H	3.209484	-0.916842	-0.871774
H	3.210239	0.899803	-0.885205
C	3.260861	0.006264	1.123667
H	4.353602	0.006788	1.251304
H	2.872626	0.899274	1.616750
H	2.871909	-0.879050	1.629879
H	-3.409092	0.006422	0.776010

⁵TS-β-ethox

Ni	-0.924108	-0.677210	-1.112702
Ni	0.481637	1.470842	-0.172256
Ni	1.275844	-0.931317	0.390930
O	-1.350877	1.032614	-0.281206
C	-2.121673	0.774647	0.916925
C	-1.469117	-0.170199	1.907235
H	-2.309470	1.743278	1.400939
H	-3.092332	0.376900	0.602489
H	-0.655204	0.263218	2.487519
H	-2.168085	-0.728640	2.530948
H	-0.882725	-1.239579	1.146512
O	-0.308526	-1.832805	0.317281
O	2.219509	0.694230	0.095513
H	2.754792	0.688736	-0.706056

⁵TS-α-ethox

Ni	1.174278	-1.252201	-0.302455
Ni	-0.748346	0.655189	-0.806392
Ni	1.436970	1.172213	0.436697
O	2.719773	-0.204636	0.065215
H	3.270398	-0.481657	0.804942
O	-0.720734	-1.189470	-0.081700
O	-0.325626	1.496614	0.861177
C	-1.217434	-0.883447	1.198203
H	-0.849635	0.458880	1.308150
H	-0.618637	-1.344104	1.992038
C	-2.702146	-1.102291	1.354058
H	-3.033900	-0.753677	2.335958
H	-2.952986	-2.167535	1.267129
H	-3.268544	-0.560503	0.592159

⁵PC-α-ethox

Ni	0.562588	0.859874	-0.323248
Ni	-0.061290	-1.627243	0.154372
Ni	-1.845500	-0.008771	-0.866499
O	-1.012350	1.683057	-0.982215
H	-1.385290	2.409069	-0.472746
O	1.477516	-0.577886	0.519107
O	-1.888105	-1.813379	-0.310662

C	2.148157	-0.582132	1.716649
H	-2.504454	-2.062809	0.384740
H	1.592807	-0.221451	2.579769
C	3.629403	-0.477373	1.652725
H	4.066475	-0.595488	2.647532
H	3.959575	0.498315	1.256055
H	4.051720	-1.244428	0.994665

³TS-cle-ethox

Ni	0.694387	-1.324759	0.191449
Ni	-1.129996	0.667529	-0.263147
O	-1.092748	-1.421851	-0.395437
O	0.298396	1.998906	-0.323384
Ni	1.609694	0.788064	0.246628
O	2.390855	-0.813453	0.389434
C	-2.288658	-1.011976	0.116774
H	-2.429246	-1.230375	1.176282
H	-3.115441	-1.364239	-0.498420
C	-3.125377	0.811129	0.159095
H	-3.946745	0.290699	0.646242
H	-2.856980	1.653083	0.810161
H	-3.462163	1.160352	-0.819949
H	0.447971	2.590921	-1.065494

³PC-cle-ethox

Ni	-1.117758	1.172104	-0.028197
Ni	1.318147	-0.270575	-0.046264
O	0.395824	2.138450	0.001611
O	0.342387	-1.992728	0.085215
Ni	-1.299492	-1.160119	0.038868
O	-2.536565	0.092583	-0.076211
C	1.652104	1.667975	0.161348
H	2.067531	1.803935	1.165447
H	2.346034	1.976805	-0.627369
C	3.244564	-0.588317	-0.053915
H	3.819588	0.127951	0.531706
H	3.381287	-1.598634	0.338379
H	3.560603	-0.547756	-1.100738
H	0.606648	-2.906178	-0.040345

