Supplementary Information for

Structures, energetics, and reaction barriers for CH_x bound to the Nickel (111) Surface.

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Contents

1. Pseudopotentials

Carbon

```
type number, label:
 1 C
notes4
 Constructed by Peter A. Schultz, 29-January-2002
 Hamann-type ppot [D.R. Hamann,  PRB 40, 2980 (1989)]
 generated by fhi98PP [M.Fuchs,M.Scheffler, Comput.Phys.Commun. 119,67(1999)]
 basis refined in bulk diamond calculations, a0=6.74 bohr
effective nuclear charge (s2p2 to  9.0)
  4.00000000d+00
pseudopotentials: Lmax, and effective gaussian range
  1    3.6900000d+00
functional type used in generating potential:
PBE
radial mesh: number of points for local and non-local pot integrals
 120 102
mesh points for nuclear potential;  ham1fh
     0.02500000  0.02626767  0.02759962  0.02899911  0.03046956  0.03201457
     0.03363793  0.03534360  0.03713576  0.03901879  0.04099731  0.04307615
     0.04526040  0.04755541  0.04996679  0.05250045  0.05516258  0.05795969
     0.06089864  0.06398662  0.06723117  0.07064025  0.07422219  0.07798576
     0.08194016  0.08609508  0.09046069  0.09504766  0.09986722  0.10493116
     0.11025188  0.11584240  0.12171640  0.12788824  0.13437304  0.14118667
     0.14834579  0.15586792  0.16377148  0.17207581  0.18080122  0.18996907
     0.19960178  0.20972295  0.22035732  0.23153093  0.24327112  0.25560661
     0.26856760  0.28218580  0.29649453  0.31152882  0.32732544  0.34392306
     0.36136229  0.37968580  0.39893845  0.41916733  0.44042195  0.46275433
     0.48621911  0.51087372  0.53677848  0.56399678  0.59259524  0.62264384
     0.65421610  0.68738929  0.72224459  0.75886728  0.79734700  0.83777789
     0.88025891  0.92489400  0.97179240  1.02106886  1.07284397  1.12724443
     1.18440336  1.24446064  1.30756323  1.37386554  1.44352984  1.51672659
     1.59363490  1.67444299  1.75934860  1.84855950  1.94229399  2.04078146
     2.14426291  2.25299158  2.36723352  2.48726830  2.61338966  2.74590623
     2.88514229  3.03143855  3.18515303  3.34666188  3.51636032  3.69466362
     3.88200811  4.07885223  4.28567768  4.50299058  4.73132272  4.97123285
     5.22330805  5.48816517  5.76645234  6.05885055  6.36607534  6.68887851
     7.02804998  7.38441975  7.75885987  8.15228666  8.56566284  9.00000000
radwts: weights for radial points
     0.00123658  0.00129928  0.00136516  0.00143438  0.00150712  0.00158354
     0.00166383  0.00174820  0.00183685  0.00192999  0.00202785  0.00213068
```

```
     0.00223872  0.00235224  0.00247151  0.00259683  0.00272851  0.00286686
     0.00301223  0.00316497  0.00332546  0.00349408  0.00367126  0.00385741
     0.00405301  0.00425853  0.00447446  0.00470135  0.00493974  0.00519022
     0.00545340  0.00572992  0.00602047  0.00632574  0.00664650  0.00698352
     0.00733764  0.00770970  0.00810064  0.00851140  0.00894298  0.00939645
     0.00987291  0.01037354  0.01089955  0.01145223  0.01203293  0.01264309
     0.01328418  0.01395777  0.01466553  0.01540917  0.01619052  0.01701149
     0.01787408  0.01878042  0.01973272  0.02073330  0.02178462  0.02288924
     0.02404988  0.02526938  0.02655071  0.02789701  0.02931157  0.03079787
     0.03235953  0.03400038  0.03572443  0.03753590  0.03943922  0.04143906
     0.04354030  0.04574809  0.04806782  0.05050519  0.05306614  0.05575696
     0.05858421  0.06155483  0.06467608  0.06795559  0.07140140  0.07502194
     0.07882606  0.08282307  0.08702276  0.09143541  0.09607180  0.10094329
     0.10606180  0.11143986  0.11709061  0.12302790  0.12926625  0.13582092
     0.14270796  0.14994422  0.15754741  0.16553613  0.17392994  0.18274936
     0.19201600  0.20175251  0.21198273  0.22273169  0.23402570  0.24589238
     0.25836079  0.27146144  0.28522637  0.29968928  0.31488556  0.33085239
     0.34762885  0.36525599  0.38377694  0.40323704  0.42368389  0.44516753
non-local potential: l,potential*integration weight
 0   0.39100562  0.39067485  0.39033823  0.38999879  0.38965989  0.38932513
     0.38899826  0.38868306  0.38838318  0.38810195  0.38784228  0.38760641
     0.38739581  0.38721103  0.38705165  0.38691622  0.38680233  0.38670671
     0.38662533  0.38655366  0.38648687  0.38642000  0.38634820  0.38626692
     0.38617199  0.38605973  0.38592700  0.38577121  0.38559025  0.38538254
     0.38514689  0.38488257  0.38458924  0.38426700  0.38391647  0.38353887
     0.38313623  0.38271152  0.38226892  0.38181401  0.38135384  0.38089688
     0.38045258  0.38003039  0.37963798  0.37927841  0.37894605  0.37862117
     0.37826346  0.37780501  0.37714367  0.37613777  0.37460355  0.37231704
     0.36902414  0.36446416  0.35841004  0.35071546  0.34133721  0.33029684
     0.31759520  0.30316281  0.28690444  0.26875136  0.24853666  0.22574941
     0.19972621  0.17051837  0.13937241  0.10806813  0.07821471  0.05122470
     0.02840363  0.01081157 -0.00100516 -0.00724855 -0.00892743 -0.00764520
    -0.00514007 -0.00276292 -0.00116667 -0.00036807 -0.00007497 -0.00000151
     0.00000748  0.00000523  0.00000292  0.00000155  0.00000081  0.00000043
     0.00000024  0.00000016  0.00000011  0.00000009  0.00000008  0.00000006
     0.00000005  0.00000005  0.00000004  0.00000004  0.00000003  0.00000003
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
non-local potential: l,potential*integration weight
 1   0.36560953  0.36397730  0.36227137  0.36049107  0.35863582  0.35670508
     0.35469817  0.35261419  0.35045178  0.34820898  0.34588303  0.34347014
     0.34096536  0.33836235  0.33565334  0.33282904  0.32987859  0.32678968
     0.32354862  0.32014045  0.31654912  0.31275762  0.30874814  0.30450211
     0.30000028  0.29522270  0.29014867  0.28475665  0.27902413  0.27292752
     0.26644201  0.25954148  0.25219842  0.24438401  0.23606814  0.22721973
     0.21780705  0.20779831  0.19716246  0.18587020  0.17389525  0.16121597
     0.14781711  0.13369188  0.11884413  0.10329073  0.08706410  0.07021526
     0.05281777  0.03497340  0.01682029 -0.00145547 -0.01960454 -0.03729506
    -0.05408874 -0.06941146 -0.08252220 -0.09249895 -0.09828416 -0.09883540
    -0.09337182 -0.08162951 -0.06406125 -0.04206903 -0.01838077  0.00287417
     0.01747263  0.02350852  0.02232316  0.01698540  0.01056097  0.00526361
     0.00203413  0.00063797  0.00029470  0.00031888  0.00036305  0.00033630
     0.00025811  0.00017000  0.00009990  0.00005521  0.00003035  0.00001705
     0.00000966  0.00000539  0.00000293  0.00000155  0.00000081  0.00000043
     0.00000024  0.00000016  0.00000011  0.00000009  0.00000008  0.00000006
     0.00000005  0.00000005  0.00000004  0.00000004  0.00000003  0.00000003
```

```
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
number of radial functions    ****  C_pbe  basis - XXFeb02-pas  ****
 5
angular momentum, number of alphas
 0  5
alphas - s - 5s/2/5s312 (Eopt + reopt c2,c1)
  0.15583000d+00  0.45832000d+00  1.40253800d+00  2.80520000d+00
  5.61040000d+00
wave function coefficients
  0.21950000d+00  0.69562300d+00  0.36253700d+00 -1.29642800d+00
  0.45026100d+00
angular momentum, number of alphas
 0  1
alphas - p - second zeta p polarization
  0.15583000d+00
wave function coefficients
  1.00000000d+00
angular momentum, number of alphas
 1  4
alphas - p - 4p/2/4p304(Eopt + reopt c2,c1)
  0.15470100d+00  0.52390800d+00  1.44226700d+00  4.60469500d+00
wave function coefficients
  0.10763100d+00  0.52463000d+00  1.00250300d+00  1.67541100d+00
angular momentum, number of alphas
 1  1
alphas - p - second zeta p polarization
  0.15470100d+00
wave function coefficients
  1.00000000d+00
angular momentum, number of alphas
 2  1
alphas - d - angular polarization (dzp Eopt)
  0.77000000d+00
wave function coefficients
  1.00000000d+00
shell occupation numbers for C, carbon - s(2.00)p(2.00)
     2.00000000  0.00000000  2.00000000  0.00000000  0.00000000  0.00000000
end atom file
```

Hydrogen

```
type number, label:
 1 H
notes2
 bare nuclear potential
 generated March-2001, by Peter A. Schultz
effective nuclear charge (s1 to 10.0)
  1.00000000d+00
pseudopotentials: Lmax, and effective gaussian range
 -1   1.71000000d+00
radial mesh: number of points for local and non-local pot integrals
 100  80
mesh points for nuclear potential
     0.00200000  0.00217968  0.00237551  0.00258893  0.00282152  0.00307501
     0.00335127  0.00365236  0.00398049  0.00433810  0.00472785  0.00515260
     0.00561552  0.00612003  0.00666986  0.00726909  0.00792215  0.00863389
```

```
     0.00940957  0.01025494  0.01117626  0.01218036  0.01327466  0.01446727
     0.01576703  0.01718357  0.01872736  0.02040986  0.02224351  0.02424190
     0.02641983  0.02879343  0.03138027  0.03419952  0.03727205  0.04062063
     0.04427005  0.04824734  0.05258195  0.05730599  0.06245444  0.06806544
     0.07418054  0.08084503  0.08810827  0.09602405  0.10465099  0.11405299
     0.12429968  0.13546694  0.14763749  0.16090146  0.17535709  0.19111143
     0.20828116  0.22699345  0.24738688  0.26961248  0.29383487  0.32023343
     0.34900367  0.38035868  0.41453067  0.45177272  0.49236064  0.53659505
     0.58480355  0.63734316  0.69460302  0.75700718  0.82501783  0.89913865
     0.97991859  1.06795593  1.16390267  1.26846941  1.38243058  1.50663019
     1.64198808  1.78950672  1.95027865  2.12549457  2.31645214  2.52456563
     2.75137635  2.99856407  3.26795950  3.56155782  3.88153345  4.23025616
     4.61030863  5.02450558  5.47591460  5.96787887  6.50404194  7.08837469
     7.72520477  8.41924860  9.17564635 10.00000000
radwts: weights for radial points
     0.00017206  0.00018752  0.00020437  0.00022273  0.00024274  0.00026455
     0.00028832  0.00031422  0.00034245  0.00037322  0.00040675  0.00044329
     0.00048312  0.00052652  0.00057382  0.00062538  0.00068156  0.00074279
     0.00080953  0.00088226  0.00096152  0.00104790  0.00114205  0.00124465
     0.00135647  0.00147834  0.00161116  0.00175591  0.00191366  0.00208559
     0.00227296  0.00247716  0.00269972  0.00294226  0.00320660  0.00349468
     0.00380865  0.00415083  0.00452374  0.00493016  0.00537310  0.00585582
     0.00638192  0.00695528  0.00758015  0.00826117  0.00900336  0.00981224
     0.01069378  0.01165453  0.01270159  0.01384272  0.01508637  0.01644175
     0.01791890  0.01952876  0.02128325  0.02319537  0.02527928  0.02755040
     0.03002557  0.03272311  0.03566301  0.03886703  0.04235890  0.04616448
     0.05031197  0.05483207  0.05975826  0.06512703  0.07097814  0.07735492
     0.08430461  0.09187866  0.10013317  0.10912928  0.11893362  0.12961879
     0.14126394  0.15395530  0.16778687  0.18286109  0.19928960  0.21719407
     0.23670711  0.25797323  0.28114992  0.30640885  0.33393707  0.36393847
     0.39663525  0.43226954  0.47110528  0.51343007  0.55955739  0.60982886
     0.66461678  0.72432694  0.78940154  0.86032254
number of radial functions  **** H PBE bare-core basis 11Apr01-PAS ****
 4
angular momentum, number of alphas
 0  5
alphas - s - Ham-II/PBE/4s408 + a5(19.22) + full recontract in H2
  0.10247400d+00  0.37230400d+00  1.23085800d+00  4.78332400d+00
 19.22000000d+00
wave function coefficients
  0.10406000d+00  0.48010000d+00  0.58535000d+00  0.39756300d+00
  0.26913000d+00
angular momentum, number of alphas
 0  2
alphas - s - second zeta s polarization (H2O Eopt)
  0.10247400d+00  0.37230400d+00
wave function coefficients
  0.07528100d+00  0.12093900d+00
angular momentum, number of alphas
 0  1
alphas - s - second zeta s polarization (H2O Eopt)
  0.10247400d+00
wave function coefficients
  1.00000000d+00
angular momentum, number of alphas
 1  1
alphas - p - angular polarization (dzp Eopt H2)
```

```
  1.10000000d+00
wave function coefficients
  1.00000000d+00
shell occupancies for hydrogen, H: s(1.00)p(0.00)
     1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
end atom file
```

Nickel

```
type number, label:
 1 Ni
notes6
 Constructed by Peter A. Schultz, 3-October-2005
 Hamann-type ppot [D.R. Hamann,  PRB 40, 2980 (1989)]
 Troullier/Martins-type ppot [N.Troullier,J.L.Martins, PRB 43,8861(1991)]
 generated by fhi98PP [M.Fuchs,M.Scheffler, Comput.Phys.Commun. 119,67(1999)]
 Pot'l: d8.0s1.0[+1.0], Rpc=0.6, Rs(H)=1.15,Rp0(TM)=2.38,Rd(TM)=1.5
 Basis: refined in 5l fcc slab
effective nuclear charge (d8.0s1.0[+1.0],Rpc=0.6 to 11.0)
 10.00000000d+00
pseudopotentials: Lmax, and effective gaussian range
  2   1.18000000d+00
functional type used in generating potential:
PBE
radial mesh: number of points for local and non-local pot integrals
 120 103
mesh points for nuclear potential;  tm91fh
     0.01000000  0.01060615  0.01124905  0.01193092  0.01265411  0.01342115
     0.01423467  0.01509751  0.01601266  0.01698327  0.01801272  0.01910456
     0.02026259  0.02149082  0.02279349  0.02417513  0.02564052  0.02719472
     0.02884314  0.03059148  0.03244580  0.03441251  0.03649844  0.03871080
     0.04105727  0.04354598  0.04618553  0.04898509  0.05195434  0.05510357
     0.05844369  0.06198628  0.06574360  0.06972868  0.07395531  0.07843814
     0.08319269  0.08823545  0.09358388  0.09925650  0.10527297  0.11165413
     0.11842209  0.12560029  0.13321360  0.14128839  0.14985264  0.15893602
     0.16856998  0.17878792  0.18962521  0.20111942  0.21331035  0.22624024
     0.23995388  0.25449877  0.26992531  0.28628694  0.30364033  0.32204561
     0.34156653  0.36227071  0.38422989  0.40752013  0.43222212  0.45842143
     0.48620882  0.51568055  0.54693873  0.58009163  0.61525411  0.65254797
     0.69210241  0.73405447  0.77854946  0.82574153  0.87579417  0.92888077
     0.98518524  1.04490262  1.10823979  1.17541617  1.24666447  1.32223151
     1.40237908  1.48738483  1.57754323  1.67316661  1.77458625  1.88215347
     1.99624093  2.11724383  2.24558138  2.38169816  2.52606570  2.67918414
     2.84158391  3.01382761  3.19651192  3.39026972  3.59577222  3.81373133
     4.04490211  4.29008540  4.55013057  4.82593848  5.11846459  5.42872228
     5.75778636  6.10679678  6.47696260  6.86956617  7.28596756  7.72760927
     8.19602127  8.69282623  9.21974522  9.77860361 10.37133741 11.00000000
radwts: weights for radial points
     0.00058849  0.00062416  0.00066200  0.00070213  0.00074469  0.00078982
     0.00083770  0.00088848  0.00094233  0.00099945  0.00106004  0.00112429
     0.00119244  0.00126472  0.00134138  0.00142269  0.00150893  0.00160039
     0.00169740  0.00180029  0.00190941  0.00202515  0.00214791  0.00227810
     0.00241619  0.00256265  0.00271799  0.00288274  0.00305748  0.00324281
     0.00343937  0.00364785  0.00386896  0.00410348  0.00435222  0.00461603
     0.00489583  0.00519259  0.00550734  0.00584117  0.00619524  0.00657077
     0.00696906  0.00739149  0.00783953  0.00831472  0.00881872  0.00935327
     0.00992022  0.01052154  0.01115931  0.01183573  0.01255316  0.01331408
     0.01412112  0.01497707  0.01588491  0.01684778  0.01786902  0.01895216
```

```
     0.02010095  0.02131937  0.02261166  0.02398227  0.02543596  0.02697778
     0.02861304  0.03034743  0.03218696  0.03413798  0.03620727  0.03840198
     0.04072974  0.04319858  0.04581708  0.04859430  0.05153986  0.05466397
     0.05797745  0.06149178  0.06521912  0.06917241  0.07336532  0.07781239
     0.08252901  0.08753154  0.09283730  0.09846467  0.10443314  0.11076339
     0.11747736  0.12459830  0.13215087  0.14016124  0.14865717  0.15766808
     0.16722519  0.17736161  0.18811246  0.19951496  0.21160864  0.22443538
     0.23803962  0.25246848  0.26777195  0.28400305  0.30121800  0.31947645
     0.33884164  0.35938065  0.38116465  0.40426909  0.42877401  0.45476432
     0.48233003  0.51156665  0.54257546  0.57546388  0.61034584  0.64734219
non-local potential: l,potential*integration weight  fhi/H: Rs=1.15
 0   1.17216208  1.17186965  1.17155949  1.17123052  1.17088159  1.17051150
     1.17011896  1.16970260  1.16926098  1.16879255  1.16829570  1.16776867
     1.16720965  1.16661666  1.16598765  1.16532040  1.16461257  1.16386168
     1.16306509  1.16221998  1.16132336  1.16037204  1.15936265  1.15829156
     1.15715494  1.15594869  1.15466841  1.15330944  1.15186679  1.15033510
     1.14870865  1.14698131  1.14514649  1.14319710  1.14112555  1.13892362
     1.13658244  1.13409241  1.13144313  1.12862331  1.12562069  1.12242198
     1.11901272  1.11537719  1.11149822  1.10735707  1.10293325  1.09820436
     1.09314584  1.08773084  1.08192992  1.07571092  1.06903884  1.06187571
     1.05418077  1.04591052  1.03701892  1.02745735  1.01717439  1.00611530
     0.99421965  0.98141242  0.96758780  0.95261227  0.93638548  0.91889427
     0.90016415  0.88020268  0.85894779  0.83615302  0.81138294  0.78403558
     0.75366894  0.71996478  0.68261147  0.64128184  0.59567351  0.54559089
     0.49105735  0.43244959  0.37064109  0.30712362  0.24404774  0.18408603
     0.13005662  0.08449623  0.04944548  0.02541699  0.01108975  0.00390642
     0.00101086  0.00013508 -0.00003304 -0.00003452 -0.00001885 -0.00000900
    -0.00000406 -0.00000174 -0.00000071 -0.00000028 -0.00000011 -0.00000004
    -0.00000001  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
non-local potential: l,potential*integration weight  fhi/TM: Rp0=2.38
 1   1.16687109  1.16625798  1.16560771  1.16491802  1.16418652  1.16341069
     1.16258782  1.16171508  1.16078943  1.15980767  1.15876641  1.15766202
     1.15649069  1.15524835  1.15393070  1.15253317  1.15105093  1.14947883
     1.14781143  1.14604294  1.14416723  1.14217781  1.14006776  1.13782979
     1.13545611  1.13293851  1.13026823  1.12743602  1.12443204  1.12124585
     1.11786641  1.11428195  1.11048003  1.10644742  1.10217011  1.09763321
     1.09282095  1.08771658  1.08230237  1.07655950  1.07046803  1.06400685
     1.05715364  1.04988476  1.04217531  1.03399900  1.02532818  1.01613381
     1.00638552  0.99605156  0.98509896  0.97349367  0.96120076  0.94818487
     0.93441080  0.91984426  0.90445274  0.88820621  0.87107742  0.85304153
     0.83407546  0.81415787  0.79327158  0.77141122  0.74859816  0.72490110
     0.70045079  0.67542341  0.64996586  0.62406876  0.59757021  0.57019102
     0.54186780  0.51271374  0.48288665  0.45253624  0.42179222  0.39076638
     0.35955395  0.32823017  0.29684478  0.26541997  0.23395175  0.20239829
     0.17066745  0.13881483  0.10760584  0.07814192  0.05171360  0.02979783
     0.01373520  0.00418183  0.00042258 -0.00003872 -0.00001909 -0.00000901
    -0.00000406 -0.00000174 -0.00000071 -0.00000028 -0.00000011 -0.00000004
    -0.00000001  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
non-local potential: l,potential*integration weight  fhi/TM: Rd=1.5
 2   1.14178107  1.13964712  1.13738382  1.13498333  1.13243733  1.12973701
     1.12687300  1.12383539  1.12061365  1.11719663  1.11357248  1.10972865
     1.10565183  1.10132788  1.09674184  1.09187781  1.08671894  1.08124737
     1.07544413  1.06928913  1.06276105  1.05583727  1.04849381  1.04070523
```

```
     1.03244458  1.02368324  1.01439089  1.00453537  0.99408257  0.98299635
     0.97123839  0.95876808  0.94554239  0.93151572  0.91663982  0.90086358
     0.88413297  0.86639085  0.84757689  0.82762747  0.80647559  0.78405081
     0.76027935  0.73508407  0.70838475  0.68009842  0.65013981  0.61842222
     0.58485852  0.54936277  0.51185225  0.47225031  0.43049027  0.38652044
     0.34031086  0.29186192  0.24121526  0.18846703  0.13378387  0.07742158
     0.01974728 -0.03873428 -0.09734869 -0.15521302 -0.21119062 -0.26384565
    -0.31141600 -0.35183960 -0.38287462 -0.40232292 -0.40819131 -0.39890331
    -0.37329894 -0.33107835 -0.27336188 -0.20311256 -0.12533715 -0.04696003
     0.02372247  0.07803766  0.10838416  0.11021244  0.08485439  0.04315998
     0.00698904 -0.00307351 -0.00201422 -0.00128016 -0.00078812 -0.00046643
    -0.00026453 -0.00014428 -0.00007610 -0.00003885 -0.00001910 -0.00000901
    -0.00000406 -0.00000174 -0.00000071 -0.00000028 -0.00000011 -0.00000004
    -0.00000001  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
partial core charge density, cutoff=    0.59083713
-2   5.11447569  5.11446604  5.11445455  5.11444088  5.11442462  5.11440529
     5.11438230  5.11435497  5.11432249  5.11428390  5.11423805  5.11418360
     5.11411895  5.11404222  5.11395118  5.11384319  5.11371514  5.11356337
     5.11338356  5.11317061  5.11291853  5.11262029  5.11226759  5.11185074
     5.11135835  5.11077710  5.11009138  5.10928300  5.10833073  5.10720982
     5.10589154  5.10434249  5.10252400  5.10039137  5.09789299  5.09496944
     5.09155249  5.08756395  5.08291453  5.07750246  5.07121221  5.06391301
     5.05545736  5.04567954  5.03439403  5.02139404  5.00644997  4.98930800
     4.96968865  4.94728540  4.92176318  4.89275672  4.85986831  4.82266489
     4.78067357  4.73337514  4.68019428  4.62048540  4.55351225  4.47841997
     4.39419779  4.29963160  4.19324763  4.07325154  3.93747497  3.78335273
     3.60797524  3.40829372  3.18161221  2.92658458  2.64489735  2.34214337
     2.02842098  1.71629941  1.41804124  1.14376276  0.90049567  0.69197424
     0.51893895  0.37974555  0.27109355  0.18873718  0.12809376  0.08470507
     0.05454184  0.03417236  0.02081481  0.01231399  0.00706767  0.00393051
     0.00211504  0.00109947  0.00055117  0.00026593  0.00012322  0.00005471
     0.00002322  0.00000939  0.00000361  0.00000132  0.00000045  0.00000015
     0.00000004  0.00000001  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
number of radial functions  **** Ni/pbe   - by Peter Schultz / 14Oct05 ****
 5
angular momentum, number of alphas
 2  5
alphas - d - 5d/2/5d448 Eopt + reopt(c2,c1)
  0.20943000d+00  0.56997100d+00  1.43707300d+00  3.85466600d+00
 11.08797800d+00
wave function coefficients
  0.03668000d+00  0.26331000d+00  1.77817900d+00 14.02861100d+00
 -1.40558400d+00
angular momentum, number of alphas
 0  4
alphas - s - 4s/2/4s327 Eopt + reopt(a1,a2,c1,c2)
  0.06800000d+00  0.25000000d+00  0.88470000d+00  1.76940000d+00
wave function coefficients
  0.09974000d+00  0.40080000d+00 -1.15305900d+00  0.42460100d+00
angular momentum, number of alphas
 0  1
alphas - s - second zeta s polarization
  0.06800000d+00
```

```
wave function coefficients
  1.00000000d+00
angular momentum, number of alphas
 1  2
alphas
  0.12500000d+00  0.78000000d+00
wave function coefficients
  1.00000000d+00 -0.56500000d+00
angular momentum, number of alphas
 2  1
alphas - d - second zeta d polarization
  0.20943000d+00
wave function coefficients
  1.00000000d+00
shell occupancies for nickel, Ni: d(8.53)s(s1.47)
     8.53000000  1.47000000  0.00000000  0.00000000  0.00000000  0.00000000
end atom file
```

