Supplementary Information

THEORETICAL STUDY OF ELECTROCHEMICAL REDUCTION OF CO_2 TO CO USING NICKEL-N_4-SCHIFF BASE COMPLEX

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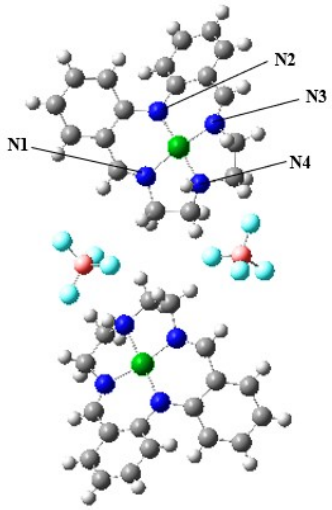
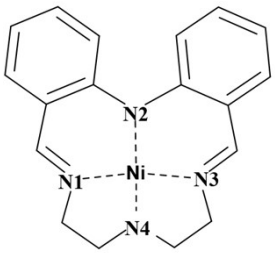


Fig. S1 Example structure of a reaction accelerator from a .cif file

Table S1 Important geometrical parameters for 1-Ni as computed by various methods including CPU time and x-ray structure.



	X-Ray	M06-2X			
		LANL2DZ, 6-31g(d,p)	SDD, 6-31g(d,p)	6-31g(d,p)	def2-TZVP
N1-Ni	1.83	1.90	1.91	1.89	1.91
N2-Ni	1.87	1.90	1.91	1.90	1.92
N3-Ni	1.86	1.91	1.91	1.90	1.92
N4-Ni	1.92	1.98	1.97	1.96	1.98
N1-Ni-N3	169.83	169.25	169.49	169.82	169.46
N2-Ni-N4	179.34	178.94	178.47	177.78	178.22
Jop cpu time(h.)	-	8.06	11.41	13.23	58.11

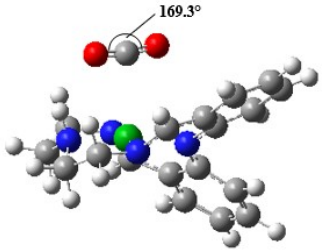
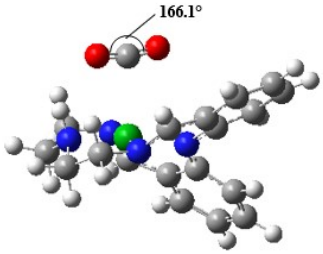
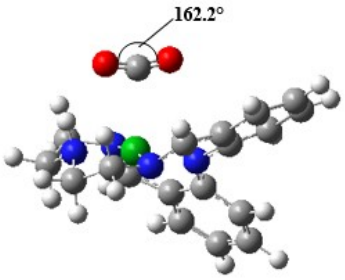
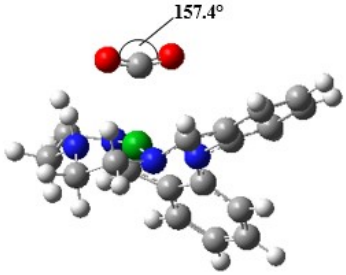
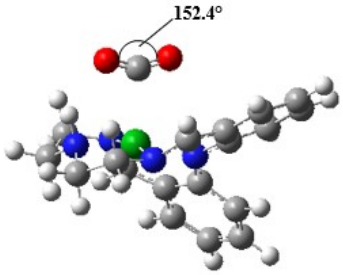
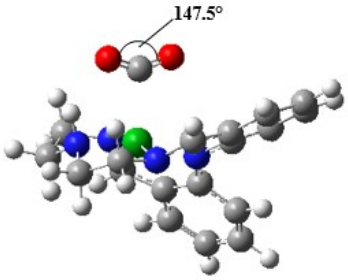
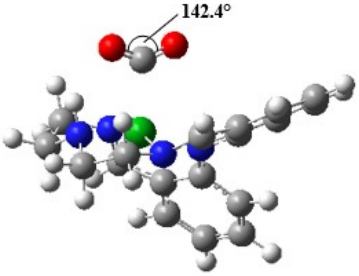
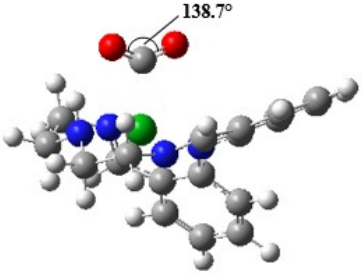
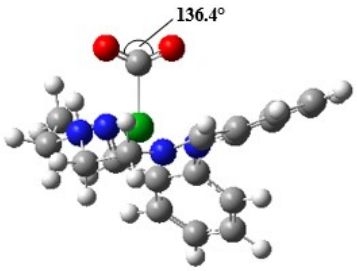
Ni-C 2.8 Å	Ni-C 2.7 Å	Ni-C 2.6 Å
		
Ni-C 2.5 Å	Ni-C 2.4 Å	Ni-C 2.3 Å
		
Ni-C 2.2 Å	Ni-C 2.1 Å	Ni-C 2.0 Å
		

Fig. S2 The distance between the nickel catalyst and the carbon dioxide molecule by considering the distance between Ni of the nickel catalyst and C of the carbon dioxide molecule and the angle of the carbon dioxide structure during adsorption.