⁷TS-act-Ni3O2

Ni	-1.215934	-0.763449	-1.029833
Ni	-1.382691	1.260155	0.127436
Ni	0.907699	-0.240289	0.952699
O	0.248645	-1.571507	-0.334786
O	0.068642	1.368706	1.134053
C	2.771867	-0.862819	0.005777
H	3.126208	-1.891737	-0.127260
H	3.203663	-0.558295	0.972320
C	3.260678	0.057926	-1.117994
H	4.352257	0.048070	-1.212500
H	2.846814	-0.248378	-2.083160

H	2.955305	1.093865	-0.949486
H	1.455672	-1.331415	-0.332860

⁵Ethylnickel-Ni3O2

Ni	-1.187385	-0.469269	1.299332
Ni	-1.487961	-0.484991	-1.051781
Ni	0.601113	0.484996	0.091329
O	0.224976	0.705819	1.972601
O	0.091743	0.165449	-1.587420
C	2.242629	-0.493713	0.078641
H	2.337106	-0.805253	1.120444
H	2.075815	-1.336855	-0.588149
C	3.330733	0.448402	-0.393118
H	4.298945	-0.072767	-0.378787
H	3.157205	0.783981	-1.417610
H	3.435840	1.324796	0.253025
H	0.075356	1.587303	2.329666

⁷Ethylnickel-Ni3O2

Ni	-1.737123	-0.373559	1.056444
Ni	-1.604368	0.167945	-1.195379
Ni	1.185229	0.743484	-0.003907
O	-0.023689	0.196411	1.557215
O	0.024340	0.642237	-1.485871
C	3.004708	0.022129	0.240231
H	3.397319	0.430967	1.182604
H	3.626230	0.434868	-0.564116
C	3.077126	-1.508243	0.243422
H	4.102694	-1.879063	0.375754
H	2.475830	-1.942982	1.049755
H	2.702420	-1.926646	-0.695538
H	0.434025	-0.185481	2.313936

⁵TS-β-Ni3O2

Ni	-1.774035	-0.671768	0.103480
Ni	0.722547	-0.548409	-0.292264
Ni	-0.957440	1.526458	0.016597
O	-0.353333	-2.055630	0.098618
O	0.884431	1.281701	-0.105884
C	2.829806	-0.702836	0.104053
C	3.284935	0.638441	0.358701
H	-0.174825	-2.632666	0.847150
H	3.080264	-1.171574	-0.847985
H	2.741976	-1.397428	0.937550
H	2.147813	1.289940	0.214806
H	3.585923	0.863808	1.381114
H	3.926929	1.088140	-0.397578

⁵Ni₃O₂H₂

Ni	-1.358556	-0.649220	0.060804
Ni	0.415637	1.390169	0.003891
Ni	0.789742	-1.280703	-0.059360
O	-1.486361	1.313263	0.026321
O	1.969377	0.291389	-0.018833
H	-1.879767	1.644339	-0.790565
H	2.476529	0.352436	0.800218

⁷TS- α -Ni3O2

Ni	0.969916	-0.250277	-0.747278
Ni	-1.369384	1.630676	-0.309506
Ni	-1.644814	-0.263320	0.850172
O	-0.253985	-1.378981	0.300432
O	0.292357	1.448050	-1.340947
H	0.908533	2.185987	-1.394507
C	2.117137	-0.750446	0.829682
H	2.319865	0.047671	1.547558
H	0.938391	-1.190147	0.974652
C	3.112311	-1.879079	0.886392
H	3.236707	-2.274826	1.903617
H	2.838035	-2.713291	0.235846
H	4.103347	-1.524338	0.570961

⁷PC- α -Ni3O2

Ni	1.150081	-0.265457	-0.381001
Ni	-1.832722	-0.937746	0.123481
Ni	-1.515249	1.256133	0.042942
O	0.386831	1.523896	-0.101823
O	-0.088188	-1.740894	0.017295
H	0.216400	-2.295837	0.743563
C	2.952572	-0.542816	0.234005
H	3.326987	-1.570901	0.270060
H	0.835076	2.028824	0.585228
C	4.016384	0.501517	0.393142
H	4.784322	0.435512	-0.393606
H	3.622123	1.522391	0.369610
H	4.553158	0.381740	1.346662