2. Final relaxed geometries with charge and spin analysis for structures presented in the text.

Bare Ni111 Slab
16 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.44325	-0.00004	4.06130
10 Ni	1.44307	2.49180	4.06130
11 Ni	3.60123	-1.24601	4.06116
12 Ni	3.60124	1.24591	4.06114
13 Ni	1.43867	0.00000	-2.03458
14 Ni	1.43867	2.49184	-2.03458
15 Ni	3.59667	-1.24592	-2.03458
16 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1497.8114218081

Total electrons from output= 160
Spin up from output= 86.0000000000
Spin down from output= 74.0000000000
Fermi level up from output= -4.9434132468
Fermi level down from output= -5.033793919
# of atoms= 16

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.012, -0.012, -0.014, 0.163, 0.150, 0.150, 0.163, 0.186, 0.789
Atom 2, 0.016, -0.012, -0.012, -0.014, 0.163, 0.150, 0.150, 0.163, 0.186, 0.789
Atom 3, 0.016, -0.012, -0.012, -0.014, 0.163, 0.150, 0.150, 0.163, 0.186, 0.789
Atom 4, 0.016, -0.012, -0.012, -0.014, 0.163, 0.150, 0.150, 0.163, 0.186, 0.789

Atom 5, 0.016, -0.012, -0.012, -0.014, 0.162, 0.150, 0.151, 0.162, 0.186, 0.789
Atom 6, 0.016, -0.012, -0.012, -0.014, 0.162, 0.150, 0.151, 0.162, 0.186, 0.788
Atom 7, 0.016, -0.012, -0.012, -0.014, 0.162, 0.150, 0.151, 0.162, 0.186, 0.788
Atom 8, 0.016, -0.012, -0.012, -0.014, 0.162, 0.150, 0.151, 0.162, 0.186, 0.788
Atom 9, 0.017, -0.010, -0.010, -0.010, 0.174, 0.112, 0.112, 0.173, 0.219, 0.776
Atom 10, 0.017, -0.010, -0.010, -0.010, 0.174, 0.112, 0.112, 0.173, 0.219, 0.776
Atom 11, 0.017, -0.010, -0.010, -0.010, 0.174, 0.112, 0.112, 0.173, 0.219, 0.776
Atom 12, 0.017, -0.010, -0.010, -0.010, 0.174, 0.112, 0.112, 0.173, 0.219, 0.776
Atom 13, 0.017, -0.010, -0.010, -0.011, 0.173, 0.111, 0.111, 0.173, 0.219, 0.774
Atom 14, 0.017, -0.010, -0.010, -0.011, 0.173, 0.111, 0.111, 0.173, 0.219, 0.774
Atom 15, 0.017, -0.010, -0.010, -0.011, 0.173, 0.111, 0.111, 0.173, 0.219, 0.773
Atom 16, 0.017, -0.010, -0.010, -0.011, 0.173, 0.111, 0.111, 0.173, 0.219, 0.774
total spin= 12.5092888627538

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.332, 0.339, 1.741, 1.771, 1.771, 1.742, 1.701, 10.001
Atom 2, 0.272, 0.332, 0.332, 0.339, 1.741, 1.771, 1.771, 1.742, 1.701, 10.001
Atom 3, 0.272, 0.332, 0.332, 0.339, 1.741, 1.771, 1.771, 1.742, 1.701, 10.001
Atom 4, 0.272, 0.332, 0.332, 0.339, 1.741, 1.771, 1.771, 1.742, 1.701, 10.001
Atom 5, 0.269, 0.333, 0.333, 0.340, 1.742, 1.770, 1.770, 1.743, 1.702, 10.002
Atom 6, 0.269, 0.333, 0.333, 0.340, 1.742, 1.771, 1.770, 1.743, 1.702, 10.002
Atom 7, 0.269, 0.333, 0.333, 0.340, 1.742, 1.771, 1.770, 1.743, 1.702, 10.002
Atom 8, 0.269, 0.333, 0.333, 0.340, 1.742, 1.770, 1.770, 1.743, 1.702, 10.002
Atom 9, 0.442, 0.305, 0.304, 0.165, 1.729, 1.809, 1.808, 1.729, 1.702, 9.993
Atom 10, 0.442, 0.305, 0.304, 0.165, 1.729, 1.809, 1.808, 1.729, 1.702, 9.993
Atom 11, 0.442, 0.305, 0.304, 0.165, 1.729, 1.809, 1.808, 1.729, 1.702, 9.993
Atom 12, 0.442, 0.305, 0.304, 0.165, 1.729, 1.809, 1.808, 1.729, 1.702, 9.993
Atom 13, 0.445, 0.304, 0.304, 0.165, 1.729, 1.809, 1.810, 1.729, 1.701, 9.997
Atom 14, 0.445, 0.304, 0.304, 0.165, 1.729, 1.809, 1.810, 1.729, 1.701, 9.997
Atom 15, 0.445, 0.304, 0.304, 0.165, 1.729, 1.809, 1.810, 1.729, 1.701, 9.997
Atom 16, 0.445, 0.304, 0.304, 0.165, 1.729, 1.809, 1.810, 1.729, 1.701, 9.997
total charge= 159.972

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.268, -3.961, -3.961, -4.121, -2.102, -1.827, -1.827, -2.102, -2.248, -2.226
Atom 2, -5.268, -3.961, -3.961, -4.121, -2.102, -1.827, -1.827, -2.095, -2.248, -2.226
Atom 3, -5.268, -3.961, -3.961, -4.121, -2.102, -1.827, -1.827, -2.095, -2.248, -2.226
Atom 4, -5.268, -3.961, -3.961, -4.121, -2.102, -1.827, -1.827, -2.095, -2.248, -2.226
Atom 5, -5.268, -3.968, -3.975, -4.135, -2.102, -1.834, -1.841, -2.102, -2.255, -2.233
Atom 6, -5.268, -3.968, -3.975, -4.135, -2.102, -1.834, -1.841, -2.102, -2.255, -2.233
Atom 7, -5.268, -3.968, -3.975, -4.135, -2.102, -1.834, -1.841, -2.102, -2.255, -2.233
Atom 8, -5.268, -3.968, -3.975, -4.135, -2.102, -1.834, -1.841, -2.102, -2.255, -2.233
Atom 9, -4.193, -3.141, -3.148, -1.798, -1.935, -1.500, -1.500, -1.935, -1.623, -1.747
Atom 10, -4.193, -3.141, -3.148, -1.798, -1.935, -1.500, -1.500, -1.928, -1.623, -1.747
Atom 11, -4.193, -3.141, -3.148, -1.798, -1.935, -1.500, -1.500, -1.935, -1.623, -1.747
Atom 12, -4.193, -3.148, -3.148, -1.798, -1.935, -1.500, -1.500, -1.935, -1.623, -1.747
Atom 13, -4.193, -3.126, -3.126, -1.790, -1.928, -1.493, -1.493, -1.928, -1.616, -1.739
Atom 14, -4.193, -3.126, -3.126, -1.790, -1.928, -1.493, -1.493, -1.928, -1.616, -1.739
Atom 15, -4.193, -3.126, -3.126, -1.790, -1.928, -1.493, -1.493, -1.928, -1.616, -1.739
Atom 16, -4.193, -3.126, -3.126, -1.790, -1.928, -1.493, -1.493, -1.928, -1.616, -1.739

H binding at top site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.43867	0.00000	4.06187
10 Ni	1.43666	2.49184	4.07155
11 Ni	3.59767	-1.24418	4.07158
12 Ni	3.59766	1.24421	4.07155
13 H	1.43867	0.00000	5.54164
14 Ni	1.43867	0.00000	-2.03458
15 Ni	1.43867	2.49184	-2.03458
16 Ni	3.59667	-1.24592	-2.03458
17 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1498.9786106543

Total electrons from output= 161
Spin up from output= 86.5000000000
Spin down from output= 74.5000000000
Fermi level up from output= -5.0204334162
Fermi level down from output= -5.1569772106
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.013, -0.012, -0.014, 0.166, 0.154, 0.156, 0.165, 0.185, 0.802
Atom 2, 0.019, -0.013, -0.013, -0.012, 0.170, 0.158, 0.158, 0.170, 0.178, 0.815
Atom 3, 0.016, -0.012, -0.013, -0.014, 0.165, 0.155, 0.154, 0.166, 0.185, 0.802
Atom 4, 0.016, -0.012, -0.013, -0.014, 0.165, 0.155, 0.154, 0.166, 0.185, 0.802
Atom 5, 0.016, -0.011, -0.011, -0.013, 0.159, 0.124, 0.150, 0.160, 0.199, 0.773
Atom 6, 0.016, -0.011, -0.011, -0.013, 0.159, 0.124, 0.150, 0.160, 0.199, 0.773
Atom 7, 0.016, -0.010, -0.012, -0.013, 0.160, 0.163, 0.112, 0.159, 0.199, 0.773
Atom 8, 0.016, -0.011, -0.011, -0.012, 0.162, 0.157, 0.157, 0.162, 0.192, 0.813
Atom 9, 0.009, -0.009, -0.009, -0.005, 0.153, 0.054, 0.054, 0.153, 0.074, 0.473
Atom 10, 0.020, -0.010, -0.009, -0.002, 0.175, 0.135, 0.119, 0.179, 0.212, 0.820
Atom 11, 0.020, -0.009, -0.009, -0.002, 0.178, 0.123, 0.131, 0.176, 0.212, 0.820
Atom 12, 0.020, -0.009, -0.009, -0.002, 0.178, 0.123, 0.131, 0.176, 0.212, 0.820
Atom 13, 0.012, -0.000, -0.000, 0.012, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 14, 0.018, -0.010, -0.010, -0.009, 0.174, 0.112, 0.112, 0.174, 0.225, 0.786
Atom 15, 0.019, -0.010, -0.010, -0.007, 0.173, 0.107, 0.126, 0.172, 0.229, 0.799
Atom 16, 0.019, -0.010, -0.010, -0.007, 0.172, 0.121, 0.112, 0.173, 0.229, 0.799
Atom 17, 0.019, -0.010, -0.010, -0.007, 0.172, 0.121, 0.112, 0.173, 0.229, 0.799
total spin= 12.4701755543262

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.333, 0.341, 1.739, 1.767, 1.769, 1.740, 1.701, 9.994
Atom 2, 0.272, 0.331, 0.331, 0.338, 1.735, 1.768, 1.768, 1.735, 1.713, 9.991
Atom 3, 0.272, 0.333, 0.332, 0.341, 1.739, 1.769, 1.768, 1.739, 1.701, 9.994
Atom 4, 0.272, 0.333, 0.332, 0.341, 1.739, 1.769, 1.768, 1.739, 1.701, 9.994
Atom 5, 0.270, 0.331, 0.331, 0.338, 1.740, 1.781, 1.766, 1.742, 1.696, 9.996
Atom 6, 0.270, 0.331, 0.331, 0.338, 1.740, 1.781, 1.766, 1.742, 1.696, 9.996

Atom 7, 0.270, 0.331, 0.332, 0.338, 1.743, 1.758, 1.788, 1.739, 1.696, 9.996
Atom 8, 0.274, 0.333, 0.333, 0.340, 1.742, 1.764, 1.764, 1.742, 1.701, 9.991
Atom 9, 0.434, 0.323, 0.323, 0.383, 1.738, 1.872, 1.872, 1.738, 1.598, 10.280
Atom 10, 0.431, 0.300, 0.288, 0.156, 1.728, 1.791, 1.812, 1.723, 1.714, 9.943
Atom 11, 0.431, 0.291, 0.297, 0.156, 1.724, 1.807, 1.796, 1.726, 1.714, 9.943
Atom 12, 0.431, 0.291, 0.297, 0.156, 1.724, 1.807, 1.796, 1.726, 1.714, 9.943
Atom 13, 0.903, 0.002, 0.002, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.911
Atom 14, 0.444, 0.304, 0.304, 0.166, 1.726, 1.812, 1.812, 1.726, 1.699, 9.994
Atom 15, 0.447, 0.304, 0.303, 0.169, 1.727, 1.811, 1.798, 1.728, 1.696, 9.982
Atom 16, 0.447, 0.304, 0.304, 0.169, 1.727, 1.801, 1.807, 1.727, 1.696, 9.982
Atom 17, 0.447, 0.304, 0.304, 0.169, 1.727, 1.801, 1.807, 1.727, 1.696, 9.982
total charge= 160.912

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.285, -3.955, -3.940, -4.118, -2.122, -1.848, -1.848, -2.122, -2.277, -2.262
Atom 2, -5.263, -3.992, -3.992, -4.199, -2.137, -1.863, -1.863, -2.137, -2.225, -2.255
Atom 3, -5.285, -3.962, -3.962, -4.118, -2.122, -1.848, -1.848, -2.122, -2.277, -2.262
Atom 4, -5.285, -3.962, -3.962, -4.118, -2.122, -1.848, -1.848, -2.122, -2.277, -2.262
Atom 5, -5.271, -3.962, -3.984, -4.044, -2.107, -1.834, -1.841, -2.107, -2.262, -2.233
Atom 6, -5.271, -3.962, -3.984, -4.044, -2.107, -1.834, -1.841, -2.107, -2.262, -2.233
Atom 7, -5.271, -3.977, -3.948, -4.044, -2.107, -1.848, -1.826, -2.107, -2.262, -2.233
Atom 8, -5.285, -3.940, -3.940, -4.066, -2.115, -1.856, -1.856, -2.115, -2.262, -2.248
Atom 9, -5.285, -2.891, -2.891, -3.194, -1.885, -1.664, -1.664, -1.885, -3.253, -2.078
Atom 10, -4.169, -3.016, -3.253, -2.506, -1.959, -1.412, -1.516, -1.959, -1.627, -1.752
Atom 11, -4.169, -3.186, -3.075, -2.506, -1.959, -1.486, -1.435, -1.959, -1.627, -1.752
Atom 12, -4.169, -3.186, -3.075, -2.506, -1.959, -1.486, -1.435, -1.959, -1.627, -1.752
Atom 13, -3.659, -1.671, -1.671, -3.689, -9.092, -9.092, -9.092, -9.092, -9.092, -9.092
Atom 14, -4.221, -3.142, -3.142, -1.841, -1.952, -1.516, -1.516, -1.952, -1.634, -1.760
Atom 15, -4.199, -3.149, -3.149, -1.819, -1.959, -1.508, -1.516, -1.952, -1.656, -1.767
Atom 16, -4.199, -3.149, -3.149, -1.819, -1.952, -1.516, -1.516, -1.959, -1.656, -1.767
Atom 17, -4.199, -3.149, -3.149, -1.819, -1.952, -1.516, -1.516, -1.959, -1.656, -1.767

H binding at bridge site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000   0.00000   0.00000
 2 Ni   0.00000   2.49184   0.00000
 3 Ni   2.15800 -1.24592   0.00000
 4 Ni   2.15800   1.24592   0.00000
 5 Ni   0.71933   1.24592   2.03458
 6 Ni   0.71933   3.73777   2.03458
 7 Ni   2.87733   0.00000   2.03458
 8 Ni   2.87733   2.49184   2.03458
 9 Ni   1.43246 -0.00550   4.08071
10 Ni   1.44344   2.48874   4.07070
11 Ni   3.59568 -1.23906   4.07171
12 Ni   3.60927   1.25131   4.08009
13 H   2.52401   0.61858   5.13893
14 Ni   1.43867   0.00000 -2.03458
15 Ni   1.43867   2.49184 -2.03458
16 Ni   3.59667 -1.24592 -2.03458
17 Ni   3.59667   1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1499.0101030521

Total electrons from output= 161
Spin up from output= 86.5000000000
Spin down from output= 74.5000000000
Fermi level up from output= -4.9255493566
Fermi level down from output= -5.0895216374
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.012, -0.013, 0.164, 0.152, 0.154, 0.162, 0.184, 0.794
Atom 2, 0.018, -0.013, -0.013, -0.013, 0.164, 0.163, 0.162, 0.164, 0.182, 0.815
Atom 3, 0.018, -0.012, -0.013, -0.013, 0.164, 0.165, 0.160, 0.165, 0.182, 0.816
Atom 4, 0.016, -0.012, -0.012, -0.013, 0.164, 0.153, 0.153, 0.163, 0.185, 0.796
Atom 5, 0.016, -0.012, -0.011, -0.012, 0.161, 0.147, 0.151, 0.160, 0.195, 0.795
Atom 6, 0.016, -0.010, -0.010, -0.008, 0.161, 0.122, 0.106, 0.155, 0.191, 0.722
Atom 7, 0.017, -0.012, -0.012, -0.015, 0.164, 0.154, 0.146, 0.164, 0.212, 0.815
Atom 8, 0.016, -0.012, -0.011, -0.012, 0.157, 0.141, 0.157, 0.164, 0.195, 0.795
Atom 9, 0.013, -0.007, -0.009, -0.003, 0.150, 0.091, 0.103, 0.150, 0.112, 0.599
Atom 10, 0.019, -0.011, -0.009, -0.004, 0.183, 0.127, 0.124, 0.177, 0.197, 0.803
Atom 11, 0.019, -0.011, -0.009, -0.003, 0.182, 0.122, 0.119, 0.180, 0.209, 0.807
Atom 12, 0.013, -0.008, -0.009, -0.003, 0.149, 0.098, 0.096, 0.151, 0.112, 0.598
Atom 13, 0.009, 0.000, -0.000, 0.009, 0.000, 0.000, 0.000, 0.000, 0.000, 0.017
Atom 14, 0.019, -0.011, -0.010, -0.007, 0.172, 0.118, 0.111, 0.173, 0.226, 0.790
Atom 15, 0.020, -0.010, -0.011, -0.006, 0.173, 0.113, 0.118, 0.173, 0.225, 0.795
Atom 16, 0.020, -0.010, -0.010, -0.007, 0.173, 0.117, 0.123, 0.173, 0.239, 0.816
Atom 17, 0.019, -0.011, -0.010, -0.007, 0.172, 0.115, 0.114, 0.173, 0.225, 0.790
total spin= 12.3634748699292

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.332, 0.339, 1.741, 1.772, 1.772, 1.742, 1.705, 10.007
Atom 2, 0.273, 0.333, 0.332, 0.340, 1.741, 1.761, 1.765, 1.741, 1.708, 9.994
Atom 3, 0.273, 0.333, 0.332, 0.340, 1.742, 1.763, 1.763, 1.740, 1.708, 9.994
Atom 4, 0.271, 0.333, 0.333, 0.341, 1.742, 1.770, 1.770, 1.742, 1.702, 10.003
Atom 5, 0.274, 0.331, 0.331, 0.340, 1.741, 1.775, 1.771, 1.743, 1.698, 10.004
Atom 6, 0.267, 0.327, 0.329, 0.343, 1.739, 1.782, 1.795, 1.744, 1.690, 10.015
Atom 7, 0.284, 0.331, 0.330, 0.333, 1.741, 1.774, 1.783, 1.741, 1.691, 10.008
Atom 8, 0.274, 0.331, 0.331, 0.340, 1.745, 1.778, 1.768, 1.739, 1.698, 10.005
Atom 9, 0.424, 0.353, 0.323, 0.230, 1.726, 1.812, 1.756, 1.740, 1.796, 10.161
Atom 10, 0.419, 0.297, 0.290, 0.166, 1.718, 1.799, 1.804, 1.725, 1.730, 9.949
Atom 11, 0.416, 0.295, 0.290, 0.166, 1.720, 1.801, 1.807, 1.722, 1.717, 9.934
Atom 12, 0.423, 0.347, 0.329, 0.230, 1.728, 1.803, 1.765, 1.739, 1.796, 10.161
Atom 13, 0.811, 0.003, 0.003, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.821
Atom 14, 0.446, 0.304, 0.304, 0.167, 1.728, 1.806, 1.812, 1.727, 1.700, 9.994
Atom 15, 0.447, 0.303, 0.303, 0.169, 1.727, 1.808, 1.804, 1.727, 1.703, 9.992
Atom 16, 0.446, 0.304, 0.304, 0.167, 1.728, 1.806, 1.801, 1.728, 1.687, 9.969
Atom 17, 0.446, 0.304, 0.304, 0.167, 1.727, 1.808, 1.810, 1.727, 1.700, 9.994
total charge= 161.005

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.249, -3.981, -3.981, -4.077, -2.139, -1.874, -1.867, -2.139, -2.294, -2.264
Atom 2, -5.256, -3.981, -3.981, -4.121, -2.132, -1.903, -1.896, -2.147, -2.301, -2.272
Atom 3, -5.256, -3.989, -3.996, -4.121, -2.147, -1.903, -1.903, -2.132, -2.301, -2.272
Atom 4, -5.264, -3.996, -3.989, -4.011, -2.132, -1.881, -1.874, -2.139, -2.301, -2.272
Atom 5, -5.404, -4.011, -4.018, -4.063, -2.124, -1.830, -1.837, -2.124, -2.272, -2.250

Atom 6, -5.308, -3.996, -3.981, -3.930, -2.088, -1.808, -1.785, -2.080, -2.294, -2.220
Atom 7, -5.131, -3.959, -3.945, -3.908, -2.139, -1.844, -1.837, -2.139, -2.301, -2.272
Atom 8, -5.404, -4.011, -3.996, -4.063, -2.124, -1.830, -1.844, -2.124, -2.272, -2.250
Atom 9, -6.023, -4.011, -3.908, -3.473, -2.058, -1.542, -1.609, -2.043, -1.690, -1.881
Atom 10, -4.195, -3.171, -3.237, -2.287, -1.977, -1.528, -1.535, -1.992, -1.660, -1.785
Atom 11, -4.195, -3.186, -3.267, -2.331, -1.933, -1.491, -1.513, -1.977, -1.660, -1.778
Atom 12, -6.030, -4.004, -3.864, -3.473, -2.029, -1.535, -1.616, -2.073, -1.697, -1.881
Atom 13, -5.529, -1.343, -1.601, -5.558, -9.140, -9.140, -9.140, -9.140, -9.140, -5.522
Atom 14, -4.232, -3.156, -3.156, -1.830, -1.970, -1.535, -1.528, -1.977, -1.668, -1.785
Atom 15, -4.225, -3.171, -3.163, -1.815, -1.970, -1.528, -1.520, -1.970, -1.660, -1.778
Atom 16, -4.203, -3.171, -3.163, -1.837, -1.977, -1.535, -1.535, -1.970, -1.682, -1.793
Atom 17, -4.232, -3.163, -3.163, -1.830, -1.977, -1.528, -1.535, -1.970, -1.668, -1.785