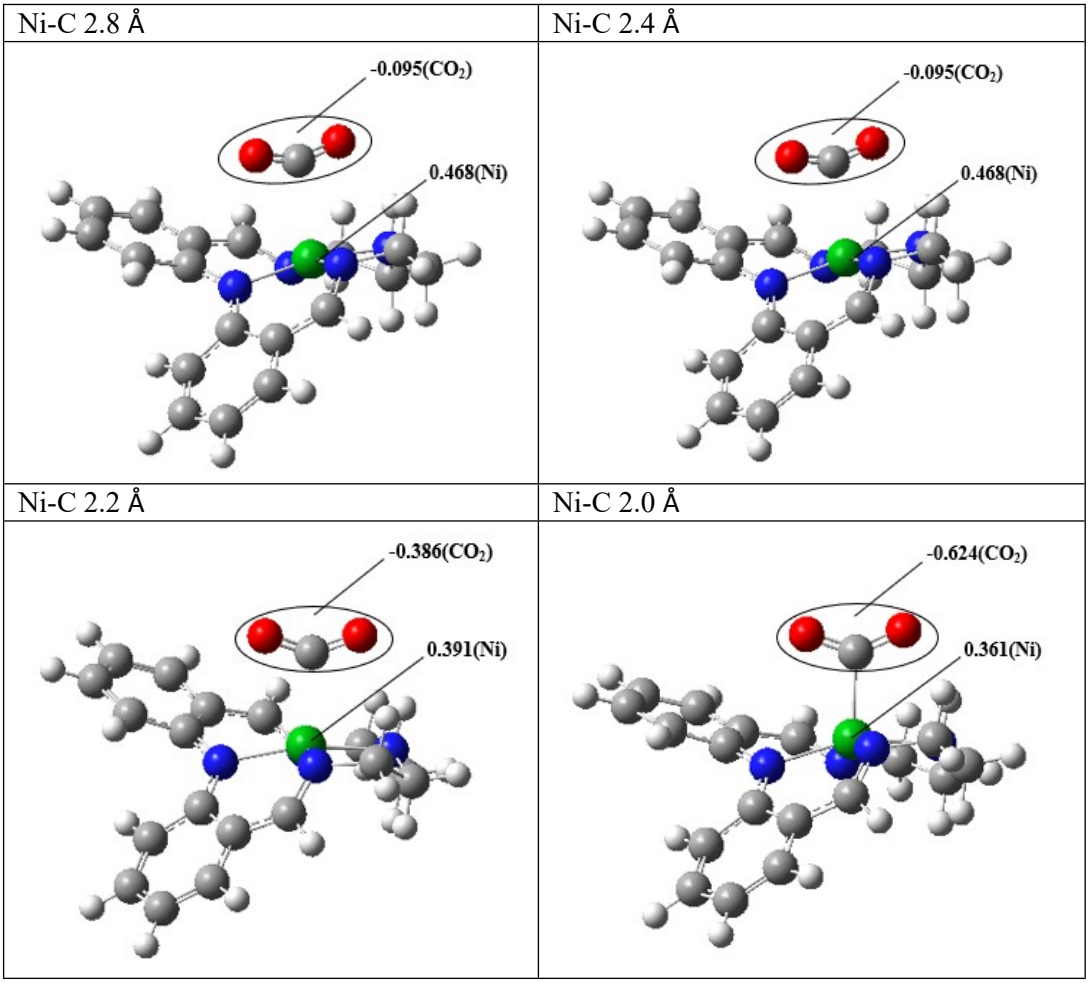


Fig. S3 NBO charges observed during the adsorption of CO_2.

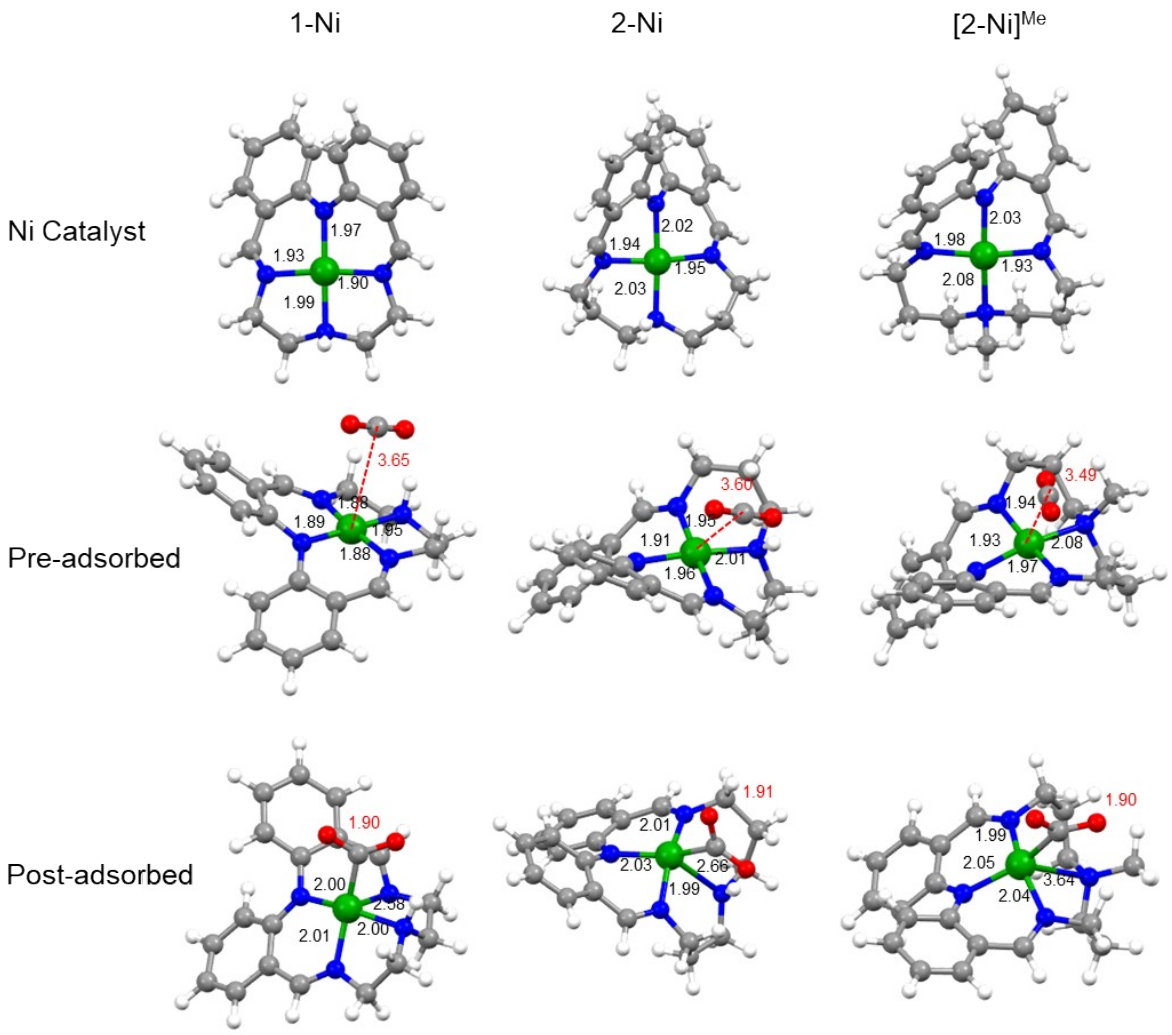


Fig. S4 The structure of Ni catalyst, Pre-adsorbed and Post-adsorbed, with black letters indicating the N-Ni distance and red letters indicating the Ni-C distance of the carbon dioxide molecule in angstrom units.