⁵TS-cle-Ni3O2

Ni	-1.630975	-0.575481	-0.456174
Ni	0.970179	-0.721403	0.226362
O	-0.623300	-1.799648	0.200344
Ni	-0.312483	1.400574	-0.027373
C	0.979394	0.564494	-1.242051
H	1.541710	1.480955	-1.445943
H	0.763810	0.050738	-2.177167
C	2.764592	-0.233380	-0.541300
H	3.237034	0.671769	-0.169070
H	3.046055	-1.081884	0.114216
H	3.099787	-0.469809	-1.547588
O	0.559153	0.808240	1.577135
H	1.283260	1.340233	1.923934

⁵PC-cle-Ni3O2

Ni	-1.080347	1.432959	-0.106228
Ni	1.173966	-0.246635	-0.292860
O	0.516444	1.537168	-0.691878
Ni	-1.232359	-0.940306	0.283589
C	0.328769	-0.712538	1.379731
H	0.634045	-1.692663	1.766335
H	0.428321	0.056964	2.140895
C	2.818171	0.126062	0.618970
H	3.226837	-0.719967	1.172707
H	3.449468	0.360229	-0.249868
H	2.726229	1.003391	1.255551
O	-0.360429	-1.225044	-1.382934
H	-0.200711	-2.140645	-1.640990

⁵TS-iso-Ni3O2

Ni	0.880477	0.869754	-0.483092
Ni	-1.466491	-0.106208	0.034728
O	-0.469132	0.387293	-1.520957
Ni	-0.060695	0.156297	1.849152
O	1.717060	0.787210	1.205805
C	1.233197	-0.259160	-2.295443
H	2.251448	0.038152	-2.005471
H	0.933719	0.246819	-3.203260
C	1.017655	-1.743977	-2.267099
H	1.699833	-2.224691	-2.982055
H	1.222287	-2.168268	-1.281951
H	-0.005316	-1.993325	-2.548525
H	2.511272	0.265132	1.353445

⁵Ethoxide-Ni3O2

O	0.294667	1.564833	-0.254345
Ni	-1.586898	1.061727	-0.006445
Ni	-1.795234	-1.167646	0.145605
O	-0.025794	-2.017228	0.116925
Ni	0.740121	-0.273930	-0.061034
H	0.190887	-2.425231	0.964557
C	0.743286	2.370614	-1.347838
C	2.263366	2.435019	-1.392785
H	0.357671	1.979879	-2.299493
H	0.338309	3.381458	-1.216776
H	2.600253	3.079116	-2.211151
H	2.657561	2.831409	-0.453939
H	2.686381	1.437260	-1.551372

⁵TS-act-Ni3O1

Ni	-0.645314	1.323848	0.016029
Ni	-1.927162	-0.663612	0.317270

Ni	0.435242	-0.674254	-0.345222
O	0.788808	1.086604	-1.109357
C	2.598405	-0.600078	-0.125142
H	3.301353	-0.511500	-0.960330
H	2.404984	-1.687617	-0.053915
C	3.197010	-0.087958	1.188993
H	4.127903	-0.602152	1.452798
H	3.418444	0.980679	1.120623
H	2.503607	-0.218871	2.025094
H	1.780149	0.401362	-0.621606

³Ethylnickel-Ni3O1

Ni	1.702584	-0.308906	0.384222
Ni	0.523723	1.562382	-0.332452
Ni	-0.701085	-0.673566	-0.441163
O	0.598526	-1.905655	0.298663
C	-2.574877	-0.179918	-0.229843
H	-3.131889	-1.093580	-0.484341
H	-2.817134	0.563655	-0.999964
C	-2.958305	0.323474	1.163044
H	-4.030962	0.545916	1.237987
H	-2.727255	-0.415285	1.936045
H	-2.421471	1.240836	1.424254
H	0.833359	-2.695114	-0.199483