H binding at fcc site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44012 -0.00864 4.07970
10 Ni 1.44014 2.49959 4.07970
11 Ni 3.60263 -1.24633 4.05757
12 Ni 3.61194 1.24551 4.08001
13 H 2.16390 1.24551 5.01437
14 Ni 1.43867 0.00000 -2.03458
15 Ni 1.43867 2.49184 -2.03458
16 Ni 3.59667 -1.24592 -2.03458
17 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1499.0198844722

Total electrons from output= 161
Spin up from output= 86.5000000000
Spin down from output= 74.5000000000
Fermi level up from output= -4.9001344694
Fermi level down from output= -5.0734808708
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.018, -0.013, -0.012, -0.013, 0.167, 0.162, 0.164, 0.165, 0.187, 0.825
Atom 2, 0.018, -0.013, -0.012, -0.013, 0.167, 0.162, 0.164, 0.165, 0.187, 0.825
Atom 3, 0.018, -0.012, -0.013, -0.013, 0.164, 0.166, 0.161, 0.167, 0.187, 0.825
Atom 4, 0.015, -0.012, -0.012, -0.012, 0.165, 0.153, 0.152, 0.165, 0.187, 0.801
Atom 5, 0.016, -0.012, -0.012, -0.013, 0.163, 0.150, 0.160, 0.163, 0.201, 0.817
Atom 6, 0.016, -0.010, -0.010, -0.006, 0.161, 0.108, 0.108, 0.161, 0.192, 0.718
Atom 7, 0.017, -0.012, -0.012, -0.013, 0.163, 0.157, 0.154, 0.163, 0.201, 0.817
Atom 8, 0.017, -0.012, -0.012, -0.013, 0.163, 0.157, 0.154, 0.163, 0.201, 0.817
Atom 9, 0.015, -0.009, -0.007, -0.003, 0.161, 0.100, 0.105, 0.156, 0.150, 0.668
Atom 10, 0.015, -0.009, -0.007, -0.003, 0.161, 0.100, 0.105, 0.156, 0.150, 0.668
Atom 11, 0.020, -0.011, -0.011, -0.004, 0.189, 0.125, 0.126, 0.189, 0.225, 0.848

Atom 12, 0.015, -0.006, -0.010, -0.003, 0.153, 0.105, 0.099, 0.164, 0.150, 0.668
Atom 13, 0.006, 0.000, 0.000, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 14, 0.019, -0.010, -0.011, -0.006, 0.174, 0.115, 0.118, 0.173, 0.229, 0.803
Atom 15, 0.019, -0.010, -0.011, -0.006, 0.174, 0.115, 0.118, 0.173, 0.229, 0.803
Atom 16, 0.021, -0.010, -0.010, -0.006, 0.173, 0.123, 0.123, 0.173, 0.250, 0.837
Atom 17, 0.019, -0.011, -0.010, -0.006, 0.173, 0.120, 0.114, 0.174, 0.229, 0.803
total spin= 12.5397215176507

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.273, 0.332, 0.333, 0.339, 1.739, 1.762, 1.763, 1.741, 1.704, 9.986
Atom 2, 0.273, 0.332, 0.333, 0.339, 1.739, 1.762, 1.763, 1.741, 1.704, 9.986
Atom 3, 0.273, 0.333, 0.332, 0.339, 1.741, 1.763, 1.762, 1.738, 1.704, 9.986
Atom 4, 0.270, 0.333, 0.333, 0.340, 1.740, 1.770, 1.770, 1.740, 1.699, 9.995
Atom 5, 0.277, 0.330, 0.332, 0.337, 1.740, 1.777, 1.766, 1.741, 1.695, 9.994
Atom 6, 0.266, 0.327, 0.326, 0.345, 1.738, 1.792, 1.791, 1.739, 1.683, 10.007
Atom 7, 0.277, 0.332, 0.330, 0.337, 1.740, 1.769, 1.773, 1.740, 1.695, 9.994
Atom 8, 0.277, 0.332, 0.330, 0.337, 1.740, 1.769, 1.773, 1.740, 1.695, 9.994
Atom 9, 0.426, 0.318, 0.334, 0.206, 1.718, 1.781, 1.805, 1.733, 1.770, 10.093
Atom 10, 0.426, 0.318, 0.334, 0.206, 1.718, 1.781, 1.805, 1.733, 1.770, 10.092
Atom 11, 0.426, 0.289, 0.288, 0.159, 1.717, 1.801, 1.800, 1.717, 1.704, 9.901
Atom 12, 0.427, 0.344, 0.309, 0.206, 1.739, 1.819, 1.767, 1.712, 1.770, 10.093
Atom 13, 0.778, 0.004, 0.004, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.790
Atom 14, 0.446, 0.303, 0.303, 0.168, 1.727, 1.808, 1.805, 1.726, 1.698, 9.985
Atom 15, 0.447, 0.303, 0.303, 0.168, 1.727, 1.808, 1.805, 1.726, 1.698, 9.985
Atom 16, 0.446, 0.303, 0.303, 0.167, 1.727, 1.800, 1.800, 1.727, 1.676, 9.950
Atom 17, 0.447, 0.303, 0.303, 0.168, 1.726, 1.803, 1.809, 1.727, 1.698, 9.985
total charge= 160.816

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.249, -3.986, -3.979, -4.119, -2.147, -1.903, -1.903, -2.154, -2.302, -2.280
Atom 2, -5.249, -3.986, -3.979, -4.119, -2.147, -1.903, -1.903, -2.154, -2.302, -2.280
Atom 3, -5.249, -3.994, -4.001, -4.119, -2.154, -1.903, -1.903, -2.140, -2.302, -2.280
Atom 4, -5.264, -4.009, -4.009, -3.972, -2.140, -1.874, -1.874, -2.140, -2.302, -2.273
Atom 5, -5.301, -3.994, -4.016, -3.994, -2.140, -1.844, -1.866, -2.132, -2.287, -2.265
Atom 6, -5.309, -4.009, -4.009, -3.927, -2.088, -1.792, -1.800, -2.088, -2.354, -2.236
Atom 7, -5.294, -4.009, -4.001, -3.986, -2.140, -1.859, -1.852, -2.140, -2.287, -2.265
Atom 8, -5.294, -4.009, -4.001, -3.986, -2.140, -1.859, -1.852, -2.140, -2.287, -2.265
Atom 9, -5.301, -3.366, -3.536, -3.041, -2.058, -1.608, -1.541, -2.058, -1.645, -1.852
Atom 10, -5.301, -3.366, -3.528, -3.041, -2.058, -1.608, -1.541, -2.058, -1.645, -1.852
Atom 11, -4.245, -3.189, -3.189, -2.036, -1.970, -1.549, -1.556, -1.970, -1.689, -1.792
Atom 12, -5.301, -4.193, -3.942, -3.033, -2.066, -1.497, -1.637, -2.051, -1.645, -1.852
Atom 13, -5.855, -1.696, -1.696, -5.877, -9.172, -9.172, -9.172, -9.172, -9.172, -9.172
Atom 14, -4.230, -3.174, -3.166, -1.829, -1.977, -1.534, -1.534, -1.977, -1.667, -1.785
Atom 15, -4.230, -3.174, -3.166, -1.829, -1.977, -1.534, -1.534, -1.977, -1.667, -1.785
Atom 16, -4.215, -3.181, -3.181, -1.837, -1.977, -1.541, -1.541, -1.977, -1.696, -1.800
Atom 17, -4.230, -3.174, -3.174, -1.829, -1.977, -1.534, -1.534, -1.970, -1.667, -1.785

H binding at hcp site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000

5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.43151	0.00001	4.08418
10 Ni	1.43864	2.49185	4.05433
11 Ni	3.60019	-1.25206	4.08414
12 Ni	3.60020	1.25210	4.08418
13 H	2.87723	0.00016	5.02120
14 Ni	1.43867	0.00000	-2.03458
15 Ni	1.43867	2.49184	-2.03458
16 Ni	3.59667	-1.24592	-2.03458
17 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1499.0191911430

Total electrons from output= 161
Spin up from output= 86.5000000000
Spin down from output= 74.5000000000
Fermi level up from output= -4.9073861476
Fermi level down from output= -5.0767053506
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.012, -0.012, -0.013, 0.164, 0.150, 0.150, 0.164, 0.187, 0.793
Atom 2, 0.017, -0.012, -0.013, -0.013, 0.165, 0.165, 0.162, 0.166, 0.185, 0.823
Atom 3, 0.017, -0.012, -0.012, -0.013, 0.166, 0.163, 0.164, 0.165, 0.185, 0.823
Atom 4, 0.017, -0.012, -0.012, -0.013, 0.166, 0.163, 0.164, 0.165, 0.185, 0.823
Atom 5, 0.016, -0.011, -0.011, -0.011, 0.164, 0.147, 0.134, 0.159, 0.193, 0.781
Atom 6, 0.016, -0.011, -0.011, -0.011, 0.164, 0.147, 0.134, 0.159, 0.194, 0.781
Atom 7, 0.016, -0.013, -0.013, -0.016, 0.166, 0.151, 0.151, 0.166, 0.216, 0.825
Atom 8, 0.016, -0.011, -0.011, -0.011, 0.157, 0.128, 0.153, 0.166, 0.193, 0.781
Atom 9, 0.014, -0.005, -0.011, -0.003, 0.155, 0.098, 0.103, 0.161, 0.149, 0.661
Atom 10, 0.021, -0.011, -0.011, -0.005, 0.185, 0.132, 0.132, 0.185, 0.209, 0.836
Atom 11, 0.014, -0.009, -0.007, -0.003, 0.160, 0.102, 0.099, 0.157, 0.149, 0.662
Atom 12, 0.014, -0.009, -0.007, -0.003, 0.160, 0.102, 0.099, 0.157, 0.149, 0.662
Atom 13, 0.006, -0.000, -0.000, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 14, 0.019, -0.011, -0.010, -0.008, 0.173, 0.123, 0.112, 0.174, 0.234, 0.806
Atom 15, 0.021, -0.010, -0.010, -0.005, 0.174, 0.116, 0.116, 0.174, 0.233, 0.808
Atom 16, 0.019, -0.010, -0.011, -0.008, 0.174, 0.115, 0.120, 0.173, 0.234, 0.806
Atom 17, 0.019, -0.010, -0.011, -0.008, 0.174, 0.115, 0.120, 0.173, 0.234, 0.806
total spin= 12.4763703881117

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.332, 0.338, 1.741, 1.775, 1.775, 1.741, 1.703, 10.007
Atom 2, 0.272, 0.333, 0.332, 0.340, 1.741, 1.759, 1.764, 1.740, 1.705, 9.987
Atom 3, 0.272, 0.333, 0.333, 0.340, 1.740, 1.763, 1.760, 1.741, 1.705, 9.987
Atom 4, 0.272, 0.333, 0.333, 0.340, 1.740, 1.763, 1.760, 1.741, 1.705, 9.987
Atom 5, 0.271, 0.330, 0.331, 0.341, 1.738, 1.772, 1.781, 1.742, 1.695, 10.002
Atom 6, 0.271, 0.330, 0.331, 0.341, 1.738, 1.772, 1.781, 1.742, 1.695, 10.002
Atom 7, 0.286, 0.329, 0.329, 0.321, 1.738, 1.779, 1.779, 1.738, 1.689, 9.989
Atom 8, 0.271, 0.331, 0.330, 0.341, 1.745, 1.786, 1.767, 1.736, 1.695, 10.002
Atom 9, 0.426, 0.350, 0.307, 0.205, 1.736, 1.825, 1.759, 1.717, 1.770, 10.095
Atom 10, 0.426, 0.291, 0.291, 0.160, 1.719, 1.797, 1.797, 1.719, 1.720, 9.919

Atom 11, 0.426, 0.318, 0.340, 0.205, 1.721, 1.776, 1.809, 1.731, 1.770, 10.095
Atom 12, 0.426, 0.318, 0.340, 0.205, 1.721, 1.776, 1.809, 1.731, 1.770, 10.095
Atom 13, 0.776, 0.004, 0.004, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.787
Atom 14, 0.445, 0.304, 0.304, 0.167, 1.727, 1.802, 1.811, 1.727, 1.692, 9.979
Atom 15, 0.448, 0.303, 0.303, 0.170, 1.726, 1.805, 1.805, 1.726, 1.697, 9.982
Atom 16, 0.445, 0.304, 0.304, 0.167, 1.727, 1.809, 1.804, 1.727, 1.692, 9.980
Atom 17, 0.445, 0.304, 0.304, 0.167, 1.727, 1.809, 1.804, 1.727, 1.692, 9.980
total charge= 160.875

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.233, -3.990, -3.990, -4.071, -2.143, -1.863, -1.863, -2.143, -2.298, -2.268
Atom 2, -5.255, -3.975, -3.990, -4.108, -2.143, -1.915, -1.908, -2.150, -2.312, -2.276
Atom 3, -5.255, -3.997, -3.990, -4.108, -2.150, -1.908, -1.915, -2.143, -2.312, -2.276
Atom 4, -5.255, -3.997, -3.990, -4.108, -2.150, -1.908, -1.915, -2.143, -2.312, -2.276
Atom 5, -5.395, -4.019, -4.012, -4.049, -2.121, -1.827, -1.819, -2.121, -2.276, -2.246
Atom 6, -5.395, -4.019, -4.012, -4.049, -2.121, -1.827, -1.819, -2.121, -2.276, -2.246
Atom 7, -5.094, -3.946, -3.946, -3.828, -2.150, -1.834, -1.834, -2.150, -2.305, -2.268
Atom 8, -5.395, -3.997, -4.019, -4.049, -2.114, -1.812, -1.834, -2.121, -2.276, -2.246
Atom 9, -5.263, -4.262, -4.019, -2.938, -2.084, -1.488, -1.577, -1.996, -1.643, -1.849
Atom 10, -4.233, -3.151, -3.151, -2.055, -1.981, -1.569, -1.569, -1.981, -1.680, -1.805
Atom 11, -5.263, -3.445, -3.600, -2.938, -2.025, -1.554, -1.510, -2.070, -1.643, -1.849
Atom 12, -5.263, -3.445, -3.600, -2.938, -2.025, -1.554, -1.510, -2.070, -1.643, -1.849
Atom 13, -5.866, -1.532, -1.532, -5.881, -9.170, -9.170, -9.170, -9.170, -9.170, -9.170
Atom 14, -4.218, -3.144, -3.151, -1.834, -1.974, -1.540, -1.532, -1.981, -1.680, -1.790
Atom 15, -4.240, -3.173, -3.173, -1.819, -1.974, -1.525, -1.525, -1.974, -1.672, -1.783
Atom 16, -4.218, -3.166, -3.158, -1.834, -1.974, -1.532, -1.540, -1.974, -1.680, -1.790
Atom 17, -4.218, -3.166, -3.158, -1.834, -1.974, -1.532, -1.540, -1.974, -1.680, -1.790

C binding at top site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43867 0.00000 4.04141
10 Ni 1.43819 2.49184 4.10543
11 Ni 3.59690 -1.24552 4.10544
12 Ni 3.59692 1.24548 4.10543
13 C 1.43867 0.00000 5.67696
14 Ni 1.43867 0.00000 -2.03458
15 Ni 1.43867 2.49184 -2.03458
16 Ni 3.59667 -1.24592 -2.03458
17 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1508.9648238294

Total electrons from output= 164
Spin up from output= 87.5000000000
Spin down from output= 76.5000000000
Fermi level up from output= -5.2576299598

Fermi level down from output= -5.3597929084
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.012, -0.012, -0.015, 0.161, 0.161, 0.151, 0.162, 0.177, 0.788
Atom 2, 0.017, -0.012, -0.012, -0.014, 0.169, 0.140, 0.140, 0.169, 0.159, 0.757
Atom 3, 0.016, -0.012, -0.012, -0.015, 0.162, 0.153, 0.158, 0.161, 0.177, 0.788
Atom 4, 0.016, -0.012, -0.012, -0.015, 0.162, 0.153, 0.158, 0.161, 0.177, 0.788
Atom 5, 0.015, -0.012, -0.012, -0.011, 0.153, 0.093, 0.119, 0.157, 0.195, 0.695
Atom 6, 0.015, -0.012, -0.012, -0.011, 0.153, 0.093, 0.119, 0.157, 0.195, 0.695
Atom 7, 0.015, -0.013, -0.012, -0.011, 0.159, 0.131, 0.080, 0.151, 0.195, 0.695
Atom 8, 0.013, -0.012, -0.012, -0.017, 0.157, 0.147, 0.147, 0.157, 0.179, 0.760
Atom 9, -0.001, -0.010, -0.010, -0.017, 0.047, 0.010, 0.010, 0.047, 0.012, 0.089
Atom 10, 0.016, -0.012, 0.002, -0.003, 0.173, 0.086, 0.112, 0.158, 0.168, 0.700
Atom 11, 0.016, -0.001, -0.009, -0.003, 0.162, 0.105, 0.093, 0.170, 0.168, 0.700
Atom 12, 0.016, -0.001, -0.009, -0.003, 0.162, 0.105, 0.093, 0.170, 0.168, 0.700
Atom 13, 0.002, 0.004, 0.004, -0.015, -0.000, -0.000, -0.000, -0.000, -0.000, -0.004
Atom 14, 0.015, -0.013, -0.013, -0.012, 0.168, 0.112, 0.112, 0.168, 0.227, 0.763
Atom 15, 0.015, -0.013, -0.013, -0.013, 0.170, 0.112, 0.121, 0.166, 0.223, 0.769
Atom 16, 0.015, -0.013, -0.013, -0.013, 0.167, 0.119, 0.114, 0.169, 0.223, 0.769
Atom 17, 0.015, -0.013, -0.013, -0.013, 0.167, 0.119, 0.114, 0.169, 0.223, 0.769
total spin= 11.2201628675572

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.334, 0.338, 1.744, 1.759, 1.769, 1.742, 1.708, 9.998
Atom 2, 0.269, 0.333, 0.333, 0.333, 1.736, 1.777, 1.777, 1.736, 1.719, 10.013
Atom 3, 0.272, 0.333, 0.333, 0.338, 1.743, 1.767, 1.762, 1.743, 1.708, 9.998
Atom 4, 0.272, 0.333, 0.333, 0.338, 1.743, 1.767, 1.762, 1.743, 1.708, 9.998
Atom 5, 0.267, 0.327, 0.325, 0.337, 1.736, 1.807, 1.792, 1.736, 1.685, 10.011
Atom 6, 0.267, 0.327, 0.325, 0.337, 1.736, 1.807, 1.792, 1.736, 1.685, 10.011
Atom 7, 0.267, 0.323, 0.328, 0.337, 1.736, 1.784, 1.814, 1.736, 1.685, 10.011
Atom 8, 0.288, 0.327, 0.328, 0.324, 1.737, 1.777, 1.777, 1.737, 1.703, 9.997
Atom 9, 0.286, 0.457, 0.457, 0.356, 1.852, 1.729, 1.729, 1.852, 1.576, 10.295
Atom 10, 0.401, 0.285, 0.273, 0.147, 1.709, 1.822, 1.808, 1.707, 1.739, 9.891
Atom 11, 0.401, 0.276, 0.282, 0.147, 1.707, 1.811, 1.818, 1.708, 1.739, 9.891
Atom 12, 0.401, 0.276, 0.282, 0.147, 1.707, 1.811, 1.818, 1.708, 1.739, 9.891
Atom 13, 1.809, 0.607, 0.607, 0.918, 0.001, 0.006, 0.006, 0.001, 0.008, 3.964
Atom 14, 0.443, 0.301, 0.301, 0.167, 1.727, 1.806, 1.806, 1.727, 1.698, 9.978
Atom 15, 0.443, 0.300, 0.302, 0.167, 1.725, 1.807, 1.797, 1.727, 1.701, 9.970
Atom 16, 0.443, 0.301, 0.300, 0.167, 1.727, 1.799, 1.804, 1.726, 1.701, 9.970
Atom 17, 0.443, 0.301, 0.300, 0.167, 1.727, 1.799, 1.804, 1.726, 1.701, 9.970
total charge= 163.857

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.253, -3.942, -3.927, -4.012, -2.100, -1.915, -1.869, -2.107, -2.254, -2.231
Atom 2, -5.260, -3.865, -3.865, -4.027, -2.107, -1.869, -1.869, -2.107, -2.239, -2.223
Atom 3, -5.253, -3.896, -3.904, -4.012, -2.107, -1.884, -1.907, -2.100, -2.254, -2.231
Atom 4, -5.253, -3.896, -3.904, -4.012, -2.107, -1.884, -1.907, -2.100, -2.254, -2.231
Atom 5, -5.253, -3.942, -3.942, -3.996, -2.054, -1.683, -1.714, -2.054, -2.215, -2.146
Atom 6, -5.253, -3.942, -3.942, -3.996, -2.054, -1.683, -1.714, -2.054, -2.215, -2.146
Atom 7, -5.253, -3.935, -3.927, -3.996, -2.046, -1.730, -1.676, -2.054, -2.215, -2.146
Atom 8, -5.338, -3.865, -3.865, -4.066, -2.107, -1.722, -1.722, -2.107, -2.215, -2.177
Atom 9, -5.260, -3.534, -3.534, -6.024, -2.609, -3.935, -3.935, -2.609, -4.027, -3.564

Atom 10, -4.598, -3.218, -3.457, -3.025, -1.845, -1.290, -1.452, -1.938, -1.514, -1.653
Atom 11, -4.598, -3.426, -3.310, -3.025, -1.907, -1.406, -1.321, -1.869, -1.514, -1.653
Atom 12, -4.598, -3.426, -3.310, -3.025, -1.907, -1.406, -1.321, -1.869, -1.514, -1.653
Atom 13, -10.140, -3.672, -3.672, -1.930, -2.524, -3.965, -3.965, -2.524, -3.881, -3.988
Atom 14, -4.166, -3.171, -3.171, -1.807, -1.938, -1.514, -1.514, -1.938, -1.614, -1.753
Atom 15, -4.197, -3.179, -3.171, -1.807, -1.946, -1.506, -1.498, -1.938, -1.637, -1.753
Atom 16, -4.197, -3.171, -3.179, -1.807, -1.938, -1.498, -1.506, -1.938, -1.637, -1.753
Atom 17, -4.197, -3.171, -3.179, -1.807, -1.938, -1.498, -1.506, -1.938, -1.637, -1.753

C binding at bridge site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.33118	-0.01485	4.06221
10 Ni	1.47226	2.43282	4.14927
11 Ni	-0.65365	-1.16076	4.06223
12 Ni	-0.78436	1.35778	4.15132
13 C	2.49077	0.66841	5.14006
14 Ni	1.43867	0.00000	-2.03458
15 Ni	1.43867	2.49184	-2.03458
16 Ni	3.59667	-1.24592	-2.03458
17 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1509.0905987387

Total electrons from output= 164
Spin up from output= 87.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -5.2785414596
Fermi level down from output= -5.3587452926
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.012, -0.011, -0.017, 0.159, 0.155, 0.152, 0.159, 0.167, 0.769
Atom 2, 0.017, -0.011, -0.012, -0.016, 0.161, 0.129, 0.145, 0.163, 0.172, 0.747
Atom 3, 0.017, -0.011, -0.012, -0.016, 0.162, 0.144, 0.130, 0.162, 0.172, 0.747
Atom 4, 0.016, -0.012, -0.012, -0.018, 0.160, 0.150, 0.148, 0.159, 0.176, 0.767
Atom 5, 0.013, -0.012, -0.011, -0.010, 0.157, 0.112, 0.123, 0.151, 0.171, 0.696
Atom 6, 0.014, -0.012, -0.011, -0.009, 0.148, 0.105, 0.097, 0.144, 0.143, 0.619
Atom 7, 0.015, -0.011, -0.011, -0.008, 0.158, 0.130, 0.115, 0.160, 0.196, 0.745
Atom 8, 0.013, -0.011, -0.011, -0.010, 0.147, 0.110, 0.125, 0.161, 0.171, 0.696
Atom 9, -0.002, -0.007, -0.008, -0.009, 0.024, 0.021, 0.020, 0.039, 0.016, 0.096
Atom 10, 0.015, -0.005, -0.001, -0.003, 0.105, 0.081, 0.095, 0.112, 0.114, 0.514
Atom 11, -0.002, -0.006, -0.008, -0.009, 0.032, 0.026, 0.016, 0.032, 0.016, 0.096
Atom 12, 0.017, -0.004, -0.001, -0.002, 0.110, 0.108, 0.093, 0.102, 0.124, 0.547
Atom 13, 0.006, -0.016, -0.017, 0.003, -0.000, -0.000, -0.000, -0.000, -0.000, -0.024
Atom 14, 0.012, -0.014, -0.013, -0.014, 0.168, 0.118, 0.113, 0.167, 0.217, 0.755
Atom 15, 0.015, -0.014, -0.014, -0.012, 0.167, 0.117, 0.123, 0.167, 0.218, 0.769