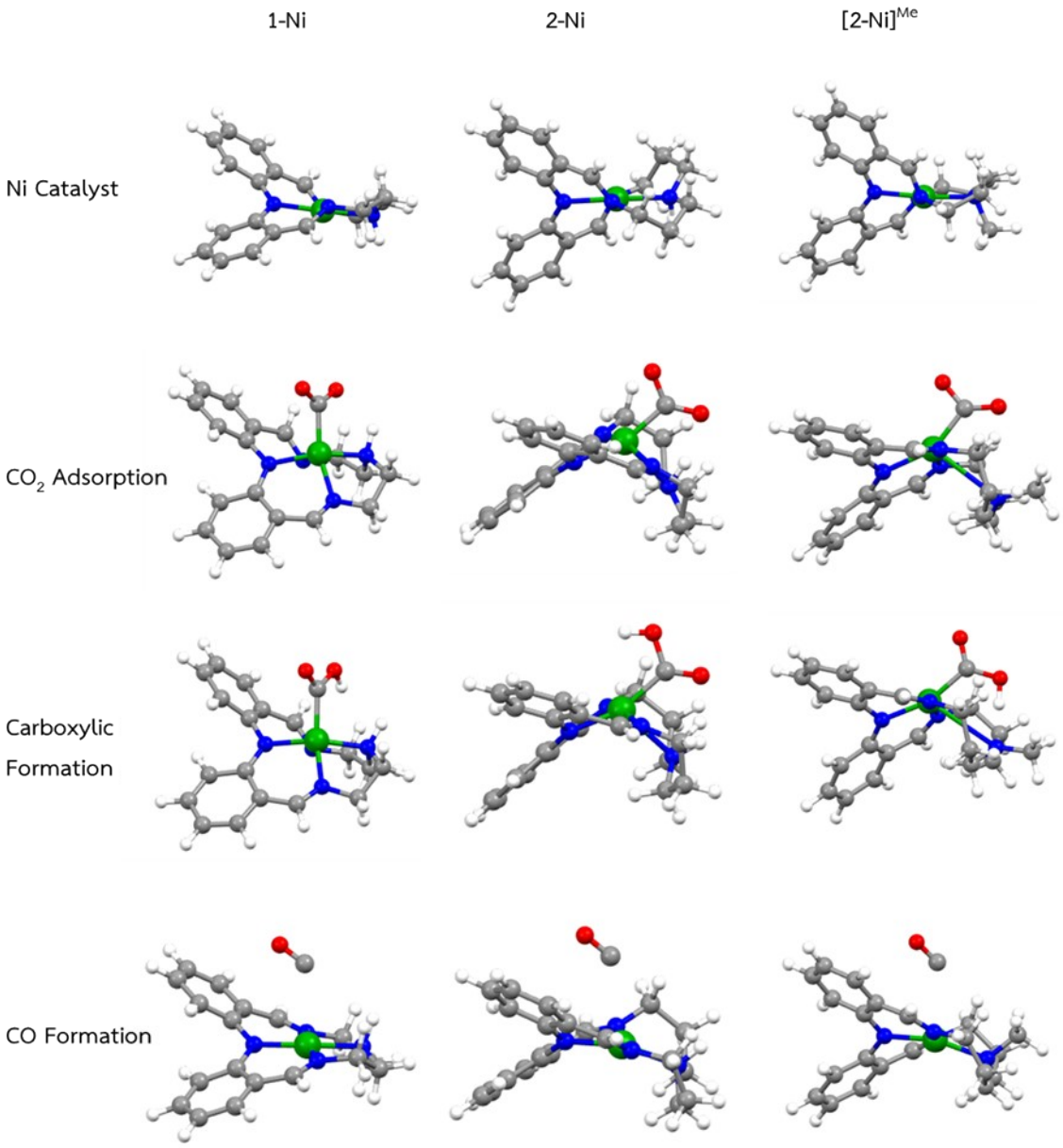


Fig. S5 The arrangement in every stage of the external proton transfer pathway(A).

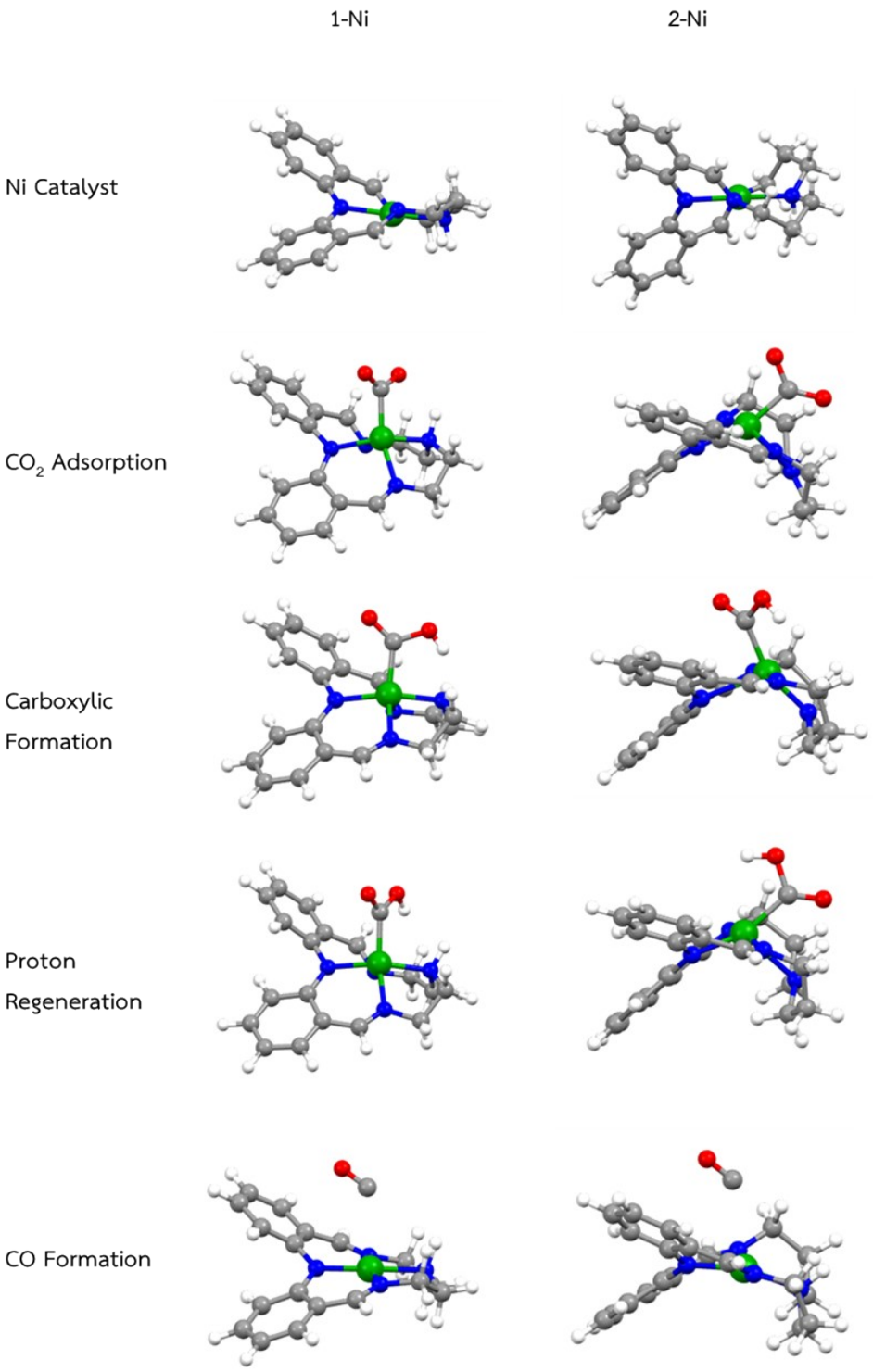


Fig. S6 The arrangement in every stage of the internal proton transfer pathway(B).