⁵Ethylnickel-Ni3O1

Ni	1.889946	0.094482	0.260170
Ni	0.044655	1.401525	-0.095466
Ni	-0.583478	-0.943020	-0.311716
O	1.118416	-1.680889	0.208602
C	-2.487144	-0.533574	-0.343041
H	-2.976762	-1.504800	-0.180626
H	-2.723752	-0.245267	-1.377200
C	-3.042673	0.505064	0.638379
H	-4.130699	0.620195	0.550224
H	-2.826860	0.237749	1.676721
H	-2.612884	1.502777	0.472547
H	1.493780	-2.467947	-0.195871

³TS-β-Ni3O1

Ni	1.105691	0.717545	-0.709037
Ni	0.278407	-1.336579	-1.455639
Ni	-1.175496	0.073193	-0.072020
O	-0.192585	1.654758	0.366316
C	-2.959895	-0.904323	0.263962
H	-2.861284	-1.778416	0.900234
H	-3.568544	-1.068355	-0.619960
C	-2.889055	0.383762	0.837063
H	-3.403652	1.211861	0.359638
H	-2.681157	0.505091	1.894767
H	-0.606795	2.446816	0.009547
H	-1.577503	-1.266261	-0.556642

³Ni₃O₁H₂

Ni	-0.581028	-1.223307	-0.002154
Ni	1.584636	-0.110682	0.006649
Ni	-0.379555	1.207325	0.000189
O	-1.996130	0.202297	-0.084578
H	-2.636709	0.287007	0.628392
H	1.116223	1.639254	-0.078129

³TS-α-Ni3O1

Ni	-0.654957	-0.517919	-1.036310
Ni	0.093708	-0.232139	1.212943
Ni	1.686779	0.630459	-0.363530
O	-0.136417	-1.945018	0.294586
H	0.663374	-2.443389	0.100778
C	-1.586602	0.484213	0.358322
C	-1.865116	1.954964	0.147300
H	-2.463699	-0.041828	0.749597
H	-1.033678	2.477529	-0.333910
H	-2.771602	2.142370	-0.437692
H	-2.013679	2.426336	1.128706
H	-2.093888	-0.287191	-1.364784

³PC-α-Ni3O1

C	-0.523604	1.080984	0.296020
C	-0.400611	2.409828	-0.413336
Ni	-2.216268	0.007948	0.080115
O	-1.244173	-1.635407	-0.165819
Ni	0.388180	-0.567985	-0.315979
Ni	2.553122	-0.176735	0.379550
H	-1.477402	-2.545127	-0.359498
H	-0.375609	1.208304	1.375026
H	-0.546620	2.339342	-1.494156
H	-1.131219	3.125520	-0.017531
H	0.588462	2.849943	-0.238035
H	-3.111019	0.958163	0.832084

⁵TS-cle-Ni3O1

Ni	1.732846	-0.484114	-0.103892
Ni	-0.965114	-0.555551	-0.090511
Ni	0.510107	1.443508	0.171180
C	-2.895390	-0.359007	0.362609
C	-1.495483	1.227454	0.147188
H	-3.043300	-1.306366	-0.180824
H	-2.990639	-0.523546	1.434698
H	-3.646157	0.343850	0.017897
H	-1.856158	1.660329	1.083723
H	-1.975862	1.728195	-0.696520
O	0.376812	-1.872498	-0.421836

H	0.388496	-2.274050	-1.297259
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⁵PC-cl-Ni3O1

Ni	-1.498947	-0.924557	0.012593
Ni	1.128486	-0.205039	-0.194477
Ni	-1.006986	1.316276	0.009551
C	3.044799	-0.180156	0.085120
C	0.915127	1.601523	0.290625
H	3.324930	-1.163805	-0.305160
H	3.541510	0.612661	-0.471701
H	3.265539	-0.099689	1.148344
H	1.416781	2.282958	-0.407688
H	1.219451	1.838819	1.314455
O	0.219530	-1.845854	0.163352
H	0.446271	-2.383663	0.928581