Atom 16, 0.014, -0.014, -0.014, -0.013, 0.168, 0.117, 0.122, 0.169, 0.217, 0.767
Atom 17, 0.012, -0.013, -0.014, -0.014, 0.166, 0.119, 0.113, 0.169, 0.217, 0.755
total spin= 10.0603429303229

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.273, 0.332, 0.333, 0.339, 1.746, 1.760, 1.762, 1.745, 1.713, 10.005
Atom 2, 0.270, 0.333, 0.331, 0.336, 1.743, 1.781, 1.765, 1.741, 1.712, 10.012
Atom 3, 0.270, 0.332, 0.332, 0.336, 1.742, 1.765, 1.781, 1.742, 1.712, 10.012
Atom 4, 0.272, 0.332, 0.333, 0.336, 1.746, 1.767, 1.769, 1.746, 1.707, 10.008
Atom 5, 0.285, 0.325, 0.329, 0.330, 1.738, 1.782, 1.784, 1.741, 1.704, 10.019
Atom 6, 0.256, 0.326, 0.328, 0.330, 1.740, 1.784, 1.790, 1.744, 1.723, 10.021
Atom 7, 0.280, 0.325, 0.325, 0.318, 1.736, 1.783, 1.791, 1.735, 1.696, 9.991
Atom 8, 0.285, 0.329, 0.326, 0.330, 1.744, 1.791, 1.775, 1.735, 1.704, 10.019
Atom 9, 0.246, 0.364, 0.345, 0.245, 1.780, 1.801, 1.715, 1.768, 1.762, 10.025
Atom 10, 0.419, 0.292, 0.274, 0.157, 1.748, 1.814, 1.816, 1.728, 1.768, 10.016
Atom 11, 0.246, 0.353, 0.356, 0.245, 1.766, 1.792, 1.723, 1.782, 1.762, 10.025
Atom 12, 0.414, 0.281, 0.279, 0.156, 1.745, 1.792, 1.826, 1.739, 1.765, 9.998
Atom 13, 1.674, 0.848, 0.772, 0.775, 0.006, 0.006, 0.008, 0.006, 0.007, 4.101
Atom 14, 0.441, 0.302, 0.301, 0.167, 1.727, 1.801, 1.806, 1.729, 1.702, 9.976
Atom 15, 0.444, 0.300, 0.301, 0.170, 1.728, 1.801, 1.796, 1.728, 1.707, 9.975
Atom 16, 0.444, 0.300, 0.301, 0.169, 1.727, 1.800, 1.795, 1.728, 1.705, 9.969
Atom 17, 0.441, 0.302, 0.301, 0.167, 1.729, 1.801, 1.805, 1.726, 1.702, 9.976
total charge= 164.148

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.230, -3.914, -3.906, -4.055, -2.076, -1.894, -1.894, -2.084, -2.250, -2.217
Atom 2, -5.247, -3.889, -3.906, -4.063, -2.084, -1.852, -1.885, -2.092, -2.250, -2.208
Atom 3, -5.247, -3.881, -3.881, -4.063, -2.092, -1.869, -1.869, -2.084, -2.250, -2.208
Atom 4, -5.272, -3.922, -3.922, -4.013, -2.084, -1.910, -1.910, -2.084, -2.258, -2.217
Atom 5, -5.280, -3.906, -3.897, -3.889, -2.035, -1.753, -1.670, -2.035, -2.175, -2.142
Atom 6, -5.296, -3.964, -3.930, -3.906, -1.977, -1.645, -1.629, -1.977, -2.142, -2.092
Atom 7, -5.280, -3.897, -3.881, -3.947, -2.026, -1.670, -1.629, -2.018, -2.159, -2.134
Atom 8, -5.280, -3.856, -3.939, -3.889, -2.026, -1.695, -1.728, -2.043, -2.175, -2.142
Atom 9, -5.156, -3.632, -3.583, -3.343, -2.399, -2.109, -2.448, -2.432, -2.432, -2.457
Atom 10, -4.775, -3.235, -3.492, -3.094, -1.811, -1.182, -1.198, -1.885, -1.339, -1.604
Atom 11, -5.156, -3.483, -3.475, -3.343, -2.448, -2.150, -2.432, -2.391, -2.432, -2.457
Atom 12, -4.742, -3.285, -3.417, -3.036, -1.794, -1.256, -1.165, -1.861, -1.389, -1.587
Atom 13, -11.191, -4.295, -4.394, -3.334, -2.035, -4.667, -4.088, -2.150, -3.947, -4.684
Atom 14, -4.195, -3.152, -3.160, -1.786, -1.919, -1.496, -1.488, -1.919, -1.621, -1.736
Atom 15, -4.195, -3.177, -3.177, -1.778, -1.927, -1.496, -1.496, -1.919, -1.621, -1.736
Atom 16, -4.187, -3.194, -3.185, -1.778, -1.927, -1.488, -1.496, -1.927, -1.621, -1.745
Atom 17, -4.195, -3.160, -3.160, -1.786, -1.919, -1.496, -1.496, -1.919, -1.621, -1.736

C binding at fcc site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458

 9 Ni 1.43360 -0.02558 4.13352
10 Ni 1.43357 2.51738 4.13349
11 Ni 3.63697 1.24594 4.13363
12 Ni 3.60559 -1.24595 4.05033
13 C 2.16875 1.24592 5.14000
14 Ni 1.43867 0.00000 -2.03458
15 Ni 1.43867 2.49184 -2.03458
16 Ni 3.59667 -1.24592 -2.03458
17 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1509.1229796738

Total electrons from output= 164
Spin up from output= 87.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -5.2981060248
Fermi level down from output= -5.4039696422
# of atoms= 17

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.012, -0.011, -0.016, 0.161, 0.138, 0.146, 0.163, 0.171, 0.757
Atom 2, 0.017, -0.012, -0.011, -0.016, 0.161, 0.138, 0.146, 0.163, 0.171, 0.757
Atom 3, 0.017, -0.011, -0.012, -0.016, 0.165, 0.151, 0.133, 0.160, 0.171, 0.757
Atom 4, 0.016, -0.012, -0.012, -0.019, 0.157, 0.147, 0.146, 0.157, 0.182, 0.763
Atom 5, 0.014, -0.012, -0.010, -0.010, 0.163, 0.103, 0.145, 0.153, 0.172, 0.719
Atom 6, 0.013, -0.010, -0.010, -0.007, 0.148, 0.095, 0.095, 0.149, 0.117, 0.590
Atom 7, 0.014, -0.010, -0.011, -0.010, 0.156, 0.134, 0.114, 0.161, 0.173, 0.719
Atom 8, 0.014, -0.010, -0.011, -0.010, 0.156, 0.134, 0.114, 0.161, 0.173, 0.719
Atom 9, -0.000, -0.006, -0.005, -0.009, 0.043, 0.029, 0.033, 0.041, 0.032, 0.157
Atom 10, -0.000, -0.006, -0.005, -0.009, 0.043, 0.029, 0.033, 0.041, 0.032, 0.157
Atom 11, -0.000, -0.005, -0.007, -0.009, 0.039, 0.035, 0.027, 0.044, 0.031, 0.156
Atom 12, 0.025, 0.001, 0.001, 0.001, 0.119, 0.128, 0.130, 0.119, 0.183, 0.707
Atom 13, 0.011, -0.015, -0.015, 0.012, -0.000, -0.000, -0.000, -0.000, -0.000, -0.007
Atom 14, 0.013, -0.013, -0.013, -0.013, 0.168, 0.111, 0.120, 0.166, 0.222, 0.762
Atom 15, 0.013, -0.013, -0.013, -0.013, 0.168, 0.111, 0.120, 0.166, 0.222, 0.762
Atom 16, 0.014, -0.013, -0.013, -0.014, 0.169, 0.125, 0.125, 0.169, 0.210, 0.772
Atom 17, 0.013, -0.013, -0.013, -0.013, 0.165, 0.125, 0.107, 0.170, 0.221, 0.761
total spin= 10.0089694758463

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.333, 0.333, 0.337, 1.743, 1.775, 1.766, 1.741, 1.713, 10.012
Atom 2, 0.272, 0.333, 0.333, 0.337, 1.743, 1.775, 1.766, 1.741, 1.713, 10.012
Atom 3, 0.272, 0.333, 0.333, 0.337, 1.740, 1.761, 1.779, 1.745, 1.713, 10.012
Atom 4, 0.270, 0.333, 0.333, 0.335, 1.749, 1.770, 1.771, 1.749, 1.701, 10.010
Atom 5, 0.284, 0.325, 0.327, 0.327, 1.734, 1.801, 1.766, 1.742, 1.709, 10.015
Atom 6, 0.269, 0.322, 0.322, 0.318, 1.737, 1.791, 1.790, 1.737, 1.738, 10.024
Atom 7, 0.284, 0.327, 0.325, 0.327, 1.740, 1.776, 1.792, 1.736, 1.709, 10.015
Atom 8, 0.284, 0.327, 0.325, 0.327, 1.740, 1.776, 1.792, 1.736, 1.709, 10.015
Atom 9, 0.354, 0.331, 0.331, 0.224, 1.756, 1.738, 1.808, 1.758, 1.760, 10.060
Atom 10, 0.354, 0.331, 0.331, 0.224, 1.756, 1.738, 1.808, 1.758, 1.760, 10.060
Atom 11, 0.354, 0.333, 0.329, 0.223, 1.758, 1.845, 1.702, 1.756, 1.760, 10.060
Atom 12, 0.374, 0.274, 0.273, 0.141, 1.760, 1.800, 1.798, 1.761, 1.732, 9.915
Atom 13, 1.646, 0.790, 0.790, 0.774, 0.007, 0.007, 0.007, 0.007, 0.007, 4.035
Atom 14, 0.443, 0.301, 0.301, 0.169, 1.727, 1.808, 1.800, 1.730, 1.699, 9.978

Atom 15, 0.443, 0.301, 0.301, 0.169, 1.727, 1.808, 1.800, 1.730, 1.699, 9.978
Atom 16, 0.443, 0.301, 0.301, 0.169, 1.728, 1.793, 1.793, 1.728, 1.711, 9.966
Atom 17, 0.443, 0.302, 0.301, 0.169, 1.732, 1.796, 1.812, 1.726, 1.700, 9.979
total charge= 164.146

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.247, -3.908, -3.908, -4.091, -2.104, -1.896, -1.896, -2.112, -2.286, -2.237
Atom 2, -5.247, -3.908, -3.908, -4.091, -2.104, -1.896, -1.896, -2.112, -2.286, -2.237
Atom 3, -5.247, -3.883, -3.891, -4.091, -2.112, -1.896, -1.896, -2.095, -2.286, -2.237
Atom 4, -5.288, -3.925, -3.925, -4.024, -2.087, -1.879, -1.879, -2.087, -2.278, -2.228
Atom 5, -5.272, -3.933, -3.933, -3.941, -2.054, -1.655, -1.763, -2.054, -2.162, -2.153
Atom 6, -5.205, -3.908, -3.908, -3.700, -1.937, -1.513, -1.521, -1.937, -2.095, -2.037
Atom 7, -5.272, -3.933, -3.941, -3.941, -2.054, -1.721, -1.679, -2.045, -2.153, -2.153
Atom 8, -5.272, -3.933, -3.941, -3.941, -2.054, -1.721, -1.679, -2.045, -2.153, -2.153
Atom 9, -4.848, -3.459, -3.409, -3.343, -2.253, -1.995, -1.646, -2.170, -2.120, -2.162
Atom 10, -4.848, -3.459, -3.409, -3.343, -2.253, -1.995, -1.646, -2.170, -2.120, -2.162
Atom 11, -4.848, -3.293, -3.384, -3.334, -2.137, -1.513, -2.286, -2.286, -2.120, -2.162
Atom 12, -4.415, -3.268, -3.276, -2.528, -1.630, -1.314, -1.330, -1.630, -1.555, -1.613
Atom 13, -11.284, -4.432, -4.432, -3.575, -2.004, -4.207, -4.207, -2.012, -3.975, -4.615
Atom 14, -4.199, -3.176, -3.176, -1.804, -1.937, -1.505, -1.497, -1.937, -1.638, -1.754
Atom 15, -4.199, -3.176, -3.176, -1.804, -1.937, -1.505, -1.497, -1.937, -1.638, -1.754
Atom 16, -4.199, -3.210, -3.210, -1.796, -1.946, -1.497, -1.497, -1.946, -1.605, -1.771
Atom 17, -4.199, -3.168, -3.168, -1.804, -1.929, -1.497, -1.505, -1.937, -1.638, -1.754

C binding at hcp site on Ni111
17 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.41273 -0.00051 4.12025
10 Ni 1.44670 2.49147 4.04447
11 Ni 3.62455 1.27816 4.11838
12 Ni 3.62431 -1.27935 4.11821
13 C 2.89022 -0.00066 5.11065
14 Ni 1.43867 0.00000 -2.03458
15 Ni 1.43867 2.49184 -2.03458
16 Ni 3.59667 -1.24592 -2.03458
17 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1509.1279669723

Total electrons from output= 164
Spin up from output= 87.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -5.2670993182
Fermi level down from output= -5.3836839908
# of atoms= 17

spin:

Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.012, -0.012, -0.018, 0.157, 0.151, 0.150, 0.157, 0.165, 0.753
Atom 2, 0.017, -0.012, -0.013, -0.016, 0.160, 0.129, 0.146, 0.163, 0.168, 0.743
Atom 3, 0.017, -0.013, -0.012, -0.016, 0.162, 0.142, 0.133, 0.161, 0.169, 0.743
Atom 4, 0.017, -0.013, -0.012, -0.016, 0.162, 0.142, 0.133, 0.161, 0.169, 0.743
Atom 5, 0.013, -0.012, -0.011, -0.010, 0.152, 0.123, 0.103, 0.146, 0.157, 0.660
Atom 6, 0.013, -0.012, -0.011, -0.010, 0.152, 0.123, 0.103, 0.146, 0.157, 0.660
Atom 7, 0.017, -0.010, -0.011, -0.006, 0.163, 0.115, 0.116, 0.163, 0.206, 0.753
Atom 8, 0.013, -0.012, -0.012, -0.010, 0.144, 0.093, 0.134, 0.155, 0.157, 0.661
Atom 9, 0.000, -0.005, -0.009, -0.008, 0.022, 0.026, 0.041, 0.050, 0.022, 0.138
Atom 10, 0.024, -0.001, -0.001, 0.001, 0.123, 0.119, 0.121, 0.123, 0.148, 0.658
Atom 11, 0.000, -0.008, -0.006, -0.008, 0.043, 0.037, 0.030, 0.028, 0.021, 0.137
Atom 12, 0.000, -0.008, -0.006, -0.008, 0.043, 0.037, 0.030, 0.028, 0.021, 0.137
Atom 13, 0.011, -0.014, -0.014, 0.010, -0.000, -0.000, -0.000, -0.000, -0.000, -0.007
Atom 14, 0.012, -0.014, -0.013, -0.014, 0.167, 0.120, 0.104, 0.167, 0.215, 0.745
Atom 15, 0.017, -0.014, -0.014, -0.011, 0.167, 0.120, 0.120, 0.167, 0.218, 0.771
Atom 16, 0.012, -0.013, -0.014, -0.014, 0.167, 0.108, 0.116, 0.167, 0.215, 0.745
Atom 17, 0.012, -0.013, -0.014, -0.014, 0.167, 0.108, 0.116, 0.167, 0.215, 0.745
total spin= 9.78480915867934

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.331, 0.332, 0.338, 1.748, 1.766, 1.767, 1.748, 1.715, 10.017
Atom 2, 0.271, 0.333, 0.331, 0.336, 1.744, 1.781, 1.768, 1.742, 1.714, 10.021
Atom 3, 0.271, 0.332, 0.333, 0.336, 1.743, 1.771, 1.778, 1.744, 1.714, 10.021
Atom 4, 0.271, 0.332, 0.333, 0.336, 1.743, 1.771, 1.778, 1.744, 1.714, 10.021
Atom 5, 0.272, 0.329, 0.329, 0.331, 1.743, 1.771, 1.788, 1.747, 1.718, 10.027
Atom 6, 0.272, 0.329, 0.329, 0.331, 1.743, 1.771, 1.788, 1.747, 1.718, 10.027
Atom 7, 0.277, 0.322, 0.321, 0.298, 1.731, 1.799, 1.799, 1.731, 1.691, 9.968
Atom 8, 0.272, 0.331, 0.327, 0.332, 1.749, 1.798, 1.760, 1.741, 1.718, 10.028
Atom 9, 0.340, 0.354, 0.317, 0.223, 1.774, 1.858, 1.683, 1.740, 1.773, 10.062
Atom 10, 0.380, 0.276, 0.276, 0.139, 1.753, 1.805, 1.803, 1.754, 1.764, 9.951
Atom 11, 0.338, 0.328, 0.345, 0.224, 1.749, 1.726, 1.814, 1.766, 1.773, 10.062
Atom 12, 0.338, 0.328, 0.345, 0.224, 1.749, 1.726, 1.814, 1.766, 1.773, 10.062
Atom 13, 1.644, 0.791, 0.792, 0.763, 0.007, 0.008, 0.008, 0.007, 0.007, 4.026
Atom 14, 0.442, 0.301, 0.301, 0.167, 1.730, 1.800, 1.814, 1.729, 1.702, 9.986
Atom 15, 0.445, 0.300, 0.300, 0.170, 1.730, 1.799, 1.799, 1.730, 1.710, 9.982
Atom 16, 0.442, 0.301, 0.301, 0.167, 1.729, 1.810, 1.804, 1.730, 1.702, 9.986
Atom 17, 0.442, 0.301, 0.301, 0.167, 1.729, 1.810, 1.804, 1.730, 1.702, 9.986
total charge= 164.233

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.253, -3.959, -3.950, -4.109, -2.088, -1.871, -1.871, -2.088, -2.263, -2.230
Atom 2, -5.278, -3.884, -3.892, -4.076, -2.113, -1.871, -1.896, -2.121, -2.288, -2.247
Atom 3, -5.278, -3.909, -3.909, -4.076, -2.121, -1.887, -1.871, -2.121, -2.288, -2.247
Atom 4, -5.278, -3.909, -3.909, -4.076, -2.121, -1.887, -1.871, -2.121, -2.288, -2.247
Atom 5, -5.354, -3.942, -3.892, -3.909, -2.046, -1.771, -1.737, -2.038, -2.188, -2.163
Atom 6, -5.354, -3.942, -3.892, -3.909, -2.046, -1.771, -1.737, -2.038, -2.188, -2.163
Atom 7, -5.287, -3.775, -3.783, -3.984, -1.996, -1.629, -1.637, -1.996, -2.163, -2.113
Atom 8, -5.362, -3.783, -3.959, -3.917, -2.038, -1.712, -1.804, -2.046, -2.188, -2.171
Atom 9, -4.953, -3.458, -3.658, -3.408, -2.163, -1.604, -2.330, -2.330, -2.171, -2.222
Atom 10, -4.410, -3.332, -3.332, -2.648, -1.687, -1.328, -1.345, -1.687, -1.445, -1.637
Atom 11, -4.953, -3.525, -3.449, -3.416, -2.305, -2.105, -1.729, -2.222, -2.180, -2.222
Atom 12, -4.953, -3.525, -3.449, -3.416, -2.305, -2.105, -1.729, -2.222, -2.180, -2.222
Atom 13, -11.359, -4.485, -4.485, -3.808, -2.038, -4.218, -4.226, -2.038, -4.067, -4.660

Atom 14, -4.218, -3.174, -3.182, -1.804, -1.938, -1.520, -1.503, -1.938, -1.645, -1.754
Atom 15, -4.201, -3.224, -3.224, -1.787, -1.938, -1.512, -1.512, -1.938, -1.645, -1.754
Atom 16, -4.218, -3.190, -3.190, -1.804, -1.938, -1.512, -1.520, -1.938, -1.645, -1.754
Atom 17, -4.218, -3.190, -3.190, -1.804, -1.938, -1.512, -1.520, -1.938, -1.645, -1.754

CH binding at top site on Ni111
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.43867	0.00000	3.97424
10 Ni	1.43573	2.49185	4.13585
11 Ni	3.59814	-1.24336	4.13589
12 Ni	3.59815	1.24337	4.13590
13 C	1.43867	0.00000	5.63543
14 H	1.43867	0.00001	6.72915
15 Ni	1.43867	0.00000	-2.03458
16 Ni	1.43867	2.49184	-2.03458
17 Ni	3.59667	-1.24592	-2.03458
18 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1510.2161610433

Total electrons from output= 165
Spin up from output= 88.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -4.2710615896
Fermi level down from output= -4.3130750648
# of atoms= 18

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.012, -0.017, 0.160, 0.150, 0.148, 0.160, 0.169, 0.758
Atom 2, 0.017, -0.012, -0.012, -0.015, 0.164, 0.126, 0.126, 0.164, 0.155, 0.712
Atom 3, 0.015, -0.012, -0.013, -0.017, 0.160, 0.148, 0.149, 0.160, 0.169, 0.758
Atom 4, 0.015, -0.012, -0.013, -0.017, 0.160, 0.148, 0.149, 0.160, 0.169, 0.758
Atom 5, 0.014, -0.013, -0.013, -0.014, 0.148, 0.087, 0.106, 0.151, 0.205, 0.671
Atom 6, 0.014, -0.013, -0.013, -0.014, 0.148, 0.087, 0.106, 0.151, 0.205, 0.671
Atom 7, 0.014, -0.013, -0.013, -0.014, 0.152, 0.116, 0.077, 0.147, 0.205, 0.671
Atom 8, 0.012, -0.013, -0.013, -0.018, 0.150, 0.131, 0.131, 0.150, 0.190, 0.723
Atom 9, 0.003, -0.010, -0.010, -0.012, 0.066, 0.032, 0.032, 0.066, 0.052, 0.217
Atom 10, 0.009, -0.019, -0.004, -0.007, 0.191, 0.109, 0.123, 0.185, 0.140, 0.726
Atom 11, 0.009, -0.008, -0.015, -0.007, 0.186, 0.120, 0.113, 0.189, 0.140, 0.726
Atom 12, 0.009, -0.008, -0.015, -0.007, 0.186, 0.120, 0.113, 0.189, 0.140, 0.726
Atom 13, 0.028, 0.080, 0.080, 0.009, -0.000, 0.000, 0.000, -0.000, -0.000, 0.197
Atom 14, -0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.010, -0.016, -0.016, -0.013, 0.162, 0.111, 0.111, 0.162, 0.220, 0.732
Atom 16, 0.012, -0.015, -0.016, -0.012, 0.166, 0.110, 0.120, 0.161, 0.211, 0.736
Atom 17, 0.012, -0.016, -0.016, -0.012, 0.162, 0.118, 0.112, 0.165, 0.211, 0.736
Atom 18, 0.012, -0.016, -0.016, -0.012, 0.162, 0.118, 0.112, 0.165, 0.211, 0.736

total spin= 11.2551080100977

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.331, 0.333, 0.337, 1.746, 1.763, 1.767, 1.744, 1.711, 10.005
Atom 2, 0.266, 0.330, 0.330, 0.333, 1.739, 1.781, 1.781, 1.739, 1.716, 10.016
Atom 3, 0.272, 0.333, 0.332, 0.337, 1.745, 1.766, 1.764, 1.745, 1.711, 10.005
Atom 4, 0.272, 0.333, 0.332, 0.337, 1.745, 1.766, 1.764, 1.745, 1.711, 10.005
Atom 5, 0.264, 0.326, 0.325, 0.334, 1.741, 1.788, 1.789, 1.745, 1.691, 10.003
Atom 6, 0.264, 0.326, 0.325, 0.334, 1.741, 1.788, 1.789, 1.745, 1.691, 10.002
Atom 7, 0.264, 0.325, 0.326, 0.334, 1.747, 1.789, 1.787, 1.739, 1.691, 10.002
Atom 8, 0.295, 0.324, 0.324, 0.316, 1.740, 1.778, 1.778, 1.740, 1.695, 9.989
Atom 9, 0.186, 0.404, 0.404, 0.437, 1.825, 1.740, 1.740, 1.825, 1.577, 10.139
Atom 10, 0.437, 0.279, 0.261, 0.169, 1.723, 1.800, 1.802, 1.698, 1.771, 9.940
Atom 11, 0.437, 0.266, 0.274, 0.169, 1.704, 1.802, 1.800, 1.717, 1.771, 9.940
Atom 12, 0.437, 0.266, 0.274, 0.169, 1.704, 1.802, 1.800, 1.717, 1.771, 9.940
Atom 13, 1.503, 0.850, 0.850, 1.000, 0.001, 0.003, 0.003, 0.001, 0.011, 4.221
Atom 14, 0.823, 0.003, 0.003, 0.010, 0.000, 0.000, 0.000, 0.000, 0.000, 0.839
Atom 15, 0.439, 0.299, 0.299, 0.168, 1.725, 1.808, 1.808, 1.725, 1.700, 9.972
Atom 16, 0.441, 0.298, 0.299, 0.169, 1.724, 1.805, 1.797, 1.726, 1.710, 9.970
Atom 17, 0.441, 0.299, 0.298, 0.169, 1.725, 1.799, 1.803, 1.725, 1.710, 9.970
Atom 18, 0.441, 0.299, 0.298, 0.169, 1.725, 1.799, 1.803, 1.725, 1.710, 9.970
total charge= 164.928