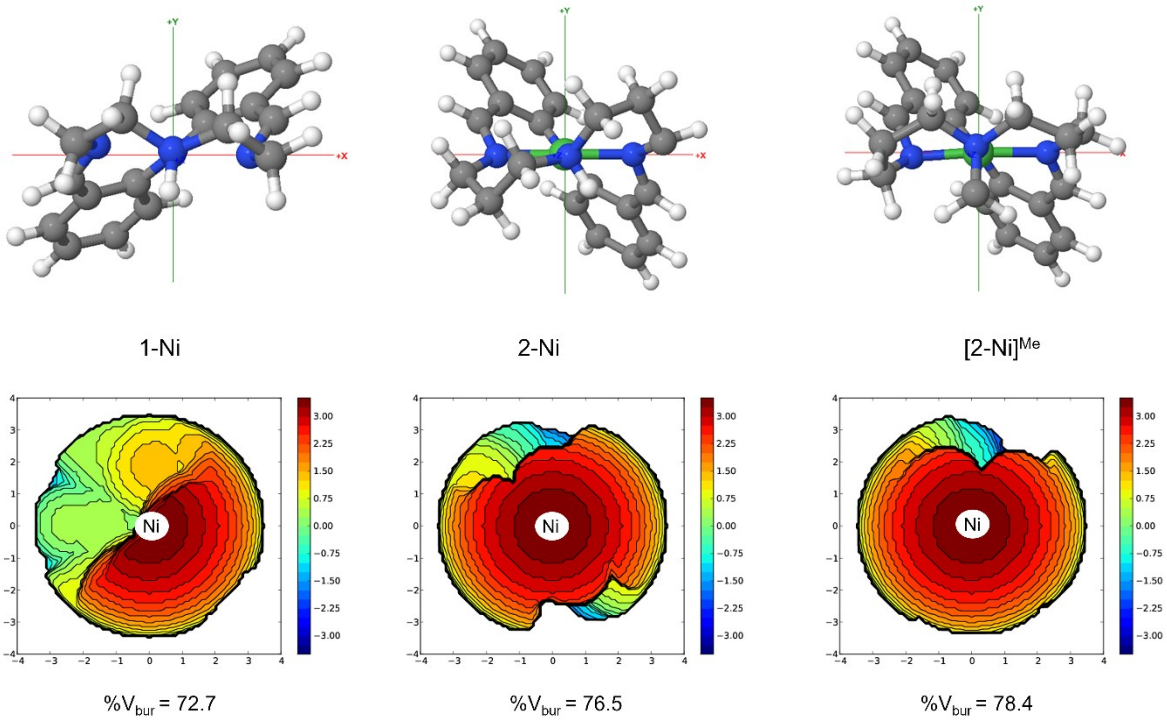


Fig. S7 Topographic steric maps of optimized pre-reaction Ni complex.

Example of input file

1-Ni (Step A2)

%chk=1A_1.chk

%mem=5GB

%nprocshared=16

#p opt m062x/genecp scrf=(solvent=acetonitrile) scf=maxcycle=99999

Title Card Required

-1 1

C	2.77814200	-2.89579000	-0.63969200
C	1.72513600	-1.95348100	-0.54555100
C	1.92434400	-0.82886500	0.30315400
C	3.09039200	-0.74966700	1.07296100
C	4.09498000	-1.71126300	0.98791800
C	3.94413500	-2.78314500	0.10247900
H	2.64328100	-3.75131200	-1.29557900
H	3.21437300	0.10286400	1.73411700
H	4.98794900	-1.61769000	1.59748700
H	4.72226500	-3.53390900	0.00823100
C	0.47548000	2.66607600	0.10089100
C	0.95343200	3.94507000	-0.25758300
C	2.18849900	4.13073600	-0.86218700
C	2.97626600	3.01040700	-1.13740600
C	2.55733100	1.73961600	-0.74676000
C	1.33996000	1.54099000	-0.07940200
H	0.30278100	4.79907300	-0.08955900
H	2.52115400	5.12610600	-1.13736600
H	3.93307000	3.12145700	-1.63838500
H	3.20282000	0.89220000	-0.93705200
N	0.95979600	0.25327100	0.42521500
C	0.50047600	-2.32413200	-1.23693000
H	0.56951800	-3.21205300	-1.87078900
C	-0.93564300	2.61034000	0.45785700
H	-1.41671500	3.57489100	0.64417700
N	-0.65878300	-1.75446500	-1.06268400
N	-1.65733100	1.53635200	0.41631100
C	-1.85367500	-2.39524100	-1.63679700
H	-2.17779200	-3.19367900	-0.95612400
H	-1.63662400	-2.85756900	-2.60679800
C	-2.97587400	-1.35698600	-1.77835500
H	-2.72418900	-0.65632200	-2.58114100
H	-3.91711300	-1.85404600	-2.04850800
C	-3.11650600	1.60754100	0.54464600
H	-3.48655400	2.63657000	0.47192000
H	-3.40055900	1.20227600	1.52210900
C	-3.72417900	0.72984900	-0.56447400
H	-3.51708100	1.18648100	-1.53746900
H	-4.81323700	0.66275400	-0.44743100
N	-3.06282500	-0.58627100	-0.52907400
H	-3.41005800	-1.14780300	0.25053700
Ni	-1.08215000	-0.25964200	0.04222200
O	-0.37091000	-0.49208100	2.67724200
O	-2.39072000	-1.41491700	2.19180000
C	-1.32103600	-0.83147500	1.92101400

Ni 0

LANL2DZ

****

C H O N 0

6-31g(d,p)

****

Ni 0

LANL2DZ

Reaction coordinates

1-Ni (Step A1)

C	1.37540000	-3.49840000	-0.77550000
C	0.82860000	-2.20680000	-0.73590000
C	1.48220000	-1.19540000	0.01670000
C	2.64880000	-1.56510000	0.71390000
C	3.18810000	-2.84010000	0.63680000
C	2.55770000	-3.82260000	-0.12840000
H	0.83700000	-4.26550000	-1.32760000
H	3.12640000	-0.81440000	1.33610000
H	4.09110000	-3.07470000	1.19250000
H	2.96360000	-4.82660000	-0.18940000
C	1.27280000	2.53140000	0.12690000
C	2.18330000	3.60820000	0.04260000
C	3.50410000	3.44870000	-0.31200000
C	3.92300000	2.15100000	-0.65720000
C	3.07970000	1.06930000	-0.55400000
C	1.73230000	1.17060000	-0.06010000
H	1.79560000	4.60650000	0.23460000
H	4.17850000	4.29460000	-0.37340000
H	4.93330000	1.99000000	-1.02470000
H	3.45010000	0.09700000	-0.85210000
N	0.94620000	0.09520000	0.16220000
C	-0.52430000	-2.07460000	-1.32300000
H	-1.12060000	-2.99400000	-1.23420000
C	-0.11030000	2.93080000	0.25640000
H	-0.27810000	4.00910000	0.38570000
N	-1.04840000	-1.01620000	-1.79470000
N	-1.12130000	2.14870000	0.15180000
C	-2.48570000	-1.06610000	-2.02520000
H	-2.93190000	-1.97710000	-1.60240000
H	-2.69040000	-1.04150000	-3.10220000
C	-3.15010000	0.17260000	-1.41990000
H	-2.69540000	1.05580000	-1.87800000
H	-4.21900000	0.17510000	-1.67290000
C	-2.47960000	2.67920000	0.14850000
H	-2.72720000	3.01120000	-0.86710000
H	-2.58540000	3.55040000	0.80670000
C	-3.44370000	1.56360000	0.58420000
H	-4.46600000	1.80160000	0.26150000
H	-3.43800000	1.47430000	1.67370000
N	-2.97180000	0.27900000	0.04090000
H	-3.38010000	-0.53550000	0.50320000
Ni	-1.02580000	0.16700000	0.49670000
O	-0.54880000	-1.67860000	2.43150000
O	-2.26250000	-2.22000000	1.07620000
C	-1.29320000	-1.48470000	1.43840000