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.193, -3.935, -3.918, -4.019, -2.069, -1.883, -1.858, -2.069, -2.229, -2.204
Atom 2, -5.201, -3.842, -3.842, -3.985, -2.060, -1.765, -1.765, -2.060, -2.153, -2.162
Atom 3, -5.193, -3.867, -3.876, -4.019, -2.069, -1.866, -1.874, -2.069, -2.229, -2.204
Atom 4, -5.193, -3.867, -3.876, -4.019, -2.069, -1.866, -1.874, -2.069, -2.229, -2.204
Atom 5, -5.150, -3.926, -3.892, -3.952, -2.043, -1.756, -1.697, -2.035, -2.178, -2.145
Atom 6, -5.150, -3.926, -3.892, -3.952, -2.043, -1.756, -1.697, -2.035, -2.178, -2.145
Atom 7, -5.150, -3.825, -3.901, -3.952, -2.035, -1.672, -1.790, -2.043, -2.178, -2.145
Atom 8, -5.370, -3.994, -3.994, -4.002, -2.035, -1.638, -1.638, -2.035, -2.162, -2.111
Atom 9, -6.864, -3.664, -3.664, -3.740, -2.466, -3.757, -3.757, -2.466, -4.103, -3.242
Atom 10, -4.610, -3.133, -3.580, -2.305, -1.832, -1.258, -1.444, -1.917, -1.419, -1.630
Atom 11, -4.610, -3.504, -3.344, -2.305, -1.883, -1.393, -1.300, -1.849, -1.419, -1.630
Atom 12, -4.610, -3.504, -3.344, -2.305, -1.883, -1.393, -1.300, -1.849, -1.419, -1.630
Atom 13, -11.652, -3.301, -3.301, -6.738, -2.297, -3.791, -3.791, -2.297, -4.804, -6.231
Atom 14, -7.489, -2.558, -2.558, -7.413, -12.116, -12.116, -12.116, -12.116, -12.116, -12.116
Atom 15, -4.196, -3.192, -3.192, -1.773, -1.908, -1.478, -1.478, -1.908, -1.596, -1.723
Atom 16, -4.188, -3.200, -3.183, -1.782, -1.917, -1.478, -1.469, -1.908, -1.596, -1.723
Atom 17, -4.188, -3.200, -3.209, -1.782, -1.908, -1.469, -1.478, -1.917, -1.596, -1.723
Atom 18, -4.188, -3.200, -3.209, -1.782, -1.908, -1.469, -1.478, -1.917, -1.596, -1.723

CH binding at bridge site on Ni111
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458

 9 Ni 1.34818 -0.00594 4.06596
10 Ni 1.46544 2.44916 4.14180
11 Ni 3.53730 -1.13937 4.16552
12 Ni 3.65037 1.32355 4.06531
13 C 2.49591 0.66528 5.27503
14 H 2.49821 0.66250 6.37309
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1510.3434588385

Total electrons from output= 165
Spin up from output= 87.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.6082034016
Fermi level down from output= -4.6466250512
# of atoms= 18

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.012, -0.012, -0.016, 0.156, 0.146, 0.146, 0.158, 0.162, 0.742
Atom 2, 0.017, -0.012, -0.012, -0.015, 0.159, 0.133, 0.143, 0.162, 0.164, 0.738
Atom 3, 0.017, -0.012, -0.012, -0.015, 0.162, 0.146, 0.131, 0.159, 0.164, 0.738
Atom 4, 0.016, -0.013, -0.012, -0.016, 0.158, 0.148, 0.150, 0.157, 0.173, 0.761
Atom 5, 0.014, -0.012, -0.011, -0.012, 0.151, 0.103, 0.116, 0.149, 0.189, 0.687
Atom 6, 0.015, -0.012, -0.011, -0.012, 0.150, 0.088, 0.083, 0.145, 0.147, 0.593
Atom 7, 0.014, -0.011, -0.012, -0.009, 0.156, 0.113, 0.102, 0.156, 0.211, 0.720
Atom 8, 0.014, -0.011, -0.012, -0.012, 0.144, 0.106, 0.113, 0.155, 0.189, 0.687
Atom 9, 0.000, -0.007, -0.009, -0.007, 0.045, 0.035, 0.039, 0.065, 0.019, 0.180
Atom 10, 0.014, -0.006, -0.003, -0.002, 0.121, 0.085, 0.100, 0.131, 0.101, 0.542
Atom 11, 0.015, -0.006, -0.003, -0.001, 0.125, 0.097, 0.091, 0.123, 0.113, 0.554
Atom 12, 0.000, -0.007, -0.009, -0.007, 0.056, 0.040, 0.034, 0.054, 0.019, 0.180
Atom 13, 0.004, -0.017, -0.019, 0.006, -0.000, -0.000, -0.000, -0.000, -0.000, -0.026
Atom 14, 0.003, -0.000, -0.000, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.013, -0.014, -0.014, -0.012, 0.165, 0.115, 0.114, 0.164, 0.208, 0.738
Atom 16, 0.012, -0.014, -0.014, -0.013, 0.164, 0.112, 0.115, 0.164, 0.202, 0.730
Atom 17, 0.017, -0.015, -0.014, -0.010, 0.167, 0.119, 0.122, 0.167, 0.217, 0.769
Atom 18, 0.013, -0.014, -0.013, -0.012, 0.164, 0.117, 0.112, 0.165, 0.208, 0.738
total spin= 10.0693790059651

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.273, 0.332, 0.333, 0.338, 1.749, 1.770, 1.769, 1.747, 1.715, 10.025
Atom 2, 0.270, 0.333, 0.331, 0.335, 1.746, 1.784, 1.769, 1.743, 1.718, 10.030
Atom 3, 0.270, 0.331, 0.333, 0.335, 1.743, 1.768, 1.785, 1.746, 1.718, 10.030
Atom 4, 0.271, 0.332, 0.333, 0.336, 1.747, 1.769, 1.769, 1.748, 1.713, 10.018
Atom 5, 0.286, 0.322, 0.329, 0.325, 1.742, 1.784, 1.801, 1.742, 1.696, 10.029
Atom 6, 0.256, 0.321, 0.325, 0.322, 1.740, 1.793, 1.810, 1.742, 1.723, 10.030
Atom 7, 0.286, 0.325, 0.325, 0.325, 1.740, 1.796, 1.798, 1.737, 1.686, 10.019
Atom 8, 0.286, 0.328, 0.323, 0.325, 1.745, 1.807, 1.778, 1.739, 1.696, 10.029
Atom 9, 0.255, 0.339, 0.323, 0.250, 1.792, 1.779, 1.683, 1.767, 1.798, 9.986
Atom 10, 0.432, 0.292, 0.279, 0.171, 1.748, 1.786, 1.799, 1.724, 1.798, 10.030
Atom 11, 0.434, 0.279, 0.279, 0.164, 1.747, 1.777, 1.817, 1.734, 1.791, 10.023
Atom 12, 0.254, 0.328, 0.334, 0.250, 1.780, 1.770, 1.692, 1.779, 1.798, 9.986

Atom 13, 1.456, 0.954, 0.881, 1.038, 0.004, 0.004, 0.005, 0.004, 0.011, 4.356
Atom 14, 0.819, 0.003, 0.003, 0.010, 0.000, 0.000, 0.000, 0.000, 0.000, 0.835
Atom 15, 0.442, 0.301, 0.300, 0.168, 1.728, 1.804, 1.804, 1.729, 1.713, 9.989
Atom 16, 0.442, 0.300, 0.300, 0.168, 1.728, 1.805, 1.803, 1.727, 1.719, 9.992
Atom 17, 0.444, 0.300, 0.301, 0.169, 1.728, 1.800, 1.798, 1.728, 1.708, 9.976
Atom 18, 0.442, 0.300, 0.301, 0.168, 1.729, 1.801, 1.807, 1.728, 1.713, 9.989
total charge= 165.372

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.171, -3.880, -3.880, -4.085, -2.058, -1.870, -1.878, -2.067, -2.212, -2.186
Atom 2, -5.188, -3.888, -3.905, -4.051, -2.067, -1.836, -1.878, -2.075, -2.220, -2.186
Atom 3, -5.188, -3.888, -3.880, -4.051, -2.075, -1.861, -1.853, -2.067, -2.220, -2.186
Atom 4, -5.214, -3.897, -3.897, -3.931, -2.067, -1.895, -1.895, -2.058, -2.229, -2.195
Atom 5, -5.248, -3.914, -3.871, -3.905, -1.998, -1.742, -1.613, -1.998, -2.152, -2.109
Atom 6, -5.223, -3.991, -3.948, -3.931, -1.913, -1.588, -1.528, -1.904, -2.092, -2.041
Atom 7, -5.154, -3.828, -3.820, -3.880, -1.998, -1.647, -1.630, -2.015, -2.144, -2.126
Atom 8, -5.248, -3.846, -3.905, -3.905, -1.990, -1.639, -1.699, -2.015, -2.152, -2.109
Atom 9, -4.624, -3.546, -3.529, -2.691, -2.169, -1.972, -2.374, -2.220, -2.186, -2.280
Atom 10, -4.650, -3.230, -3.418, -2.580, -1.810, -1.322, -1.314, -1.887, -1.340, -1.630
Atom 11, -4.615, -3.187, -3.298, -2.494, -1.759, -1.280, -1.186, -1.853, -1.331, -1.570
Atom 12, -4.624, -3.409, -3.384, -2.691, -2.203, -1.981, -2.340, -2.186, -2.186, -2.280
Atom 13, -11.800, -3.666, -3.828, -6.583, -1.870, -4.059, -3.503, -1.981, -2.092, -6.086
Atom 14, -6.831, -3.426, -3.495, -6.839, -12.210, -12.210, -12.210, -12.210, -12.210, -12.210
Atom 15, -4.162, -3.144, -3.161, -1.759, -1.895, -1.485, -1.468, -1.904, -1.588, -1.716
Atom 16, -4.230, -3.170, -3.170, -1.767, -1.895, -1.468, -1.468, -1.895, -1.579, -1.707
Atom 17, -4.188, -3.187, -3.170, -1.750, -1.913, -1.485, -1.485, -1.913, -1.605, -1.733
Atom 18, -4.162, -3.170, -3.153, -1.759, -1.904, -1.476, -1.476, -1.895, -1.588, -1.716

CH binding at fcc site on Ni111
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43770 -0.01410 4.12172
10 Ni 1.43766 2.50589 4.12168
11 Ni 3.60335 -1.24593 4.07130
12 Ni 3.62372 1.24588 4.11850
13 C 2.17152 1.24588 5.27424
14 H 2.17494 1.24585 6.37312
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1510.3707241823

Total electrons from output= 165
Spin up from output= 87.5000000000
Spin down from output= 77.5000000000

Fermi level up from output= -4.6334006024
Fermi level down from output= -4.6899718556
# of atoms= 18

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.011, -0.011, -0.015, 0.159, 0.137, 0.143, 0.163, 0.164, 0.745
Atom 2, 0.016, -0.011, -0.011, -0.015, 0.159, 0.137, 0.143, 0.163, 0.164, 0.745
Atom 3, 0.016, -0.012, -0.011, -0.015, 0.164, 0.147, 0.133, 0.158, 0.164, 0.744
Atom 4, 0.016, -0.011, -0.011, -0.016, 0.156, 0.144, 0.144, 0.156, 0.182, 0.760
Atom 5, 0.013, -0.012, -0.010, -0.010, 0.157, 0.094, 0.139, 0.151, 0.190, 0.712
Atom 6, 0.015, -0.009, -0.009, -0.010, 0.156, 0.080, 0.080, 0.156, 0.121, 0.579
Atom 7, 0.013, -0.011, -0.012, -0.010, 0.153, 0.127, 0.106, 0.155, 0.190, 0.712
Atom 8, 0.013, -0.011, -0.012, -0.010, 0.153, 0.127, 0.106, 0.155, 0.190, 0.712
Atom 9, 0.001, -0.006, -0.005, -0.008, 0.066, 0.044, 0.047, 0.063, 0.032, 0.232
Atom 10, 0.001, -0.006, -0.005, -0.008, 0.066, 0.044, 0.047, 0.063, 0.032, 0.232
Atom 11, 0.024, -0.000, -0.000, 0.002, 0.134, 0.118, 0.120, 0.134, 0.163, 0.696
Atom 12, 0.001, -0.005, -0.007, -0.009, 0.061, 0.047, 0.042, 0.067, 0.031, 0.230
Atom 13, 0.004, -0.016, -0.015, 0.006, -0.000, 0.000, 0.000, -0.000, -0.000, -0.022
Atom 14, 0.004, -0.000, -0.000, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.012, -0.012, -0.014, -0.013, 0.166, 0.109, 0.116, 0.165, 0.206, 0.734
Atom 16, 0.012, -0.012, -0.014, -0.013, 0.166, 0.109, 0.116, 0.165, 0.206, 0.734
Atom 17, 0.020, -0.014, -0.014, -0.009, 0.168, 0.126, 0.125, 0.168, 0.222, 0.792
Atom 18, 0.012, -0.014, -0.012, -0.013, 0.164, 0.120, 0.104, 0.167, 0.205, 0.734
total spin= 10.0699776807015

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.334, 0.333, 0.337, 1.746, 1.780, 1.771, 1.742, 1.716, 10.029
Atom 2, 0.272, 0.334, 0.333, 0.337, 1.746, 1.780, 1.771, 1.742, 1.716, 10.029
Atom 3, 0.272, 0.332, 0.334, 0.336, 1.740, 1.767, 1.785, 1.747, 1.716, 10.030
Atom 4, 0.269, 0.333, 0.333, 0.335, 1.749, 1.774, 1.775, 1.749, 1.705, 10.022
Atom 5, 0.286, 0.325, 0.330, 0.329, 1.737, 1.797, 1.781, 1.746, 1.700, 10.031
Atom 6, 0.266, 0.319, 0.319, 0.310, 1.734, 1.812, 1.812, 1.734, 1.738, 10.043
Atom 7, 0.285, 0.329, 0.326, 0.330, 1.744, 1.785, 1.793, 1.739, 1.700, 10.031
Atom 8, 0.285, 0.329, 0.326, 0.330, 1.744, 1.785, 1.793, 1.739, 1.700, 10.031
Atom 9, 0.346, 0.316, 0.315, 0.227, 1.771, 1.704, 1.783, 1.757, 1.805, 10.024
Atom 10, 0.346, 0.316, 0.315, 0.227, 1.771, 1.704, 1.783, 1.757, 1.805, 10.024
Atom 11, 0.413, 0.282, 0.280, 0.154, 1.756, 1.801, 1.799, 1.756, 1.756, 9.998
Atom 12, 0.344, 0.317, 0.316, 0.228, 1.750, 1.824, 1.662, 1.778, 1.805, 10.024
Atom 13, 1.431, 0.898, 0.897, 1.047, 0.004, 0.004, 0.004, 0.004, 0.011, 4.302
Atom 14, 0.822, 0.003, 0.003, 0.010, 0.000, 0.000, 0.000, 0.000, 0.000, 0.838
Atom 15, 0.442, 0.302, 0.301, 0.168, 1.728, 1.810, 1.803, 1.729, 1.716, 9.998
Atom 16, 0.442, 0.302, 0.301, 0.168, 1.728, 1.810, 1.803, 1.729, 1.716, 9.998
Atom 17, 0.445, 0.301, 0.301, 0.169, 1.728, 1.795, 1.795, 1.728, 1.705, 9.967
Atom 18, 0.442, 0.301, 0.302, 0.168, 1.730, 1.799, 1.813, 1.727, 1.716, 9.998
total charge= 165.417

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.184, -3.890, -3.890, -4.086, -2.068, -1.872, -1.872, -2.085, -2.247, -2.204
Atom 2, -5.184, -3.890, -3.890, -4.086, -2.068, -1.872, -1.872, -2.085, -2.247, -2.204
Atom 3, -5.184, -3.899, -3.882, -4.086, -2.085, -1.881, -1.872, -2.068, -2.247, -2.204
Atom 4, -5.227, -3.899, -3.899, -3.907, -2.060, -1.864, -1.855, -2.060, -2.230, -2.187
Atom 5, -5.201, -3.882, -3.890, -3.899, -2.034, -1.685, -1.719, -2.009, -2.162, -2.136
Atom 6, -5.201, -3.958, -3.958, -3.814, -1.872, -1.413, -1.413, -1.872, -2.051, -1.957

Atom 7, -5.193, -3.890, -3.899, -3.890, -2.017, -1.702, -1.694, -2.026, -2.162, -2.136
Atom 8, -5.193, -3.890, -3.899, -3.890, -2.017, -1.702, -1.694, -2.026, -2.162, -2.136
Atom 9, -4.588, -3.345, -3.286, -2.766, -2.051, -1.974, -1.617, -2.051, -1.906, -2.043
Atom 10, -4.588, -3.345, -3.286, -2.766, -2.051, -1.974, -1.617, -2.051, -1.906, -2.043
Atom 11, -4.529, -3.158, -3.167, -2.417, -1.651, -1.310, -1.319, -1.651, -1.489, -1.608
Atom 12, -4.588, -3.132, -3.252, -2.758, -2.060, -1.464, -2.264, -2.043, -1.915, -2.043
Atom 13, -11.809, -3.737, -3.746, -6.572, -1.821, -3.396, -3.388, -1.830, -2.026, -6.121
Atom 14, -6.777, -3.311, -3.311, -6.785, -12.217, -12.217, -12.217, -12.217, -12.217, -12.217
Atom 15, -4.222, -3.167, -3.167, -1.779, -1.906, -1.472, -1.472, -1.915, -1.591, -1.719
Atom 16, -4.222, -3.167, -3.167, -1.779, -1.906, -1.472, -1.472, -1.915, -1.591, -1.719
Atom 17, -4.188, -3.184, -3.175, -1.753, -1.923, -1.481, -1.481, -1.923, -1.617, -1.753
Atom 18, -4.222, -3.175, -3.158, -1.779, -1.915, -1.472, -1.472, -1.906, -1.591, -1.719

CH binding at hcp site on Ni111
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42229 -0.00003 4.12714
10 Ni 1.44333 2.49186 4.04921
11 Ni 3.61509 -1.26811 4.12272
12 Ni 3.61509 1.26819 4.12269
13 C 2.88978 0.00005 5.26423
14 H 2.90087 0.00004 6.36375
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1510.3736719006

Total electrons from output= 165
Spin up from output= 87.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.6079857152
Fermi level down from output= -4.6819174588
# of atoms= 18

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.014, -0.012, -0.012, -0.016, 0.156, 0.144, 0.144, 0.156, 0.161, 0.735
Atom 2, 0.017, -0.012, -0.013, -0.015, 0.160, 0.148, 0.144, 0.164, 0.167, 0.759
Atom 3, 0.017, -0.013, -0.012, -0.015, 0.163, 0.145, 0.147, 0.161, 0.167, 0.759
Atom 4, 0.017, -0.013, -0.012, -0.015, 0.163, 0.145, 0.147, 0.161, 0.167, 0.759
Atom 5, 0.014, -0.012, -0.011, -0.012, 0.153, 0.115, 0.103, 0.146, 0.170, 0.666
Atom 6, 0.014, -0.012, -0.011, -0.012, 0.153, 0.115, 0.103, 0.146, 0.170, 0.666
Atom 7, 0.015, -0.012, -0.012, -0.006, 0.163, 0.102, 0.102, 0.163, 0.219, 0.735
Atom 8, 0.014, -0.011, -0.012, -0.012, 0.143, 0.096, 0.121, 0.157, 0.170, 0.666
Atom 9, 0.001, -0.004, -0.010, -0.007, 0.042, 0.036, 0.053, 0.073, 0.026, 0.211
Atom 10, 0.022, -0.003, -0.003, 0.001, 0.136, 0.132, 0.132, 0.135, 0.127, 0.678

Atom 11, 0.001, -0.008, -0.006, -0.007, 0.065, 0.048, 0.041, 0.049, 0.025, 0.209
Atom 12, 0.001, -0.008, -0.006, -0.007, 0.065, 0.048, 0.041, 0.049, 0.025, 0.209
Atom 13, 0.005, -0.015, -0.015, 0.007, -0.000, -0.000, -0.000, -0.000, -0.000, -0.018
Atom 14, 0.004, -0.000, -0.000, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.015, -0.013, -0.014, -0.011, 0.166, 0.123, 0.110, 0.167, 0.220, 0.762
Atom 16, 0.013, -0.013, -0.013, -0.014, 0.165, 0.117, 0.117, 0.165, 0.198, 0.734
Atom 17, 0.015, -0.014, -0.014, -0.011, 0.167, 0.114, 0.120, 0.166, 0.220, 0.763
Atom 18, 0.015, -0.014, -0.014, -0.011, 0.167, 0.114, 0.120, 0.166, 0.220, 0.763
total spin= 10.0545325280124

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.332, 0.332, 0.336, 1.749, 1.771, 1.771, 1.749, 1.715, 10.026
Atom 2, 0.271, 0.333, 0.332, 0.336, 1.746, 1.771, 1.771, 1.742, 1.718, 10.019
Atom 3, 0.271, 0.332, 0.333, 0.336, 1.743, 1.771, 1.771, 1.745, 1.718, 10.019
Atom 4, 0.271, 0.332, 0.333, 0.336, 1.743, 1.771, 1.771, 1.745, 1.718, 10.019
Atom 5, 0.274, 0.324, 0.328, 0.324, 1.741, 1.778, 1.805, 1.745, 1.710, 10.029
Atom 6, 0.274, 0.324, 0.328, 0.324, 1.741, 1.778, 1.805, 1.745, 1.710, 10.029
Atom 7, 0.285, 0.324, 0.323, 0.315, 1.734, 1.805, 1.805, 1.733, 1.681, 10.004
Atom 8, 0.274, 0.330, 0.322, 0.324, 1.747, 1.819, 1.764, 1.740, 1.710, 10.029
Atom 9, 0.341, 0.331, 0.303, 0.223, 1.765, 1.842, 1.639, 1.767, 1.813, 10.025
Atom 10, 0.413, 0.290, 0.290, 0.158, 1.752, 1.777, 1.776, 1.753, 1.791, 9.999
Atom 11, 0.338, 0.312, 0.326, 0.224, 1.767, 1.690, 1.791, 1.766, 1.813, 10.027
Atom 12, 0.338, 0.312, 0.326, 0.224, 1.767, 1.690, 1.791, 1.766, 1.813, 10.027
Atom 13, 1.435, 0.895, 0.896, 1.027, 0.005, 0.004, 0.004, 0.005, 0.011, 4.282
Atom 14, 0.825, 0.003, 0.003, 0.010, 0.000, 0.000, 0.000, 0.000, 0.000, 0.841
Atom 15, 0.443, 0.301, 0.301, 0.168, 1.729, 1.796, 1.808, 1.729, 1.702, 9.977
Atom 16, 0.442, 0.300, 0.300, 0.167, 1.729, 1.802, 1.802, 1.729, 1.723, 9.993
Atom 17, 0.443, 0.301, 0.301, 0.168, 1.729, 1.805, 1.799, 1.729, 1.702, 9.977
Atom 18, 0.443, 0.301, 0.301, 0.168, 1.729, 1.805, 1.799, 1.729, 1.702, 9.977
total charge= 165.299