1-Ni (Step A2)

C	1.37540000	-3.49840000	-0.77550000
C	0.82860000	-2.20680000	-0.73590000
C	1.48220000	-1.19540000	0.01670000
C	2.64880000	-1.56510000	0.71390000
C	3.18810000	-2.84010000	0.63680000
C	2.55770000	-3.82260000	-0.12840000
H	0.83700000	-4.26550000	-1.32760000
H	3.12640000	-0.81440000	1.33610000
H	4.09110000	-3.07470000	1.19250000
H	2.96360000	-4.82660000	-0.18940000
C	1.27280000	2.53140000	0.12690000
C	2.18330000	3.60820000	0.04260000
C	3.50410000	3.44870000	-0.31200000
C	3.92300000	2.15100000	-0.65720000
C	3.07970000	1.06930000	-0.55400000
C	1.73230000	1.17060000	-0.06010000
H	1.79560000	4.60650000	0.23460000
H	4.17850000	4.29460000	-0.37340000
H	4.93330000	1.99000000	-1.02470000
H	3.45010000	0.09700000	-0.85210000
N	0.94620000	0.09520000	0.16220000
C	-0.52430000	-2.07460000	-1.32300000
H	-1.12060000	-2.99400000	-1.23420000
C	-0.11030000	2.93080000	0.25640000
H	-0.27810000	4.00910000	0.38570000
N	-1.04840000	-1.01620000	-1.79470000
N	-1.12130000	2.14870000	0.15180000
C	-2.48570000	-1.06610000	-2.02520000
H	-2.93190000	-1.97710000	-1.60240000
H	-2.69040000	-1.04150000	-3.10220000
C	-3.15010000	0.17260000	-1.41990000
H	-2.69540000	1.05580000	-1.87800000
H	-4.21900000	0.17510000	-1.67290000
C	-2.47960000	2.67920000	0.14850000
H	-2.72720000	3.01120000	-0.86710000
H	-2.58540000	3.55040000	0.80670000
C	-3.44370000	1.56360000	0.58420000
H	-4.46600000	1.80160000	0.26150000
H	-3.43800000	1.47430000	1.67370000
N	-2.97180000	0.27900000	0.04090000
H	-3.38010000	-0.53550000	0.50320000
Ni	-1.02580000	0.16700000	0.49670000
O	-0.54880000	-1.67860000	2.43150000
O	-2.26250000	-2.22000000	1.07620000
C	-1.29320000	-1.48470000	1.43840000

1-Ni (Step A3)

C	1.54970000	3.37610000	0.91230000
C	0.93680000	2.11340000	0.84810000
C	1.48750000	1.11830000	-0.00410000
C	2.60590000	1.47250000	-0.77800000
C	3.20530000	2.71960000	-0.68390000
C	2.68510000	3.68340000	0.18110000
H	1.10210000	4.13250000	1.55210000
H	2.99980000	0.73090000	-1.46620000
H	4.07030000	2.94620000	-1.29920000
H	3.14100000	4.66400000	0.25880000
C	1.15250000	-2.59450000	-0.09400000
C	2.01220000	-3.71280000	0.00880000
C	3.34440000	-3.59590000	0.32660000
C	3.83140000	-2.30530000	0.60580000
C	3.03550000	-1.18950000	0.49070000
C	1.67000000	-1.25700000	0.05390000
H	1.57670000	-4.69730000	-0.14470000
H	3.98450000	-4.46660000	0.40290000
H	4.86040000	-2.17730000	0.93040000
H	3.45950000	-0.22510000	0.73690000
N	0.90880000	-0.15930000	-0.15770000
C	-0.36300000	2.01560000	1.54070000
H	-0.78690000	2.99410000	1.82210000
C	-0.24270000	-2.91410000	-0.21770000
H	-0.47890000	-3.98220000	-0.28590000
N	-1.03660000	0.94810000	1.70450000
N	-1.21730000	-2.07440000	-0.18960000
C	-2.43640000	1.04380000	2.08410000
H	-2.87040000	2.02880000	1.84900000
H	-2.54970000	0.89290000	3.16360000
C	-3.20430000	-0.08790000	1.39450000
H	-2.82830000	-1.02790000	1.80270000
H	-4.27280000	-0.01730000	1.62420000
C	-2.59590000	-2.56390000	-0.20290000
H	-2.86910000	-2.90290000	0.80240000
H	-2.71230000	-3.41970000	-0.87590000
C	-3.50760000	-1.42130000	-0.65270000
H	-4.54450000	-1.61240000	-0.35510000
H	-3.46870000	-1.31680000	-1.73940000
N	-3.00650000	-0.14520000	-0.08050000
H	-3.51800000	0.62060000	-0.51650000
Ni	-1.02760000	-0.14900000	-0.47340000
O	-0.51140000	1.58950000	-2.59570000
O	-1.71830000	2.65580000	-1.10750000
C	-1.02830000	1.52330000	-1.49770000
H	-2.05110000	2.51690000	-0.21250000

1-Ni (Step B3)

C	-1.18531500	-3.52862200	0.82667600
C	-0.71607200	-2.20992700	0.74959100
C	-1.41640000	-1.26318600	-0.03865000
C	-2.54849400	-1.71847700	-0.73924600
C	-3.01561200	-3.01963500	-0.62650500
C	-2.34000900	-3.93882100	0.17692300
H	-0.61095700	-4.24617900	1.40820000
H	-3.05976300	-1.01641400	-1.39097200
H	-3.89644600	-3.32314700	-1.18416800
H	-2.68979800	-4.96155300	0.26668300
C	-1.42184900	2.46394500	-0.17701600
C	-2.38293700	3.49493600	-0.09673300
C	-3.69814200	3.26435700	0.23940500
C	-4.05437100	1.94435000	0.56618700
C	-3.15526100	0.90661400	0.46798600
C	-1.80858400	1.08400500	0.00059500
H	-2.04277600	4.51234000	-0.27753600
H	-4.41618600	4.07370000	0.29862300
H	-5.06061400	1.72822300	0.91561700
H	-3.48207600	-0.08441300	0.75342200
N	-0.95194600	0.05672700	-0.21028400
C	0.62159900	-1.96889000	1.34427100
H	1.31146000	-2.81902200	1.21030100
C	-0.05783800	2.92015700	-0.29656500
H	0.06918500	4.00388800	-0.41439400
N	1.03209800	-0.89881400	1.89379500
N	0.98763500	2.18413600	-0.19928600
C	2.46518300	-0.80936500	2.14670700
H	2.99480400	-1.71160100	1.80076200
H	2.63290300	-0.70077300	3.22450400
C	3.03429200	0.43382300	1.45228200
H	2.50955500	1.29934200	1.89527000
H	4.09277500	0.53100400	1.75154700
C	2.32450600	2.78460200	-0.20902100
H	2.53809400	3.17379400	0.79350600
H	2.37603300	3.63068500	-0.90525700
C	3.32180100	1.66759900	-0.57863700
H	4.33434700	1.97308800	-0.26435100
H	3.33924200	1.55912500	-1.67057900
N	2.92065000	0.39114300	-0.00237600
H	3.09353300	-1.03887700	-0.80822100
Ni	1.01957900	0.22967600	-0.44521600
O	0.68410800	-2.14900200	-2.13467700
O	2.72320500	-1.78591300	-1.36072900
C	1.40699100	-1.45199000	-1.43268800

2-Ni (Step A1)

C	1.50360000	-3.70080000	-0.48240000
C	0.93720000	-2.46950000	-0.02160000
C	1.64120000	-1.23320000	-0.32570000
C	2.86990000	-1.34400000	-1.05070000
C	3.37900000	-2.54950000	-1.46400000
C	2.68590000	-3.76060000	-1.16720000
H	0.96380000	-4.61830000	-0.25110000
H	3.38430000	-0.42130000	-1.30610000
H	4.29760000	-2.57810000	-2.04310000
H	3.09010000	-4.71540000	-1.48950000
C	1.22540000	2.39250000	0.06000000
C	1.96430000	3.53220000	0.52580000
C	3.19130000	3.42840000	1.12070000
C	3.76540000	2.14090000	1.32970000
C	3.08270000	1.01840000	0.91990000
C	1.81490000	1.07790000	0.27290000
H	1.51880000	4.51430000	0.37080000
H	3.72160000	4.32080000	1.44140000
H	4.71960000	2.04280000	1.83870000
H	3.49840000	0.03350000	1.11800000
N	1.08810000	-0.04110000	-0.00680000
C	-0.23650000	-2.50540000	0.74840000
H	-0.65270000	-3.50060000	0.95800000
C	0.00260000	2.58100000	-0.59110000
H	-0.36850000	3.61230000	-0.65560000
N	-0.87730000	-1.44080000	1.24800000
N	-0.73660000	1.59930000	-1.16630000
C	-2.97830000	-0.65640000	2.30720000
H	-2.51850000	0.29510000	2.60620000
H	-3.69190000	-0.92530000	3.09230000
C	-3.72800000	-0.47480000	0.99510000
H	-3.90680000	-1.45690000	0.54280000
H	-4.70790000	-0.00620000	1.15620000
C	-2.73510000	0.91150000	-2.39810000
H	-3.37650000	1.21600000	-3.23080000
H	-2.05780000	0.13530000	-2.77190000
C	-3.62170000	0.33610000	-1.29660000
H	-3.89510000	-0.69550000	-1.53580000
H	-4.55650000	0.90800000	-1.21610000
N	-2.95190000	0.32170000	0.02450000
H	-2.95650000	1.28530000	0.36540000
Ni	-0.93100000	0.08100000	0.02400000
C	-1.91620000	-1.74570000	2.21360000
H	-2.42240000	-2.69910000	1.97240000
H	-1.47090000	-1.88270000	3.21120000
C	-1.87550000	2.08060000	-1.92660000
H	-1.52760000	2.64270000	-2.80590000
H	-2.50570000	2.79270000	-1.35190000

2-Ni (Step A2)

C	0.92470000	3.96210000	0.11290000
C	0.62370000	2.61630000	-0.17810000
C	1.54640000	1.58670000	0.17900000
C	2.73010000	2.00590000	0.85220000
C	2.98890000	3.33200000	1.13040000
C	2.08700000	4.33920000	0.75520000
H	0.20430000	4.72120000	-0.18330000
H	3.43340000	1.24660000	1.17650000
H	3.90100000	3.59210000	1.66050000
H	2.29200000	5.38150000	0.97060000
C	2.09740000	-1.99820000	0.25620000
C	3.13490000	-2.93100000	0.10130000
C	4.31970000	-2.60610000	-0.53540000
C	4.47840000	-1.29850000	-1.01160000
C	3.48550000	-0.35180000	-0.83620000
C	2.26010000	-0.65290000	-0.18790000
H	2.98380000	-3.93600000	0.48820000
H	5.10310000	-3.34440000	-0.66260000
H	5.38990000	-1.01830000	-1.53170000
H	3.62960000	0.65330000	-1.21910000
N	1.24990000	0.27680000	-0.04930000
C	-0.64220000	2.40490000	-0.86200000
H	-1.15840000	3.34160000	-1.10840000
C	0.90510000	-2.43790000	0.97350000
H	1.04980000	-3.23690000	1.71120000
N	-1.22570000	1.30720000	-1.18720000
N	-0.26300000	-1.94580000	0.80700000
C	-3.73720000	1.10680000	-0.87530000
H	-4.06400000	0.08680000	-1.08990000
H	-4.56090000	1.77580000	-1.14410000
C	-3.50220000	1.19750000	0.63660000
H	-3.03170000	2.15650000	0.90310000
H	-4.49070000	1.18480000	1.13030000
C	-1.59340000	-1.26730000	2.79570000
H	-1.80780000	-1.75300000	3.75330000
H	-0.66740000	-0.69630000	2.92720000
C	-2.74150000	-0.30530000	2.45960000
H	-2.66210000	0.58080000	3.10140000
H	-3.71020000	-0.78040000	2.70410000
N	-2.66020000	0.09430000	1.07010000
H	-2.87890000	-0.71550000	0.48320000
Ni	-0.58720000	-0.47450000	-0.49680000
C	-2.54480000	1.46000000	-1.80390000
H	-2.65700000	2.49610000	-2.14900000
H	-2.57270000	0.80430000	-2.67680000
C	-1.31980000	-2.36280000	1.73570000
H	-1.00650000	-3.28470000	2.24090000
H	-2.21070000	-2.57280000	1.13780000
O	-1.49190000	-1.63870000	-2.63520000
O	-2.93750000	-2.02200000	-0.95320000
C	-1.89050000	-1.50620000	-1.44620000

2-Ni (Step A3)