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.186, -3.904, -3.904, -4.117, -2.065, -1.852, -1.843, -2.065, -2.236, -2.202
Atom 2, -5.212, -3.904, -3.912, -4.049, -2.091, -1.886, -1.886, -2.100, -2.262, -2.219
Atom 3, -5.212, -3.904, -3.904, -4.049, -2.100, -1.886, -1.886, -2.100, -2.262, -2.219
Atom 4, -5.212, -3.904, -3.904, -4.049, -2.100, -1.886, -1.886, -2.100, -2.262, -2.219
Atom 5, -5.306, -3.981, -3.921, -4.006, -1.997, -1.706, -1.655, -1.988, -2.159, -2.125
Atom 6, -5.306, -3.981, -3.921, -4.006, -1.997, -1.706, -1.655, -1.988, -2.151, -2.125
Atom 7, -5.135, -3.750, -3.758, -3.869, -2.005, -1.638, -1.646, -2.005, -2.159, -2.125
Atom 8, -5.306, -3.835, -3.972, -4.015, -1.988, -1.629, -1.749, -2.005, -2.159, -2.125
Atom 9, -4.639, -3.262, -3.408, -2.758, -2.074, -1.492, -2.347, -2.091, -1.894, -2.057
Atom 10, -4.553, -3.228, -3.228, -2.407, -1.715, -1.484, -1.484, -1.715, -1.433, -1.672
Atom 11, -4.647, -3.373, -3.297, -2.766, -2.091, -2.048, -1.629, -2.082, -1.911, -2.065
Atom 12, -4.647, -3.373, -3.297, -2.766, -2.091, -2.048, -1.629, -2.082, -1.911, -2.065
Atom 13, -11.864, -3.861, -3.861, -6.640, -1.834, -3.425, -3.442, -1.834, -2.185, -6.195
Atom 14, -6.811, -3.459, -3.450, -6.819, -12.274, -12.274, -12.274, -12.274, -12.274, -12.274
Atom 15, -4.211, -3.168, -3.177, -1.775, -1.920, -1.518, -1.492, -1.920, -1.621, -1.740
Atom 16, -4.254, -3.194, -3.194, -1.775, -1.911, -1.484, -1.484, -1.911, -1.586, -1.723
Atom 17, -4.211, -3.185, -3.177, -1.775, -1.920, -1.492, -1.510, -1.920, -1.621, -1.740
Atom 18, -4.211, -3.185, -3.177, -1.775, -1.920, -1.492, -1.510, -1.920, -1.621, -1.740

CH2 binding at top site on Ni111
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.43867	0.00000	4.11323
10 Ni	1.43681	2.49186	4.02081
11 Ni	3.59698	-1.24295	4.09476
12 Ni	3.59701	1.24294	4.09476
13 C	1.43867	0.00000	5.89724
14 H	1.43295	0.91591	6.50161
15 H	1.43334	-0.91539	6.50242
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1511.4754297562

Total electrons from output= 166
Spin up from output= 89.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -4.3811020648
Fermi level down from output= -4.5419451036
# of atoms= 19

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.012, -0.014, 0.163, 0.146, 0.144, 0.163, 0.178, 0.770
Atom 2, 0.018, -0.013, -0.013, -0.013, 0.169, 0.155, 0.144, 0.170, 0.167, 0.783
Atom 3, 0.016, -0.013, -0.013, -0.015, 0.165, 0.155, 0.162, 0.163, 0.181, 0.800
Atom 4, 0.016, -0.013, -0.013, -0.015, 0.165, 0.155, 0.162, 0.163, 0.181, 0.800
Atom 5, 0.016, -0.012, -0.009, -0.013, 0.158, 0.118, 0.131, 0.159, 0.200, 0.748
Atom 6, 0.016, -0.012, -0.009, -0.013, 0.158, 0.118, 0.131, 0.159, 0.200, 0.748
Atom 7, 0.015, -0.011, -0.011, -0.013, 0.156, 0.138, 0.082, 0.158, 0.219, 0.734
Atom 8, 0.015, -0.011, -0.010, -0.015, 0.159, 0.144, 0.150, 0.156, 0.190, 0.777
Atom 9, -0.004, -0.012, -0.012, -0.012, 0.111, 0.020, 0.067, 0.115, 0.080, 0.352
Atom 10, 0.021, -0.018, -0.009, -0.006, 0.190, 0.138, 0.138, 0.186, 0.172, 0.811
Atom 11, 0.013, -0.009, -0.012, -0.003, 0.196, 0.130, 0.121, 0.171, 0.171, 0.778
Atom 12, 0.013, -0.009, -0.012, -0.003, 0.195, 0.130, 0.121, 0.171, 0.171, 0.778
Atom 13, 0.038, 0.178, 0.011, 0.034, -0.000, -0.000, 0.000, -0.000, 0.000, 0.261
Atom 14, -0.013, 0.001, 0.000, -0.012, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.013, 0.001, 0.000, -0.012, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.015, -0.013, -0.010, -0.010, 0.170, 0.116, 0.108, 0.173, 0.223, 0.773
Atom 17, 0.016, -0.012, -0.009, -0.009, 0.171, 0.113, 0.123, 0.171, 0.226, 0.791
Atom 18, 0.018, -0.013, -0.010, -0.008, 0.170, 0.120, 0.116, 0.171, 0.227, 0.790
Atom 19, 0.018, -0.013, -0.010, -0.008, 0.170, 0.120, 0.116, 0.171, 0.227, 0.790
total spin= 12.287749157131

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.270, 0.331, 0.332, 0.339, 1.741, 1.771, 1.772, 1.741, 1.704, 10.001
Atom 2, 0.270, 0.331, 0.330, 0.337, 1.736, 1.768, 1.773, 1.735, 1.714, 9.994

Atom 3, 0.272, 0.332, 0.332, 0.339, 1.741, 1.769, 1.758, 1.742, 1.704, 9.990
Atom 4, 0.272, 0.332, 0.332, 0.339, 1.741, 1.769, 1.758, 1.742, 1.704, 9.990
Atom 5, 0.271, 0.328, 0.331, 0.334, 1.739, 1.784, 1.776, 1.742, 1.697, 10.002
Atom 6, 0.271, 0.328, 0.331, 0.334, 1.739, 1.784, 1.776, 1.742, 1.697, 10.002
Atom 7, 0.278, 0.326, 0.327, 0.330, 1.745, 1.768, 1.794, 1.737, 1.682, 9.989
Atom 8, 0.276, 0.332, 0.333, 0.336, 1.741, 1.773, 1.765, 1.744, 1.699, 10.000
Atom 9, 0.295, 0.368, 0.335, 0.354, 1.772, 1.928, 1.713, 1.772, 1.542, 10.079
Atom 10, 0.409, 0.302, 0.295, 0.160, 1.729, 1.796, 1.789, 1.721, 1.755, 9.955
Atom 11, 0.438, 0.288, 0.290, 0.165, 1.701, 1.799, 1.807, 1.727, 1.743, 9.957
Atom 12, 0.438, 0.288, 0.290, 0.165, 1.701, 1.799, 1.807, 1.727, 1.743, 9.957
Atom 13, 1.369, 0.799, 1.033, 1.118, 0.000, 0.014, 0.002, 0.003, 0.003, 4.341
Atom 14, 0.814, 0.003, 0.008, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.829
Atom 15, 0.814, 0.003, 0.008, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.829
Atom 16, 0.442, 0.302, 0.303, 0.166, 1.725, 1.807, 1.814, 1.726, 1.699, 9.985
Atom 17, 0.443, 0.301, 0.304, 0.168, 1.725, 1.806, 1.797, 1.728, 1.697, 9.970
Atom 18, 0.445, 0.300, 0.304, 0.168, 1.726, 1.802, 1.804, 1.728, 1.698, 9.974
Atom 19, 0.445, 0.300, 0.304, 0.168, 1.726, 1.802, 1.804, 1.728, 1.698, 9.974
total charge= 165.818

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.307, -3.977, -3.968, -4.143, -2.131, -1.851, -1.843, -2.123, -2.289, -2.262
Atom 2, -5.272, -3.986, -3.995, -4.170, -2.140, -1.878, -1.895, -2.140, -2.245, -2.262
Atom 3, -5.307, -3.968, -3.977, -4.135, -2.140, -1.895, -1.904, -2.140, -2.297, -2.280
Atom 4, -5.307, -3.968, -3.977, -4.135, -2.140, -1.895, -1.904, -2.140, -2.297, -2.280
Atom 5, -5.281, -3.968, -3.916, -4.047, -2.114, -1.843, -1.816, -2.105, -2.245, -2.227
Atom 6, -5.281, -3.968, -3.916, -4.047, -2.114, -1.843, -1.816, -2.105, -2.245, -2.227
Atom 7, -5.272, -3.925, -3.933, -4.021, -2.061, -1.816, -1.781, -2.079, -2.254, -2.201
Atom 8, -5.307, -4.030, -4.012, -4.152, -2.131, -1.825, -1.878, -2.123, -2.280, -2.254
Atom 9, -5.535, -3.137, -3.417, -3.627, -2.123, -1.720, -2.980, -2.149, -3.890, -2.464
Atom 10, -4.362, -3.330, -3.540, -2.525, -1.913, -1.493, -1.659, -1.974, -1.668, -1.825
Atom 11, -4.371, -3.190, -3.076, -2.612, -1.991, -1.475, -1.379, -1.939, -1.580, -1.746
Atom 12, -4.371, -3.190, -3.076, -2.612, -1.991, -1.475, -1.379, -1.939, -1.580, -1.746
Atom 13, -12.035, -2.446, -3.610, -4.721, -2.140, -2.018, -3.015, -11.877, -3.986, -6.086
Atom 14, -6.199, -2.088, -2.980, -6.226, -12.516, -12.516, -12.516, -12.516, -12.516, -12.516
Atom 15, -6.199, -2.088, -2.980, -6.226, -12.516, -12.516, -12.516, -12.516, -12.516, -12.516
Atom 16, -4.257, -3.190, -3.172, -1.851, -1.974, -1.528, -1.536, -1.974, -1.650, -1.781
Atom 17, -4.213, -3.216, -3.172, -1.834, -1.974, -1.528, -1.528, -1.965, -1.668, -1.790
Atom 18, -4.213, -3.216, -3.172, -1.834, -1.965, -1.528, -1.528, -1.965, -1.676, -1.781
Atom 19, -4.213, -3.216, -3.172, -1.834, -1.965, -1.528, -1.528, -1.965, -1.676, -1.781

CH2 binding at bridge site on Ni111
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42902 -0.00728 4.13522
10 Ni 1.43632 2.49581 4.04403
11 Ni 3.60036 -1.25233 4.04943
12 Ni 3.60773 1.25063 4.13524

13 C 2.49967 0.65409 5.58885
14 H 2.04836 1.43569 6.22632
15 H 2.94769 -0.12188 6.23581
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1511.5325036295

Total electrons from output= 166
Spin up from output= 89.0000000000
Spin down from output= 77.0000000000
Fermi level up from output= -4.4853058234
Fermi level down from output= -4.7611689138
# of atoms= 19

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.012, -0.012, -0.014, 0.165, 0.150, 0.149, 0.164, 0.175, 0.781
Atom 2, 0.019, -0.013, -0.013, -0.014, 0.168, 0.169, 0.159, 0.169, 0.175, 0.818
Atom 3, 0.019, -0.013, -0.013, -0.014, 0.169, 0.168, 0.161, 0.169, 0.175, 0.818
Atom 4, 0.016, -0.013, -0.012, -0.014, 0.166, 0.151, 0.154, 0.163, 0.188, 0.800
Atom 5, 0.016, -0.012, -0.009, -0.012, 0.158, 0.128, 0.159, 0.159, 0.197, 0.783
Atom 6, 0.019, -0.010, -0.008, -0.010, 0.161, 0.120, 0.095, 0.157, 0.194, 0.718
Atom 7, 0.015, -0.011, -0.010, -0.009, 0.164, 0.134, 0.115, 0.166, 0.219, 0.783
Atom 8, 0.016, -0.011, -0.011, -0.012, 0.156, 0.139, 0.147, 0.161, 0.197, 0.783
Atom 9, 0.006, -0.007, -0.008, -0.001, 0.132, 0.051, 0.069, 0.131, 0.069, 0.441
Atom 10, 0.020, -0.010, -0.007, -0.002, 0.181, 0.142, 0.127, 0.177, 0.167, 0.794
Atom 11, 0.022, -0.009, -0.006, -0.000, 0.183, 0.134, 0.126, 0.179, 0.178, 0.805
Atom 12, 0.006, -0.007, -0.008, -0.001, 0.132, 0.061, 0.059, 0.130, 0.069, 0.441
Atom 13, 0.008, 0.020, 0.009, 0.018, -0.000, 0.000, 0.000, -0.000, 0.000, 0.055
Atom 14, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.018, -0.010, -0.011, -0.008, 0.172, 0.121, 0.114, 0.173, 0.231, 0.800
Atom 17, 0.015, -0.010, -0.010, -0.010, 0.174, 0.116, 0.124, 0.174, 0.222, 0.794
Atom 18, 0.024, -0.012, -0.010, -0.005, 0.172, 0.119, 0.128, 0.174, 0.252, 0.842
Atom 19, 0.018, -0.013, -0.009, -0.008, 0.171, 0.122, 0.113, 0.174, 0.231, 0.800
total spin= 12.0563933270719

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.332, 0.332, 0.339, 1.739, 1.771, 1.768, 1.740, 1.707, 10.000
Atom 2, 0.274, 0.332, 0.332, 0.338, 1.738, 1.758, 1.762, 1.737, 1.714, 9.984
Atom 3, 0.274, 0.332, 0.332, 0.338, 1.738, 1.757, 1.763, 1.737, 1.714, 9.984
Atom 4, 0.270, 0.332, 0.332, 0.338, 1.740, 1.773, 1.770, 1.742, 1.700, 9.996
Atom 5, 0.276, 0.330, 0.334, 0.337, 1.741, 1.779, 1.770, 1.743, 1.700, 10.009
Atom 6, 0.273, 0.322, 0.326, 0.322, 1.736, 1.781, 1.803, 1.738, 1.690, 9.992
Atom 7, 0.289, 0.328, 0.327, 0.333, 1.738, 1.780, 1.788, 1.735, 1.682, 10.001
Atom 8, 0.276, 0.333, 0.331, 0.337, 1.742, 1.786, 1.762, 1.742, 1.700, 10.009
Atom 9, 0.337, 0.332, 0.303, 0.248, 1.730, 1.839, 1.733, 1.756, 1.713, 9.990
Atom 10, 0.406, 0.306, 0.292, 0.163, 1.721, 1.786, 1.799, 1.727, 1.754, 9.954
Atom 11, 0.407, 0.302, 0.289, 0.158, 1.720, 1.802, 1.807, 1.724, 1.745, 9.953
Atom 12, 0.337, 0.326, 0.309, 0.248, 1.732, 1.837, 1.736, 1.754, 1.713, 9.990
Atom 13, 1.331, 1.006, 1.045, 1.037, 0.004, 0.010, 0.005, 0.003, 0.003, 4.444
Atom 14, 0.794, 0.004, 0.006, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.810

Atom 15, 0.795, 0.004, 0.006, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.810
Atom 16, 0.445, 0.303, 0.302, 0.167, 1.728, 1.804, 1.809, 1.726, 1.695, 9.980
Atom 17, 0.443, 0.302, 0.303, 0.167, 1.726, 1.805, 1.798, 1.727, 1.700, 9.971
Atom 18, 0.448, 0.301, 0.303, 0.169, 1.727, 1.804, 1.797, 1.728, 1.678, 9.955
Atom 19, 0.445, 0.301, 0.304, 0.167, 1.727, 1.803, 1.811, 1.727, 1.695, 9.980
total charge= 165.812

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.323, -4.025, -4.025, -4.141, -2.195, -1.937, -1.937, -2.195, -2.346, -2.319
Atom 2, -5.314, -4.025, -4.034, -4.185, -2.213, -2.017, -2.008, -2.222, -2.373, -2.346
Atom 3, -5.314, -4.043, -4.034, -4.185, -2.213, -2.017, -2.008, -2.213, -2.373, -2.346
Atom 4, -5.323, -4.052, -4.043, -4.061, -2.195, -1.928, -1.928, -2.186, -2.364, -2.328
Atom 5, -5.367, -4.043, -3.990, -4.150, -2.177, -1.893, -1.911, -2.168, -2.337, -2.310
Atom 6, -5.314, -4.070, -4.016, -4.123, -2.053, -1.759, -1.688, -2.053, -2.266, -2.177
Atom 7, -5.251, -3.928, -3.919, -4.008, -2.142, -1.857, -1.857, -2.168, -2.310, -2.284
Atom 8, -5.367, -3.954, -4.008, -4.150, -2.168, -1.866, -1.937, -2.177, -2.337, -2.310
Atom 9, -5.074, -3.794, -3.812, -2.692, -2.088, -1.511, -1.822, -2.062, -2.293, -2.062
Atom 10, -4.398, -3.306, -3.528, -2.977, -2.053, -1.644, -1.644, -2.062, -1.751, -1.902
Atom 11, -4.381, -3.288, -3.537, -2.772, -1.991, -1.546, -1.573, -1.999, -1.733, -1.857
Atom 12, -5.083, -3.732, -3.776, -2.692, -2.079, -1.502, -1.884, -2.070, -2.293, -2.062
Atom 13, -12.164, -2.968, -4.167, -5.207, -2.604, -2.079, -2.461, -1.831, -1.875, -6.096
Atom 14, -6.229, -3.048, -4.256, -6.256, -12.564, -12.564, -12.564, -12.564, -12.564, -12.564
Atom 15, -6.229, -3.048, -4.256, -6.256, -12.564, -12.564, -12.564, -12.564, -12.564, -12.564
Atom 16, -4.283, -3.208, -3.217, -1.893, -2.017, -1.600, -1.591, -2.026, -1.733, -1.848
Atom 17, -4.283, -3.226, -3.208, -1.902, -2.017, -1.582, -1.591, -2.017, -1.724, -1.839
Atom 18, -4.247, -3.252, -3.217, -1.875, -2.035, -1.591, -1.600, -2.026, -1.759, -1.866
Atom 19, -4.283, -3.252, -3.199, -1.893, -2.026, -1.591, -1.600, -2.017, -1.733, -1.848

CH2 binding at fcc site on Ni111
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.46811 -0.00945 4.11644
10 Ni 1.46808 2.50157 4.11642
11 Ni 3.61165 -1.24579 4.03476
12 Ni 3.64450 1.24607 4.08550
13 C 2.13363 1.24613 5.42999
14 H 3.18264 1.24607 5.88175
15 H 1.46435 1.24614 6.30358
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1511.5445693022

Total electrons from output= 166
Spin up from output= 88.5000000000

Spin down from output= 77.5000000000
Fermi level up from output= -4.382367367
Fermi level down from output= -4.4960676948
# of atoms= 19

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.012, -0.017, 0.164, 0.137, 0.161, 0.165, 0.168, 0.770
Atom 2, 0.017, -0.013, -0.012, -0.017, 0.164, 0.137, 0.161, 0.165, 0.168, 0.770
Atom 3, 0.015, -0.012, -0.011, -0.014, 0.165, 0.149, 0.125, 0.159, 0.168, 0.744
Atom 4, 0.016, -0.013, -0.012, -0.015, 0.158, 0.153, 0.143, 0.158, 0.183, 0.772
Atom 5, 0.013, -0.011, -0.011, -0.012, 0.154, 0.098, 0.133, 0.156, 0.198, 0.718
Atom 6, 0.014, -0.009, -0.010, -0.009, 0.154, 0.077, 0.103, 0.159, 0.146, 0.625
Atom 7, 0.015, -0.011, -0.012, -0.013, 0.156, 0.139, 0.123, 0.153, 0.203, 0.753
Atom 8, 0.015, -0.011, -0.012, -0.013, 0.156, 0.139, 0.123, 0.153, 0.203, 0.753
Atom 9, 0.005, -0.012, -0.008, -0.007, 0.109, 0.063, 0.069, 0.122, 0.065, 0.406
Atom 10, 0.005, -0.012, -0.008, -0.007, 0.109, 0.063, 0.069, 0.122, 0.065, 0.406
Atom 11, 0.018, -0.007, -0.006, -0.001, 0.171, 0.115, 0.124, 0.176, 0.161, 0.751
Atom 12, 0.008, -0.010, -0.012, -0.009, 0.149, 0.058, 0.076, 0.124, 0.156, 0.542
Atom 13, 0.007, 0.013, 0.003, 0.014, -0.000, 0.000, 0.001, -0.000, -0.000, 0.037
Atom 14, 0.001, 0.000, 0.000, 0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.004, 0.000, -0.000, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.014, -0.012, -0.014, -0.011, 0.170, 0.107, 0.117, 0.166, 0.216, 0.752
Atom 17, 0.014, -0.012, -0.014, -0.011, 0.170, 0.107, 0.117, 0.166, 0.216, 0.752
Atom 18, 0.019, -0.012, -0.014, -0.009, 0.170, 0.128, 0.119, 0.168, 0.226, 0.794
Atom 19, 0.011, -0.012, -0.012, -0.013, 0.166, 0.123, 0.108, 0.168, 0.202, 0.740
total spin= 11.0862933471329

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.273, 0.333, 0.332, 0.335, 1.742, 1.778, 1.762, 1.740, 1.714, 10.008
Atom 2, 0.273, 0.333, 0.332, 0.335, 1.742, 1.778, 1.762, 1.740, 1.714, 10.008
Atom 3, 0.270, 0.331, 0.334, 0.339, 1.739, 1.764, 1.781, 1.745, 1.712, 10.014
Atom 4, 0.270, 0.331, 0.333, 0.337, 1.747, 1.769, 1.771, 1.747, 1.705, 10.008
Atom 5, 0.279, 0.329, 0.329, 0.332, 1.741, 1.790, 1.778, 1.744, 1.695, 10.018
Atom 6, 0.267, 0.327, 0.319, 0.326, 1.739, 1.811, 1.780, 1.734, 1.716, 10.019
Atom 7, 0.280, 0.333, 0.327, 0.337, 1.746, 1.780, 1.785, 1.742, 1.694, 10.022
Atom 8, 0.280, 0.333, 0.327, 0.337, 1.746, 1.780, 1.785, 1.742, 1.694, 10.022
Atom 9, 0.329, 0.299, 0.310, 0.221, 1.747, 1.733, 1.801, 1.743, 1.762, 9.946
Atom 10, 0.329, 0.299, 0.310, 0.221, 1.747, 1.733, 1.801, 1.743, 1.762, 9.946
Atom 11, 0.412, 0.290, 0.284, 0.153, 1.722, 1.814, 1.800, 1.723, 1.759, 9.957
Atom 12, 0.349, 0.325, 0.337, 0.227, 1.738, 1.837, 1.764, 1.746, 1.732, 10.057
Atom 13, 1.347, 0.987, 1.008, 1.080, 0.003, 0.003, 0.010, 0.006, 0.006, 4.450
Atom 14, 0.777, 0.008, 0.004, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.795
Atom 15, 0.806, 0.006, 0.004, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.822
Atom 16, 0.443, 0.303, 0.300, 0.167, 1.728, 1.812, 1.802, 1.728, 1.706, 9.989
Atom 17, 0.443, 0.303, 0.300, 0.167, 1.728, 1.812, 1.802, 1.728, 1.706, 9.989
Atom 18, 0.444, 0.303, 0.301, 0.167, 1.729, 1.795, 1.803, 1.728, 1.698, 9.967
Atom 19, 0.441, 0.303, 0.301, 0.167, 1.730, 1.796, 1.812, 1.725, 1.716, 9.992
total charge= 166.029

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.209, -3.927, -3.936, -4.093, -2.109, -1.897, -1.915, -2.118, -2.275, -2.247
Atom 2, -5.209, -3.927, -3.936, -4.093, -2.109, -1.897, -1.915, -2.118, -2.275, -2.247
Atom 3, -5.219, -3.936, -3.918, -4.102, -2.118, -1.869, -1.860, -2.091, -2.266, -2.229

Atom 4, -5.219, -3.964, -3.945, -3.945, -2.100, -1.869, -1.851, -2.100, -2.257, -2.229
Atom 5, -5.237, -3.991, -4.038, -4.001, -2.072, -1.722, -1.805, -2.054, -2.211, -2.192
Atom 6, -5.191, -3.853, -4.001, -3.816, -1.952, -1.528, -1.648, -1.961, -2.174, -2.081
Atom 7, -5.292, -3.918, -3.945, -4.001, -2.091, -1.805, -1.823, -2.091, -2.238, -2.220
Atom 8, -5.292, -3.918, -3.945, -4.001, -2.091, -1.805, -1.823, -2.091, -2.238, -2.220
Atom 9, -4.647, -3.207, -3.272, -3.023, -2.035, -1.795, -1.519, -2.035, -1.915, -1.989
Atom 10, -4.647, -3.207, -3.272, -3.023, -2.035, -1.795, -1.519, -2.035, -1.915, -1.989
Atom 11, -4.508, -3.290, -3.309, -2.515, -1.841, -1.362, -1.445, -1.805, -1.565, -1.694
Atom 12, -4.803, -3.641, -3.401, -5.043, -2.035, -1.620, -1.814, -2.072, -2.109, -2.072
Atom 13, -12.877, -6.907, -4.600, -6.003, -1.768, -3.161, -1.998, -3.023, -2.100, -6.667
Atom 14, -6.843, -12.794, -12.785, -6.870, -13.265, -13.265, -13.265, -13.265, -13.265, -13.265
Atom 15, -7.018, -6.612, -5.985, -7.046, -13.265, -13.265, -13.265, -13.265, -13.265, -13.265
Atom 16, -4.204, -3.161, -3.189, -1.805, -1.934, -1.509, -1.500, -1.943, -1.638, -1.758
Atom 17, -4.204, -3.161, -3.189, -1.805, -1.934, -1.509, -1.500, -1.943, -1.638, -1.758
Atom 18, -4.204, -3.161, -3.189, -1.805, -1.952, -1.519, -1.519, -1.943, -1.648, -1.777
Atom 19, -4.231, -3.152, -3.179, -1.814, -1.943, -1.509, -1.509, -1.934, -1.620, -1.749

CH2 binding at hcp site on Ni111
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.42996	-0.00003	4.09463
10 Ni	1.44595	2.49184	4.02158
11 Ni	3.59744	-1.26055	4.12613
12 Ni	3.59746	1.26053	4.12618
13 C	2.94206	0.00002	5.43904
14 H	3.62061	-0.00046	6.30622
15 H	1.89790	0.00041	5.89897
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1511.5475193241

Total electrons from output= 166
Spin up from output= 88.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.373251749
Fermi level down from output= -4.4992105422
# of atoms= 19

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.013, -0.017, 0.158, 0.145, 0.145, 0.160, 0.175, 0.755
Atom 2, 0.016, -0.013, -0.013, -0.015, 0.157, 0.137, 0.142, 0.166, 0.178, 0.756
Atom 3, 0.017, -0.013, -0.013, -0.015, 0.164, 0.155, 0.155, 0.164, 0.169, 0.783
Atom 4, 0.017, -0.013, -0.013, -0.015, 0.164, 0.155, 0.155, 0.164, 0.169, 0.783
Atom 5, 0.014, -0.011, -0.013, -0.012, 0.157, 0.147, 0.107, 0.147, 0.172, 0.709

Atom 6, 0.014, -0.011, -0.013, -0.012, 0.157, 0.147, 0.107, 0.147, 0.172, 0.709
Atom 7, 0.015, -0.012, -0.013, -0.010, 0.165, 0.107, 0.111, 0.162, 0.223, 0.750
Atom 8, 0.017, -0.010, -0.013, -0.014, 0.149, 0.101, 0.134, 0.153, 0.193, 0.709
Atom 9, 0.010, -0.009, -0.015, -0.008, 0.138, 0.051, 0.086, 0.134, 0.170, 0.559
Atom 10, 0.018, -0.007, -0.008, -0.002, 0.164, 0.119, 0.139, 0.173, 0.139, 0.737
Atom 11, 0.005, -0.012, -0.008, -0.007, 0.111, 0.067, 0.057, 0.119, 0.061, 0.393
Atom 12, 0.005, -0.012, -0.008, -0.007, 0.111, 0.067, 0.057, 0.119, 0.060, 0.393
Atom 13, 0.007, 0.013, -0.005, 0.015, -0.000, 0.000, 0.001, -0.000, -0.000, 0.030
Atom 14, 0.005, 0.000, -0.000, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.002, 0.000, -0.000, 0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.014, -0.010, -0.015, -0.010, 0.169, 0.121, 0.111, 0.168, 0.226, 0.775
Atom 17, 0.013, -0.010, -0.014, -0.013, 0.169, 0.119, 0.115, 0.170, 0.209, 0.756
Atom 18, 0.017, -0.012, -0.014, -0.010, 0.169, 0.114, 0.119, 0.167, 0.222, 0.772
Atom 19, 0.017, -0.012, -0.014, -0.010, 0.169, 0.114, 0.119, 0.167, 0.222, 0.772
total spin= 11.1403954044521

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.331, 0.331, 0.335, 1.746, 1.769, 1.771, 1.744, 1.706, 10.005
Atom 2, 0.270, 0.331, 0.331, 0.337, 1.747, 1.775, 1.771, 1.739, 1.704, 10.005
Atom 3, 0.272, 0.332, 0.333, 0.337, 1.742, 1.764, 1.766, 1.742, 1.715, 10.002
Atom 4, 0.272, 0.332, 0.333, 0.337, 1.742, 1.764, 1.766, 1.742, 1.715, 10.002
Atom 5, 0.271, 0.329, 0.330, 0.333, 1.740, 1.758, 1.795, 1.747, 1.711, 10.016
Atom 6, 0.271, 0.329, 0.330, 0.333, 1.740, 1.758, 1.795, 1.747, 1.711, 10.016
Atom 7, 0.292, 0.324, 0.324, 0.326, 1.735, 1.802, 1.789, 1.737, 1.677, 10.007
Atom 8, 0.273, 0.331, 0.323, 0.324, 1.741, 1.815, 1.762, 1.745, 1.697, 10.010
Atom 9, 0.347, 0.337, 0.328, 0.220, 1.741, 1.854, 1.758, 1.740, 1.726, 10.051
Atom 10, 0.416, 0.297, 0.293, 0.157, 1.726, 1.803, 1.780, 1.723, 1.781, 9.976
Atom 11, 0.330, 0.294, 0.318, 0.216, 1.742, 1.721, 1.813, 1.745, 1.764, 9.943
Atom 12, 0.330, 0.294, 0.318, 0.216, 1.742, 1.721, 1.813, 1.745, 1.764, 9.943
Atom 13, 1.354, 0.993, 1.001, 1.070, 0.003, 0.003, 0.010, 0.006, 0.006, 4.445
Atom 14, 0.808, 0.006, 0.004, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.824
Atom 15, 0.779, 0.008, 0.004, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.797
Atom 16, 0.442, 0.304, 0.300, 0.167, 1.730, 1.798, 1.808, 1.727, 1.694, 9.970
Atom 17, 0.442, 0.303, 0.299, 0.166, 1.729, 1.800, 1.804, 1.725, 1.710, 9.978
Atom 18, 0.444, 0.301, 0.301, 0.167, 1.729, 1.806, 1.801, 1.728, 1.701, 9.980
Atom 19, 0.444, 0.301, 0.301, 0.167, 1.729, 1.806, 1.801, 1.728, 1.701, 9.980
total charge= 165.950

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.199, -3.970, -3.979, -4.090, -2.102, -1.862, -1.862, -2.102, -2.268, -2.241
Atom 2, -5.236, -3.933, -3.942, -4.034, -2.102, -1.843, -1.880, -2.120, -2.287, -2.231
Atom 3, -5.218, -3.951, -3.942, -4.108, -2.130, -1.917, -1.908, -2.130, -2.296, -2.259
Atom 4, -5.218, -3.951, -3.942, -4.108, -2.130, -1.917, -1.908, -2.130, -2.296, -2.259
Atom 5, -5.292, -3.988, -3.951, -4.044, -2.065, -1.862, -1.723, -2.056, -2.222, -2.194
Atom 6, -5.292, -3.988, -3.951, -4.044, -2.065, -1.862, -1.723, -2.056, -2.222, -2.194
Atom 7, -5.135, -3.831, -3.822, -3.942, -2.074, -1.723, -1.732, -2.056, -2.213, -2.185
Atom 8, -5.366, -3.979, -4.081, -4.044, -2.046, -1.695, -1.815, -2.028, -2.204, -2.176
Atom 9, -4.691, -3.868, -3.637, -5.061, -2.074, -1.640, -1.778, -2.074, -2.056, -2.037
Atom 10, -4.543, -3.359, -3.332, -2.472, -1.917, -1.464, -1.575, -1.871, -1.519, -1.760
Atom 11, -4.645, -3.211, -3.332, -3.017, -2.065, -1.815, -1.501, -2.065, -1.908, -1.972
Atom 12, -4.645, -3.211, -3.332, -3.017, -2.065, -1.815, -1.492, -2.065, -1.908, -1.972
Atom 13, -12.892, -6.919, -4.654, -6.022, -1.751, -3.128, -1.908, -2.980, -2.194, -6.706
Atom 14, -7.030, -6.642, -6.041, -7.058, -13.280, -13.280, -13.280, -13.280, -13.280, -13.280
Atom 15, -6.854, -12.818, -12.809, -6.882, -13.280, -13.280, -13.280, -13.280, -13.280, -13.280

Atom 16, -4.210, -3.128, -3.202, -1.806, -1.945, -1.538, -1.510, -1.954, -1.658, -1.769
Atom 17, -4.238, -3.165, -3.221, -1.825, -1.935, -1.510, -1.510, -1.945, -1.630, -1.751
Atom 18, -4.201, -3.193, -3.202, -1.806, -1.945, -1.519, -1.529, -1.945, -1.658, -1.769
Atom 19, -4.201, -3.193, -3.202, -1.806, -1.945, -1.519, -1.529, -1.945, -1.658, -1.769

CH3 binding at fcc site on Ni111
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.44732	-0.00121	4.20139
10 Ni	1.44001	2.49152	4.03982
11 Ni	-0.71537	-1.24605	4.04030
12 Ni	-0.71479	1.24549	4.04022
13 C	1.53763	-0.02023	6.16896
14 H	0.98905	0.85374	6.54375
15 H	1.06583	-0.94179	6.53374
16 H	2.58113	0.02104	6.50848
17 Ni	1.43867	0.00000	-2.03458
18 Ni	1.43867	2.49184	-2.03458
19 Ni	3.59667	-1.24592	-2.03458
20 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1512.7450415316

Total electrons from output= 167
Spin up from output= 89.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.6684753236
Fermi level down from output= -4.8215088628
# of atoms= 20

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.013, -0.012, -0.013, 0.166, 0.154, 0.153, 0.164, 0.185, 0.801
Atom 2, 0.019, -0.013, -0.013, -0.013, 0.170, 0.163, 0.165, 0.171, 0.176, 0.825
Atom 3, 0.016, -0.012, -0.013, -0.013, 0.165, 0.154, 0.153, 0.166, 0.185, 0.801
Atom 4, 0.016, -0.012, -0.013, -0.013, 0.165, 0.154, 0.153, 0.166, 0.185, 0.801
Atom 5, 0.016, -0.010, -0.010, -0.011, 0.161, 0.122, 0.149, 0.161, 0.197, 0.775
Atom 6, 0.016, -0.010, -0.010, -0.011, 0.161, 0.122, 0.149, 0.161, 0.198, 0.777
Atom 7, 0.017, -0.010, -0.010, -0.012, 0.161, 0.164, 0.111, 0.163, 0.199, 0.783
Atom 8, 0.016, -0.010, -0.010, -0.011, 0.162, 0.157, 0.158, 0.162, 0.188, 0.810
Atom 9, 0.010, -0.007, -0.007, -0.004, 0.157, 0.043, 0.044, 0.157, 0.093, 0.486
Atom 10, 0.021, -0.009, -0.009, -0.003, 0.174, 0.143, 0.121, 0.172, 0.191, 0.801
Atom 11, 0.021, -0.009, -0.009, -0.003, 0.173, 0.126, 0.138, 0.173, 0.191, 0.800
Atom 12, 0.021, -0.009, -0.009, -0.003, 0.173, 0.126, 0.138, 0.173, 0.191, 0.800
Atom 13, 0.002, 0.001, 0.001, 0.016, -0.000, -0.000, -0.000, -0.000, 0.000, 0.019
Atom 14, -0.003, 0.000, 0.000, -0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.003, 0.000, 0.000, -0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, -0.003, 0.000, 0.000, -0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000

Atom 17, 0.018, -0.009, -0.009, -0.008, 0.175, 0.113, 0.113, 0.175, 0.221, 0.787
Atom 18, 0.021, -0.009, -0.009, -0.006, 0.174, 0.109, 0.127, 0.173, 0.233, 0.813
Atom 19, 0.020, -0.009, -0.009, -0.006, 0.173, 0.123, 0.113, 0.174, 0.233, 0.811
Atom 20, 0.021, -0.009, -0.009, -0.006, 0.173, 0.123, 0.113, 0.174, 0.233, 0.811
total spin= 12.5019506475689

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.333, 0.341, 1.739, 1.769, 1.772, 1.740, 1.702, 9.998
Atom 2, 0.274, 0.331, 0.332, 0.339, 1.735, 1.764, 1.762, 1.735, 1.716, 9.989
Atom 3, 0.271, 0.332, 0.332, 0.341, 1.740, 1.771, 1.770, 1.739, 1.702, 9.998
Atom 4, 0.271, 0.332, 0.332, 0.341, 1.740, 1.771, 1.770, 1.739, 1.702, 9.998
Atom 5, 0.278, 0.330, 0.329, 0.332, 1.739, 1.785, 1.767, 1.741, 1.698, 9.998
Atom 6, 0.278, 0.330, 0.329, 0.332, 1.739, 1.785, 1.767, 1.741, 1.698, 9.998
Atom 7, 0.278, 0.329, 0.330, 0.331, 1.743, 1.758, 1.794, 1.737, 1.698, 9.998
Atom 8, 0.265, 0.337, 0.337, 0.350, 1.743, 1.764, 1.764, 1.742, 1.704, 10.006
Atom 9, 0.376, 0.307, 0.306, 0.313, 1.728, 1.906, 1.901, 1.729, 1.537, 10.102
Atom 10, 0.421, 0.308, 0.300, 0.163, 1.728, 1.782, 1.807, 1.732, 1.737, 9.979
Atom 11, 0.421, 0.301, 0.305, 0.163, 1.731, 1.801, 1.788, 1.730, 1.737, 9.976
Atom 12, 0.421, 0.302, 0.305, 0.163, 1.731, 1.801, 1.787, 1.730, 1.737, 9.977
Atom 13, 1.303, 1.067, 1.069, 1.050, 0.004, 0.005, 0.005, 0.005, 0.002, 4.513
Atom 14, 0.816, 0.004, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.831
Atom 15, 0.816, 0.004, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.831
Atom 16, 0.819, 0.008, 0.003, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.834
Atom 17, 0.445, 0.305, 0.304, 0.167, 1.726, 1.812, 1.812, 1.726, 1.703, 10.000
Atom 18, 0.449, 0.305, 0.304, 0.169, 1.727, 1.811, 1.796, 1.728, 1.694, 9.982
Atom 19, 0.447, 0.304, 0.305, 0.169, 1.728, 1.800, 1.807, 1.728, 1.694, 9.980
Atom 20, 0.447, 0.304, 0.305, 0.168, 1.728, 1.800, 1.807, 1.728, 1.693, 9.980
total charge= 166.968

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.274, -3.988, -3.979, -4.131, -2.130, -1.862, -1.844, -2.121, -2.273, -2.264
Atom 2, -5.265, -3.988, -3.988, -4.149, -2.148, -1.924, -1.924, -2.148, -2.291, -2.282
Atom 3, -5.274, -3.979, -3.979, -4.131, -2.130, -1.853, -1.853, -2.130, -2.282, -2.264
Atom 4, -5.274, -3.979, -3.979, -4.131, -2.130, -1.853, -1.853, -2.130, -2.282, -2.264
Atom 5, -5.265, -3.970, -3.970, -4.149, -2.085, -1.782, -1.835, -2.085, -2.246, -2.210
Atom 6, -5.265, -3.970, -3.970, -4.149, -2.085, -1.782, -1.835, -2.085, -2.246, -2.219
Atom 7, -5.265, -3.916, -3.934, -4.157, -2.085, -1.862, -1.773, -2.094, -2.246, -2.219
Atom 8, -5.274, -3.898, -3.898, -4.095, -2.148, -1.916, -1.924, -2.148, -2.309, -2.282
Atom 9, -4.720, -3.559, -3.586, -2.827, -1.880, -1.290, -1.308, -1.871, -2.898, -1.862
Atom 10, -4.336, -2.916, -3.309, -2.514, -1.978, -1.514, -1.585, -1.933, -1.648, -1.799
Atom 11, -4.336, -3.300, -3.175, -2.514, -1.942, -1.558, -1.531, -1.960, -1.648, -1.799
Atom 12, -4.336, -3.309, -3.175, -2.514, -1.942, -1.558, -1.531, -1.960, -1.648, -1.799
Atom 13, -12.178, -5.310, -5.310, -3.032, -5.283, -1.657, -1.612, -5.274, -3.130, -5.337
Atom 14, -5.381, -5.408, -5.354, -5.372, -12.536, -12.536, -12.536, -12.536, -12.536, -12.536
Atom 15, -5.372, -5.363, -5.319, -5.372, -12.536, -12.536, -12.536, -12.536, -12.536, -12.536
Atom 16, -5.372, -12.116, -12.152, -5.372, -12.536, -12.536, -12.536, -12.536, -12.536, -12.536
Atom 17, -4.229, -3.139, -3.139, -1.853, -1.960, -1.523, -1.523, -1.960, -1.639, -1.782
Atom 18, -4.211, -3.130, -3.148, -1.826, -1.969, -1.523, -1.523, -1.960, -1.674, -1.782
Atom 19, -4.211, -3.139, -3.130, -1.826, -1.960, -1.523, -1.523, -1.960, -1.674, -1.782
Atom 20, -4.211, -3.139, -3.130, -1.826, -1.960, -1.523, -1.523, -1.960, -1.674, -1.782

CH3 binding at bridge site on Ni111
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.47631	0.00626	4.14325
10 Ni	1.43697	2.50209	4.01944
11 Ni	3.61392	-1.26675	4.02270
12 Ni	3.60102	1.23283	4.11624
13 C	2.47427	0.57161	5.86907
14 H	2.59844	-0.40151	6.36615
15 H	3.41834	1.14154	6.07336
16 H	1.67121	1.13994	6.36104
17 Ni	1.43867	0.00000	-2.03458
18 Ni	1.43867	2.49184	-2.03458
19 Ni	3.59667	-1.24592	-2.03458
20 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1512.7516143374

Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Total electrons from output= 167
Spin up from output= 89.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.3324491544
Fermi level down from output= -4.5038499836
# of atoms= 20

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.012, -0.015, 0.166, 0.151, 0.153, 0.164, 0.187, 0.799
Atom 2, 0.019, -0.013, -0.013, -0.014, 0.167, 0.157, 0.168, 0.169, 0.181, 0.822
Atom 3, 0.017, -0.012, -0.013, -0.013, 0.167, 0.164, 0.143, 0.167, 0.186, 0.807
Atom 4, 0.015, -0.012, -0.012, -0.013, 0.165, 0.155, 0.154, 0.164, 0.183, 0.799
Atom 5, 0.016, -0.011, -0.011, -0.012, 0.160, 0.139, 0.151, 0.159, 0.194, 0.785
Atom 6, 0.014, -0.011, -0.010, -0.006, 0.157, 0.122, 0.120, 0.160, 0.179, 0.726
Atom 7, 0.018, -0.013, -0.012, -0.015, 0.164, 0.151, 0.147, 0.164, 0.222, 0.826
Atom 8, 0.016, -0.012, -0.011, -0.011, 0.163, 0.144, 0.162, 0.157, 0.188, 0.797
Atom 9, 0.011, -0.009, -0.010, -0.005, 0.161, 0.066, 0.100, 0.155, 0.130, 0.599
Atom 10, 0.021, -0.012, -0.010, -0.006, 0.184, 0.143, 0.123, 0.177, 0.174, 0.793
Atom 11, 0.020, -0.013, -0.010, -0.005, 0.184, 0.121, 0.129, 0.178, 0.176, 0.780
Atom 12, 0.013, -0.011, -0.012, -0.006, 0.163, 0.069, 0.075, 0.160, 0.224, 0.675
Atom 13, 0.005, 0.008, 0.003, 0.023, 0.000, 0.000, 0.000, -0.000, 0.000, 0.039
Atom 14, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.001, 0.000, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 17, 0.018, -0.011, -0.010, -0.008, 0.173, 0.118, 0.113, 0.174, 0.225, 0.793
Atom 18, 0.020, -0.010, -0.010, -0.006, 0.174, 0.113, 0.122, 0.173, 0.229, 0.805
Atom 19, 0.019, -0.010, -0.010, -0.008, 0.173, 0.119, 0.123, 0.173, 0.232, 0.810
Atom 20, 0.019, -0.011, -0.010, -0.008, 0.172, 0.120, 0.112, 0.174, 0.231, 0.799
total spin= 12.4530235855156

CHARGES:

Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.332, 0.337, 1.739, 1.771, 1.771, 1.740, 1.702, 9.997
Atom 2, 0.274, 0.332, 0.332, 0.339, 1.739, 1.764, 1.760, 1.737, 1.710, 9.987
Atom 3, 0.272, 0.333, 0.332, 0.340, 1.738, 1.761, 1.775, 1.738, 1.703, 9.992
Atom 4, 0.270, 0.333, 0.333, 0.339, 1.740, 1.768, 1.766, 1.742, 1.703, 9.993
Atom 5, 0.270, 0.333, 0.332, 0.341, 1.741, 1.780, 1.768, 1.744, 1.699, 10.007
Atom 6, 0.274, 0.328, 0.326, 0.341, 1.741, 1.777, 1.776, 1.738, 1.700, 10.002
Atom 7, 0.285, 0.330, 0.328, 0.332, 1.740, 1.776, 1.780, 1.740, 1.686, 9.998
Atom 8, 0.268, 0.334, 0.334, 0.346, 1.741, 1.773, 1.764, 1.745, 1.705, 10.009
Atom 9, 0.335, 0.334, 0.307, 0.237, 1.719, 1.855, 1.764, 1.734, 1.725, 10.010
Atom 10, 0.405, 0.305, 0.299, 0.163, 1.717, 1.786, 1.808, 1.726, 1.753, 9.962
Atom 11, 0.398, 0.303, 0.293, 0.162, 1.716, 1.804, 1.798, 1.725, 1.748, 9.948
Atom 12, 0.373, 0.328, 0.326, 0.235, 1.724, 1.844, 1.806, 1.735, 1.682, 10.053
Atom 13, 1.303, 1.068, 1.095, 1.088, 0.006, 0.007, 0.004, 0.004, 0.003, 4.578
Atom 14, 0.795, 0.003, 0.008, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.810
Atom 15, 0.770, 0.007, 0.005, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.787
Atom 16, 0.795, 0.006, 0.004, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.810
Atom 17, 0.445, 0.304, 0.304, 0.166, 1.727, 1.806, 1.810, 1.726, 1.699, 9.989
Atom 18, 0.448, 0.303, 0.303, 0.169, 1.727, 1.807, 1.800, 1.727, 1.699, 9.982
Atom 19, 0.445, 0.304, 0.304, 0.166, 1.727, 1.804, 1.800, 1.728, 1.693, 9.972
Atom 20, 0.446, 0.304, 0.304, 0.167, 1.727, 1.803, 1.811, 1.727, 1.694, 9.983
total charge= 166.869