C	-0.98690000	3.93670000	0.06560000
C	-0.64810000	2.58830000	0.30190000
C	-1.50610000	1.54570000	-0.14010000
C	-2.67400000	1.93910000	-0.84620000
C	-2.97650000	3.26650000	-1.07270000
C	-2.13610000	4.29100000	-0.60940000
H	-0.30980000	4.70720000	0.42560000
H	-3.33050000	1.16640000	-1.23110000
H	-3.87390000	3.51520000	-1.63140000
H	-2.37780000	5.33210000	-0.78820000
C	-2.06130000	-2.03920000	-0.21520000
C	-3.10980000	-2.95960000	-0.04640000
C	-4.28070000	-2.61070000	0.59890000
C	-4.41200000	-1.29790000	1.07140000
C	-3.40650000	-0.36760000	0.88450000
C	-2.19540000	-0.69400000	0.22430000
H	-2.97590000	-3.96830000	-0.42870000
H	-5.07570000	-3.33400000	0.73790000
H	-5.31310000	-1.00070000	1.59950000
H	-3.53310000	0.64030000	1.26480000
N	-1.17700000	0.23090000	0.06270000
C	0.60520000	2.36650000	0.98820000
H	1.10580000	3.28820000	1.30550000
C	-0.88020000	-2.48610000	-0.92870000
H	-1.00340000	-3.33070000	-1.61520000
N	1.22040000	1.25760000	1.21060000
N	0.27500000	-1.94990000	-0.80600000
C	3.65480000	1.36960000	0.57360000
H	4.25070000	0.45720000	0.67260000
H	4.33520000	2.21320000	0.71870000
C	3.11050000	1.41410000	-0.85720000
H	2.33720000	2.18680000	-0.95920000
H	3.92590000	1.69930000	-1.54260000
C	1.61380000	-1.43990000	-2.85150000
H	2.50840000	-1.81240000	-3.36300000
H	0.78740000	-1.50320000	-3.56670000
C	1.82340000	0.03020000	-2.46190000
H	0.84870000	0.52640000	-2.34530000
H	2.34540000	0.54200000	-3.28760000
N	2.52520000	0.13050000	-1.19550000
H	3.21470000	-0.60670000	-1.07240000
Ni	0.65080000	-0.45900000	0.41560000
C	2.59160000	1.40560000	1.71330000
H	2.66870000	2.35980000	2.24550000
H	2.78180000	0.61100000	2.43450000
C	1.35440000	-2.40360000	-1.68240000
H	1.10680000	-3.39030000	-2.09080000
H	2.24960000	-2.50110000	-1.06660000
O	3.18070000	-1.90860000	0.87400000
O	1.89050000	-1.77000000	2.63780000
C	2.11940000	-1.48920000	1.30210000
H	1.03270000	-1.39460000	2.87650000

2-Ni (Step B3)

C	1.51458400	3.89975300	0.06363300
C	1.02605100	2.59148300	-0.17793200
C	1.78638100	1.45626000	0.25279100
C	2.97682300	1.73275300	0.98848000
C	3.41457300	3.02280100	1.22590900
C	2.69341500	4.13188600	0.74568500
H	0.92117200	4.73936700	-0.29052200
H	3.54453900	0.90000300	1.38692100
H	4.32251200	3.17567600	1.80378400
H	3.04220100	5.14341400	0.92581400
C	1.92913300	-2.18616800	0.34283600
C	2.89595800	-3.21198300	0.27536600
C	4.15403500	-2.99759900	-0.26308800
C	4.46110500	-1.71469000	-0.74499600
C	3.54505400	-0.67876100	-0.64790900
C	2.25489900	-0.85765200	-0.07707200
H	2.62184200	-4.19940500	0.63923100
H	4.87752700	-3.80395100	-0.32393700
H	5.42704800	-1.52440000	-1.20564300
H	3.81009600	0.30007000	-1.03174500
N	1.33781700	0.18065700	0.01485800
C	-0.26648700	2.51702300	-0.80718300
H	-0.67944800	3.49261600	-1.08570800
C	0.62911200	-2.54205100	0.86700200
H	0.58874700	-3.42915300	1.50724400
N	-1.02402500	1.48157900	-1.00978800
N	-0.47050900	-1.91550900	0.61505600
C	-3.30648100	2.22228600	-0.25646800
H	-4.33203100	2.28878500	-0.64568200
H	-3.02124000	3.23352300	0.06631200
C	-3.28575800	1.29433500	0.96988600
H	-2.24136200	1.33127500	1.36720100
H	-3.87558400	1.82296000	1.76450100
C	-2.28564200	-1.36059400	2.28749700
H	-2.32298600	-1.82606600	3.28340000
H	-1.60093400	-0.50918000	2.37287100
C	-3.70351200	-0.84295600	1.88467900
H	-4.10838200	-0.33300300	2.79488000
H	-4.33386300	-1.74328600	1.75721400
N	-3.78813300	-0.02394200	0.70696800
H	-3.34228600	-0.79590400	-0.62924400
Ni	-0.53047700	-0.31811800	-0.48293800
C	-2.40099100	1.82223400	-1.44311600
H	-2.35644700	2.65917700	-2.15332600
H	-2.82307000	0.97061800	-1.96634300
C	-1.69963700	-2.38428200	1.28289000
H	-1.47908000	-3.33332400	1.78811500
H	-2.43688800	-2.58325700	0.50212800
O	-1.27193700	-1.67868800	-2.61649700
O	-3.10228600	-1.27028500	-1.41985300
C	-1.78945000	-1.17024200	-1.61956700

[2-Ni]^{Me} (Step A1)

C	-1.44680000	-3.73610000	0.61430000
C	-0.94800000	-2.49730000	0.08170000
C	-1.74290000	-1.30230000	0.33310000
C	-2.95130000	-1.44230000	1.06220000
C	-3.40880000	-2.65830000	1.52820000
C	-2.63260000	-3.82750000	1.29260000
H	-0.85230000	-4.63240000	0.43940000
H	-3.51490000	-0.53620000	1.27530000
H	-4.33330000	-2.71580000	2.09450000
H	-2.97650000	-4.79150000	1.65890000
C	-1.50580000	2.33500000	-0.10980000
C	-2.30090000	3.43180000	-0.56120000
C	-3.49630000	3.26180000	-1.20450000
C	-3.96580000	1.93580000	-1.44680000
C	-3.24560000	0.85170000	-1.01920000
C	-1.98640000	0.98230000	-0.34170000
H	-1.92860000	4.43660000	-0.36460000
H	-4.07900000	4.11780000	-1.52960000
H	-4.89490000	1.78350000	-1.98940000
H	-3.60130000	-0.15500000	-1.22080000
N	-1.23220000	-0.07190000	0.00670000
C	0.23260000	-2.46550000	-0.66050000
H	0.78500000	-3.40760000	-0.77060000
C	-0.34830000	2.60060000	0.64800000
H	-0.16510000	3.65560000	0.89550000
N	0.70390000	-1.34920000	-1.29590000
N	0.49800000	1.69430000	1.12540000
C	3.17260000	-1.88020000	-1.49240000
H	3.99370000	-1.57750000	-2.15240000
H	3.29480000	-2.95670000	-1.33070000
C	3.32020000	-1.23280000	-0.11970000
H	2.72800000	-1.79500000	0.61060000
H	4.37560000	-1.29130000	0.18870000
C	2.90390000	2.07660000	1.68000000
H	3.09890000	2.78200000	0.86640000
H	3.53310000	2.39470000	2.51890000
C	3.33980000	0.66820000	1.30230000
H	2.97510000	-0.03680000	2.05900000
H	4.43950000	0.61110000	1.30620000
N	2.86640000	0.17780000	-0.01650000
Ni	0.78480000	0.12860000	-0.05750000
C	1.82080000	-1.59120000	-2.18290000
H	1.59770000	-2.43180000	-2.85710000
H	1.93300000	-0.71570000	-2.83300000
C	1.44620000	2.16880000	2.11590000
H	1.33300000	1.57070000	3.03320000
H	1.22680000	3.20980000	2.39450000
C	3.46820000	1.00110000	-1.07940000
H	3.21380000	0.59850000	-2.05720000
H	3.07990000	2.01780000	-1.02580000
H	4.56350000	1.02790000	-0.97850000

[2-Ni]^{Me} (Step A2)

C	1.49330000	3.91550000	-0.09400000
C	1.02280000	2.59960000	-0.29650000
C	1.77520000	1.48880000	0.20080000
C	2.92490000	1.81860000	0.97780000
C	3.35030000	3.11600000	1.16690000
C	2.64810000	4.19380000	0.60560000
H	0.89950000	4.73300000	-0.49620000
H	3.47640000	1.00920000	1.44270000
H	4.23350000	3.29980000	1.77230000
H	2.98360000	5.21490000	0.74580000
C	1.99290000	-2.15520000	0.36970000
C	2.99180000	-3.14570000	0.38090000
C	4.28300000	-2.89730000	-0.04370000
C	4.58410000	-1.60860000	-0.50330000
C	3.63350000	-0.60670000	-0.48320000
C	2.30810000	-0.81350000	-0.00890000
H	2.71540000	-4.14290000	0.71530000
H	5.03230000	-3.68050000	-0.04030000
H	5.57560000	-1.38670000	-0.88780000
H	3.89750000	0.37820000	-0.85250000
N	1.36870000	0.19650000	0.00780000
C	-0.29870000	2.52220000	-0.89460000
H	-0.74090000	3.50420000	-1.11200000
C	0.65910000	-2.60680000	0.74180000
H	0.61180000	-3.52780000	1.33790000
N	-1.03290000	1.48470000	-1.07670000
N	-0.43090000	-2.04930000	0.37370000
C	-3.13730000	2.31320000	-0.07330000
H	-4.22130000	2.29470000	-0.22930000
H	-2.86580000	3.36680000	0.06530000
C	-2.74770000	1.57350000	1.20810000
H	-1.70050000	1.80740000	1.43300000
H	-3.34910000	1.97070000	2.05010000
C	-2.12360000	-2.02380000	2.18810000
H	-3.10580000	-2.43830000	2.44110000
H	-1.43360000	-2.36250000	2.97050000
C	-2.15220000	-0.49660000	2.23180000
H	-1.11800000	-0.13040000	2.20240000
H	-2.58040000	-0.18360000	3.20570000
N	-2.85220000	0.12520000	1.11690000
Ni	-0.49040000	-0.37090000	-0.66690000
C	-2.45710000	1.75460000	-1.33370000
H	-2.56480000	2.47400000	-2.15620000
H	-2.92290000	0.81040000	-1.61130000

C	-1.69570000	-2.61750000	0.84200000
H	-1.59890000	-3.70610000	0.95050000
H	-2.44040000	-2.39070000	0.07610000
C	-4.23090000	-0.30740000	1.00500000
H	-4.69570000	0.16450000	0.13670000
H	-4.27910000	-1.38600000	0.84490000
H	-4.82740000	-0.05550000	1.90330000
C	-1.63760000	-1.16310000	-1.95790000
O	-0.85040000	-1.42620000	-2.91440000
O	-2.86670000	-1.40810000	-1.90610000

[2-Ni]^{Me} (Step A3)

C	-1.17480000	3.94840000	-0.04810000
C	-0.85900000	2.60420000	0.24870000
C	-1.70060000	1.55190000	-0.21290000
C	-2.81050000	1.93520000	-1.01560000
C	-3.08310000	3.25560000	-1.30330000
C	-2.27070000	4.28990000	-0.80940000
H	-0.51730000	4.72510000	0.33410000
H	-3.44480000	1.15750000	-1.42570000
H	-3.93530000	3.49240000	-1.93340000
H	-2.49220000	5.32670000	-1.03340000
C	-2.25810000	-2.03520000	-0.27020000
C	-3.32400000	-2.94980000	-0.20280000
C	-4.55740000	-2.58830000	0.30300000
C	-4.73430000	-1.26900000	0.74080000
C	-3.71110000	-0.34400000	0.64860000
C	-2.43840000	-0.68120000	0.12570000
H	-3.15250000	-3.96590000	-0.54860000
H	-5.36510000	-3.30810000	0.36510000
H	-5.68530000	-0.96230000	1.16580000
H	-3.87310000	0.66920000	1.00040000
N	-1.40700000	0.24350000	0.06000000
C	0.35020000	2.40730000	1.01180000
H	0.81700000	3.33760000	1.35570000
C	-1.00560000	-2.52170000	-0.81750000
H	-1.06280000	-3.39850000	-1.47150000
N	0.97010000	1.30740000	1.27510000
N	0.14060000	-2.00100000	-0.58080000
C	3.43890000	1.68720000	0.85800000
H	4.28780000	1.05670000	1.14250000
H	3.78270000	2.72220000	0.94280000
C	3.10620000	1.46430000	-0.62060000
H	2.15020000	1.93870000	-0.85590000
H	3.86300000	1.97560000	-1.23230000
C	1.72770000	-1.59570000	-2.44970000
H	2.59980000	-2.04440000	-2.93650000
H	0.92990000	-1.57740000	-3.20050000
C	2.00950000	-0.14310000	-2.06870000
H	1.08210000	0.31640000	-1.70730000
H	2.30400000	0.40500000	-2.97910000
N	3.03110000	0.04310000	-1.02380000
Ni	0.36120000	-0.44780000	0.60790000
C	2.29210000	1.47870000	1.89650000
H	2.26190000	2.35160000	2.55690000
H	2.49490000	0.61140000	2.51920000
C	1.30100000	-2.52520000	-1.30630000
H	1.05950000	-3.50770000	-1.72750000
H	2.11940000	-2.65300000	-0.59620000
C	4.34640000	-0.42520000	-1.47570000
H	5.09520000	-0.18960000	-0.71510000
H	4.33760000	-1.50920000	-1.61250000
H	4.64260000	0.05320000	-2.42080000
C	1.71790000	-1.40840000	1.59300000
O	1.39470000	-1.99560000	2.61510000
O	3.01030000	-1.44820000	1.20580000
H	3.02790000	-0.90070000	0.35950000