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.285, -3.991, -3.982, -4.086, -2.132, -1.868, -1.858, -2.141, -2.302, -2.264
Atom 2, -5.266, -3.982, -3.982, -4.142, -2.141, -1.924, -1.934, -2.160, -2.311, -2.283
Atom 3, -5.275, -3.982, -3.982, -4.105, -2.151, -1.896, -1.877, -2.141, -2.302, -2.273
Atom 4, -5.266, -3.991, -3.991, -4.048, -2.141, -1.858, -1.868, -2.132, -2.302, -2.273
Atom 5, -5.303, -4.010, -4.029, -4.048, -2.141, -1.839, -1.905, -2.132, -2.292, -2.273
Atom 6, -5.256, -3.906, -3.944, -3.897, -2.066, -1.792, -1.792, -2.085, -2.264, -2.207
Atom 7, -5.256, -3.925, -3.954, -3.982, -2.132, -1.849, -1.849, -2.132, -2.311, -2.273
Atom 8, -5.285, -4.010, -4.001, -4.067, -2.151, -1.868, -1.934, -2.141, -2.302, -2.283
Atom 9, -5.200, -3.501, -3.557, -3.765, -2.019, -1.377, -1.547, -1.990, -1.943, -1.868
Atom 10, -4.293, -3.189, -3.359, -2.528, -2.019, -1.594, -1.575, -2.000, -1.651, -1.830
Atom 11, -4.284, -3.293, -3.387, -2.566, -1.971, -1.499, -1.556, -1.962, -1.651, -1.802
Atom 12, -5.398, -3.510, -3.350, -4.690, -2.000, -1.603, -1.641, -2.038, -1.971, -1.934
Atom 13, -13.128, -6.304, -6.238, -4.067, -6.295, -2.377, -1.868, -6.125, -4.256, -6.295
Atom 14, -6.257, -6.332, -6.115, -6.266, -13.506, -13.506, -13.506, -13.506, -13.506, -13.506
Atom 15, -6.389, -8.343, -13.034, -6.408, -13.506, -13.506, -13.506, -13.506, -13.506, -13.506
Atom 16, -6.257, -6.398, -6.823, -6.276, -13.506, -13.506, -13.506, -13.506, -13.506, -13.506
Atom 17, -4.246, -3.151, -3.161, -1.849, -1.971, -1.537, -1.537, -1.981, -1.669, -1.792
Atom 18, -4.180, -3.170, -3.170, -1.830, -1.971, -1.537, -1.528, -1.971, -1.669, -1.783
Atom 19, -4.190, -3.161, -3.161, -1.849, -1.981, -1.537, -1.537, -1.971, -1.679, -1.792
Atom 20, -4.218, -3.161, -3.151, -1.849, -1.981, -1.537, -1.537, -1.971, -1.679, -1.792

CH3 binding at fcc site on Ni111
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458

8 Ni	2.87733	2.49184	2.03458
9 Ni	1.44291	0.00080	4.09402
10 Ni	1.44279	2.49067	4.09422
11 Ni	3.60006	-1.24607	4.01003
12 Ni	3.59971	1.24581	4.09355
13 C	2.16958	1.24569	5.72089
14 H	1.65613	0.35422	6.14245
15 H	3.19959	1.24526	6.14032
16 H	1.65637	2.13688	6.14341
17 Ni	1.43867	0.00000	-2.03458
18 Ni	1.43867	2.49184	-2.03458
19 Ni	3.59667	-1.24592	-2.03458
20 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1512.7625335663

Total electrons from output= 167
Spin up from output= 89.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.1827217274
Fermi level down from output= -4.3754150076
# of atoms= 20

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.018, -0.013, -0.012, -0.014, 0.165, 0.147, 0.163, 0.165, 0.188, 0.807
Atom 2, 0.018, -0.013, -0.012, -0.014, 0.165, 0.147, 0.163, 0.165, 0.188, 0.807
Atom 3, 0.018, -0.011, -0.013, -0.014, 0.165, 0.170, 0.139, 0.165, 0.188, 0.807
Atom 4, 0.015, -0.012, -0.012, -0.012, 0.161, 0.153, 0.153, 0.161, 0.181, 0.787
Atom 5, 0.017, -0.011, -0.013, -0.013, 0.163, 0.153, 0.149, 0.157, 0.199, 0.803
Atom 6, 0.012, -0.010, -0.010, -0.001, 0.159, 0.113, 0.112, 0.158, 0.162, 0.695
Atom 7, 0.017, -0.012, -0.011, -0.013, 0.159, 0.150, 0.153, 0.161, 0.200, 0.803
Atom 8, 0.017, -0.012, -0.011, -0.013, 0.159, 0.150, 0.153, 0.161, 0.200, 0.803
Atom 9, 0.014, -0.013, -0.010, -0.006, 0.165, 0.085, 0.079, 0.163, 0.198, 0.675
Atom 10, 0.014, -0.013, -0.010, -0.006, 0.165, 0.085, 0.079, 0.163, 0.198, 0.675
Atom 11, 0.021, -0.013, -0.013, -0.006, 0.189, 0.123, 0.124, 0.188, 0.172, 0.784
Atom 12, 0.014, -0.008, -0.015, -0.006, 0.162, 0.074, 0.089, 0.165, 0.197, 0.672
Atom 13, 0.005, 0.007, 0.007, 0.025, -0.000, 0.000, 0.000, -0.000, -0.000, 0.045
Atom 14, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, -0.002, 0.000, 0.000, -0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 17, 0.020, -0.011, -0.011, -0.006, 0.173, 0.113, 0.119, 0.172, 0.227, 0.797
Atom 18, 0.020, -0.011, -0.011, -0.006, 0.173, 0.113, 0.119, 0.172, 0.227, 0.797
Atom 19, 0.020, -0.011, -0.011, -0.008, 0.172, 0.121, 0.121, 0.172, 0.223, 0.802
Atom 20, 0.020, -0.011, -0.011, -0.006, 0.171, 0.123, 0.109, 0.174, 0.227, 0.797
total spin= 12.3552535878716

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.273, 0.332, 0.333, 0.339, 1.740, 1.775, 1.764, 1.740, 1.704, 10.000
Atom 2, 0.273, 0.332, 0.333, 0.339, 1.740, 1.775, 1.764, 1.740, 1.704, 10.000
Atom 3, 0.273, 0.333, 0.332, 0.339, 1.741, 1.758, 1.780, 1.740, 1.704, 10.000
Atom 4, 0.270, 0.333, 0.333, 0.338, 1.744, 1.768, 1.768, 1.744, 1.704, 10.002
Atom 5, 0.275, 0.331, 0.333, 0.340, 1.740, 1.776, 1.777, 1.747, 1.699, 10.017
Atom 6, 0.270, 0.327, 0.326, 0.347, 1.739, 1.777, 1.777, 1.739, 1.709, 10.011
Atom 7, 0.275, 0.333, 0.331, 0.340, 1.745, 1.777, 1.776, 1.742, 1.699, 10.017

Atom 8, 0.275, 0.333, 0.331, 0.340, 1.745, 1.777, 1.776, 1.742, 1.699, 10.017
Atom 9, 0.350, 0.319, 0.320, 0.214, 1.722, 1.793, 1.836, 1.730, 1.716, 10.000
Atom 10, 0.350, 0.319, 0.320, 0.214, 1.722, 1.793, 1.836, 1.730, 1.716, 10.000
Atom 11, 0.417, 0.296, 0.295, 0.158, 1.715, 1.805, 1.804, 1.716, 1.757, 9.963
Atom 12, 0.349, 0.323, 0.318, 0.215, 1.733, 1.858, 1.770, 1.719, 1.716, 10.002
Atom 13, 1.301, 1.052, 1.053, 1.130, 0.006, 0.006, 0.006, 0.006, 0.003, 4.561
Atom 14, 0.787, 0.004, 0.007, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.803
Atom 15, 0.787, 0.008, 0.003, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.803
Atom 16, 0.787, 0.004, 0.007, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.803
Atom 17, 0.447, 0.304, 0.304, 0.167, 1.728, 1.811, 1.804, 1.728, 1.700, 9.993
Atom 18, 0.447, 0.304, 0.304, 0.167, 1.728, 1.811, 1.804, 1.728, 1.700, 9.993
Atom 19, 0.445, 0.305, 0.305, 0.166, 1.728, 1.803, 1.803, 1.728, 1.702, 9.984
Atom 20, 0.447, 0.304, 0.304, 0.167, 1.728, 1.800, 1.814, 1.728, 1.700, 9.993
total charge= 166.962

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.273, -3.996, -3.986, -4.111, -2.153, -1.894, -1.903, -2.162, -2.326, -2.287
Atom 2, -5.273, -3.996, -3.986, -4.111, -2.153, -1.894, -1.903, -2.162, -2.326, -2.287
Atom 3, -5.273, -3.986, -4.005, -4.111, -2.162, -1.913, -1.884, -2.143, -2.326, -2.287
Atom 4, -5.263, -4.005, -4.005, -3.977, -2.143, -1.865, -1.865, -2.143, -2.306, -2.287
Atom 5, -5.321, -4.015, -4.005, -4.053, -2.172, -1.884, -1.903, -2.143, -2.297, -2.287
Atom 6, -5.253, -3.909, -3.909, -3.794, -2.076, -1.769, -1.778, -2.076, -2.297, -2.210
Atom 7, -5.321, -3.996, -4.005, -4.053, -2.153, -1.894, -1.894, -2.162, -2.297, -2.287
Atom 8, -5.321, -3.996, -4.005, -4.053, -2.153, -1.894, -1.894, -2.162, -2.297, -2.287
Atom 9, -5.273, -3.151, -3.285, -4.524, -2.057, -1.682, -1.625, -2.057, -1.884, -1.942
Atom 10, -5.273, -3.151, -3.285, -4.514, -2.057, -1.682, -1.625, -2.057, -1.884, -1.942
Atom 11, -4.313, -3.314, -3.324, -2.278, -1.961, -1.538, -1.538, -1.961, -1.625, -1.788
Atom 12, -5.292, -3.717, -3.391, -4.524, -2.047, -1.586, -1.721, -2.057, -1.884, -1.942
Atom 13, -13.614, -6.789, -6.780, -4.860, -6.684, -2.095, -2.076, -6.684, -4.457, -6.799
Atom 14, -6.818, -6.808, -6.741, -6.837, -13.998, -13.998, -13.998, -13.998, -13.998, -13.998
Atom 15, -6.818, -13.509, -13.576, -6.837, -13.998, -13.998, -13.998, -13.998, -13.998, -13.998
Atom 16, -6.818, -6.808, -6.741, -6.837, -13.998, -13.998, -13.998, -13.998, -13.998, -13.998
Atom 17, -4.217, -3.161, -3.170, -1.846, -1.980, -1.548, -1.548, -1.980, -1.682, -1.798
Atom 18, -4.217, -3.161, -3.170, -1.846, -1.980, -1.548, -1.548, -1.980, -1.682, -1.798
Atom 19, -4.207, -3.161, -3.161, -1.855, -1.990, -1.548, -1.548, -1.990, -1.682, -1.807
Atom 20, -4.217, -3.180, -3.161, -1.846, -1.990, -1.548, -1.548, -1.980, -1.682, -1.798

CH3 binding at hcp site on Ni111
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44303 0.00035 4.10120
10 Ni 1.43596 2.49220 4.00737
11 Ni 3.58997 -1.23851 4.10210
12 Ni 3.59000 1.23940 4.10198
13 C 2.86580 0.00206 5.73798
14 H 3.37704 0.89436 6.15996
15 H 1.83457 0.00180 6.15404

16 H 3.37809 -0.88935 6.16052
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1512.7612103534

Total electrons from output= 167
Spin up from output= 89.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.2041774432
Fermi level down from output= -4.3840408312
# of atoms= 20

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.013, -0.015, 0.163, 0.148, 0.148, 0.163, 0.189, 0.788
Atom 2, 0.017, -0.012, -0.012, -0.013, 0.160, 0.154, 0.161, 0.167, 0.184, 0.806
Atom 3, 0.017, -0.012, -0.012, -0.013, 0.165, 0.159, 0.156, 0.162, 0.184, 0.806
Atom 4, 0.017, -0.012, -0.012, -0.013, 0.165, 0.159, 0.156, 0.162, 0.184, 0.806
Atom 5, 0.015, -0.011, -0.011, -0.008, 0.157, 0.150, 0.133, 0.161, 0.178, 0.765
Atom 6, 0.015, -0.011, -0.011, -0.008, 0.157, 0.150, 0.133, 0.161, 0.178, 0.764
Atom 7, 0.017, -0.013, -0.013, -0.015, 0.165, 0.144, 0.143, 0.166, 0.233, 0.827
Atom 8, 0.015, -0.011, -0.011, -0.008, 0.163, 0.126, 0.158, 0.155, 0.178, 0.765
Atom 9, 0.013, -0.008, -0.014, -0.006, 0.164, 0.061, 0.094, 0.166, 0.203, 0.675
Atom 10, 0.023, -0.012, -0.012, -0.007, 0.186, 0.133, 0.132, 0.186, 0.165, 0.795
Atom 11, 0.014, -0.012, -0.009, -0.006, 0.166, 0.087, 0.070, 0.165, 0.204, 0.678
Atom 12, 0.014, -0.012, -0.009, -0.006, 0.166, 0.087, 0.069, 0.165, 0.204, 0.677
Atom 13, 0.005, 0.007, 0.007, 0.024, -0.000, 0.000, 0.000, -0.000, -0.000, 0.043
Atom 14, -0.001, 0.000, 0.000, -0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.001, 0.000, 0.000, -0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, -0.001, 0.000, 0.000, -0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 17, 0.019, -0.010, -0.010, -0.008, 0.170, 0.123, 0.111, 0.173, 0.227, 0.795
Atom 18, 0.021, -0.010, -0.010, -0.005, 0.173, 0.116, 0.116, 0.173, 0.225, 0.801
Atom 19, 0.019, -0.010, -0.010, -0.008, 0.172, 0.114, 0.120, 0.171, 0.227, 0.795
Atom 20, 0.019, -0.010, -0.010, -0.008, 0.173, 0.114, 0.120, 0.171, 0.227, 0.795
total spin= 12.3805882488455

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.332, 0.336, 1.742, 1.775, 1.775, 1.742, 1.702, 10.008
Atom 2, 0.272, 0.333, 0.332, 0.339, 1.745, 1.766, 1.765, 1.739, 1.705, 9.997
Atom 3, 0.272, 0.332, 0.333, 0.339, 1.740, 1.765, 1.766, 1.744, 1.705, 9.997
Atom 4, 0.272, 0.332, 0.333, 0.340, 1.740, 1.765, 1.766, 1.744, 1.705, 9.997
Atom 5, 0.272, 0.331, 0.331, 0.343, 1.744, 1.768, 1.779, 1.740, 1.709, 10.015
Atom 6, 0.271, 0.331, 0.331, 0.343, 1.744, 1.768, 1.779, 1.740, 1.709, 10.015
Atom 7, 0.292, 0.329, 0.329, 0.332, 1.740, 1.785, 1.786, 1.740, 1.678, 10.010
Atom 8, 0.272, 0.331, 0.331, 0.343, 1.738, 1.783, 1.764, 1.746, 1.709, 10.015
Atom 9, 0.349, 0.327, 0.313, 0.211, 1.729, 1.871, 1.759, 1.720, 1.710, 9.990
Atom 10, 0.426, 0.303, 0.303, 0.159, 1.718, 1.800, 1.800, 1.717, 1.766, 9.990
Atom 11, 0.351, 0.315, 0.323, 0.209, 1.722, 1.788, 1.843, 1.727, 1.710, 9.987
Atom 12, 0.350, 0.316, 0.323, 0.209, 1.722, 1.787, 1.843, 1.727, 1.710, 9.987
Atom 13, 1.305, 1.053, 1.054, 1.131, 0.006, 0.006, 0.005, 0.006, 0.003, 4.568
Atom 14, 0.788, 0.004, 0.007, 0.804, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.788, 0.008, 0.003, 0.804, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000

Atom 16, 0.788, 0.004, 0.007, 0.804, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 17, 0.446, 0.304, 0.304, 0.166, 1.729, 1.802, 1.812, 1.727, 1.698, 9.989
Atom 18, 0.448, 0.303, 0.303, 0.170, 1.727, 1.804, 1.804, 1.727, 1.705, 9.991
Atom 19, 0.446, 0.304, 0.304, 0.166, 1.728, 1.810, 1.805, 1.729, 1.698, 9.989
Atom 20, 0.446, 0.304, 0.304, 0.166, 1.728, 1.810, 1.805, 1.729, 1.698, 9.989
total charge= 166.946

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.279, -4.003, -4.003, -4.042, -2.133, -1.855, -1.855, -2.133, -2.306, -2.267
Atom 2, -5.260, -3.975, -3.994, -4.099, -2.143, -1.893, -1.903, -2.162, -2.315, -2.277
Atom 3, -5.260, -3.994, -3.984, -4.099, -2.152, -1.903, -1.893, -2.143, -2.315, -2.277
Atom 4, -5.260, -3.994, -3.984, -4.099, -2.152, -1.903, -1.893, -2.143, -2.315, -2.277
Atom 5, -5.298, -3.994, -3.994, -3.994, -2.114, -1.884, -1.836, -2.133, -2.267, -2.258
Atom 6, -5.298, -3.994, -3.994, -3.994, -2.114, -1.884, -1.836, -2.133, -2.267, -2.258
Atom 7, -5.173, -3.936, -3.936, -3.984, -2.143, -1.845, -1.845, -2.143, -2.325, -2.277
Atom 8, -5.298, -4.013, -4.003, -3.994, -2.143, -1.826, -1.903, -2.114, -2.267, -2.258
Atom 9, -5.279, -3.725, -3.476, -4.521, -2.075, -1.519, -1.644, -2.008, -1.855, -1.912
Atom 10, -4.320, -3.342, -3.342, -2.123, -2.008, -1.586, -1.586, -2.008, -1.606, -1.826
Atom 11, -5.269, -3.169, -3.389, -4.512, -2.028, -1.606, -1.538, -2.066, -1.845, -1.903
Atom 12, -5.269, -3.169, -3.389, -4.512, -2.028, -1.606, -1.538, -2.066, -1.845, -1.903
Atom 13, -13.585, -6.746, -6.746, -4.838, -6.650, -2.037, -2.018, -6.650, -4.512, -6.766
Atom 14, -6.785, -6.775, -6.708, -6.804, -13.968, -13.968, -13.968, -13.968, -13.968, -13.968
Atom 15, -6.785, -13.489, -13.546, -6.804, -13.968, -13.968, -13.968, -13.968, -13.968, -13.968
Atom 16, -6.785, -6.775, -6.708, -6.804, -13.968, -13.968, -13.968, -13.968, -13.968, -13.968
Atom 17, -4.214, -3.140, -3.159, -1.845, -1.970, -1.548, -1.538, -1.980, -1.682, -1.797
Atom 18, -4.205, -3.178, -3.178, -1.817, -1.980, -1.529, -1.529, -1.980, -1.673, -1.788
Atom 19, -4.214, -3.169, -3.159, -1.845, -1.980, -1.538, -1.548, -1.970, -1.682, -1.797
Atom 20, -4.214, -3.169, -3.159, -1.845, -1.980, -1.538, -1.548, -1.970, -1.682, -1.797

CH3 to CH2 + H transition state between an fcc and an hcp sites on Ni111
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000   0.00000   0.00000
 2 Ni   0.00000   2.49184   0.00000
 3 Ni   2.15800 -1.24592   0.00000
 4 Ni   2.15800   1.24592   0.00000
 5 Ni   0.71933   1.24592   2.03458
 6 Ni   0.71933   3.73777   2.03458
 7 Ni   2.87733   0.00000   2.03458
 8 Ni   2.87733   2.49184   2.03458
 9 Ni   1.46011 -0.01338   4.13031
10 Ni   1.43560   2.50028   4.13255
11 Ni   3.60206 -1.25374   4.01454
12 Ni   3.60861   1.22265   4.08574
13 C   2.08423   1.33289   5.52096
14 H   1.38376   0.90633   6.25967
15 H   3.01789   1.56662   6.07990
16 H   1.48440   3.02828   5.53723
17 Ni   1.43867   0.00000 -2.03458
18 Ni   1.43867   2.49184 -2.03458
19 Ni   3.59667 -1.24592 -2.03458
20 Ni   3.59667   1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1512.7040407186

Total electrons from output= 167
Spin up from output= 89.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.1610891414
Fermi level down from output= -4.4414556192
# of atoms= 20

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.019, -0.013, -0.012, -0.013, 0.169, 0.145, 0.166, 0.170, 0.181, 0.813
Atom 2, 0.018, -0.013, -0.011, -0.014, 0.168, 0.154, 0.176, 0.169, 0.184, 0.831
Atom 3, 0.017, -0.011, -0.013, -0.013, 0.168, 0.170, 0.147, 0.167, 0.184, 0.815
Atom 4, 0.016, -0.012, -0.013, -0.012, 0.164, 0.157, 0.151, 0.165, 0.184, 0.800
Atom 5, 0.017, -0.009, -0.008, -0.009, 0.164, 0.124, 0.144, 0.160, 0.201, 0.782
Atom 6, 0.014, -0.008, -0.005, -0.001, 0.165, 0.093, 0.113, 0.164, 0.164, 0.699
Atom 7, 0.016, -0.011, -0.010, -0.013, 0.162, 0.157, 0.150, 0.162, 0.207, 0.821
Atom 8, 0.017, -0.009, -0.009, -0.011, 0.160, 0.156, 0.129, 0.166, 0.202, 0.800
Atom 9, 0.011, -0.010, -0.004, -0.003, 0.145, 0.105, 0.088, 0.153, 0.127, 0.613
Atom 10, 0.001, -0.015, -0.010, -0.004, 0.109, 0.025, 0.034, 0.114, 0.136, 0.391
Atom 11, 0.019, -0.009, -0.009, -0.002, 0.185, 0.133, 0.147, 0.197, 0.167, 0.829
Atom 12, 0.014, -0.005, -0.014, -0.004, 0.165, 0.095, 0.107, 0.160, 0.176, 0.693
Atom 13, 0.012, 0.012, 0.042, 0.022, -0.000, 0.000, 0.000, -0.000, -0.000, 0.088
Atom 14, 0.002, 0.000, 0.000, 0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, -0.001, 0.000, 0.000, -0.001, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.016, -0.000, -0.000, 0.016, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 17, 0.020, -0.009, -0.009, -0.005, 0.174, 0.114, 0.132, 0.173, 0.235, 0.825
Atom 18, 0.019, -0.009, -0.009, -0.005, 0.175, 0.110, 0.123, 0.173, 0.233, 0.810
Atom 19, 0.021, -0.009, -0.009, -0.006, 0.174, 0.134, 0.126, 0.174, 0.244, 0.849
Atom 20, 0.019, -0.010, -0.008, -0.005, 0.172, 0.133, 0.115, 0.175, 0.233, 0.825
total spin= 12.2835204660643

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.331, 0.332, 0.339, 1.736, 1.774, 1.760, 1.736, 1.710, 9.990
Atom 2, 0.274, 0.332, 0.333, 0.340, 1.738, 1.767, 1.753, 1.738, 1.708, 9.983
Atom 3, 0.273, 0.333, 0.333, 0.340, 1.738, 1.757, 1.772, 1.739, 1.704, 9.989
Atom 4, 0.269, 0.332, 0.332, 0.339, 1.742, 1.767, 1.768, 1.741, 1.703, 9.994
Atom 5, 0.281, 0.328, 0.331, 0.336, 1.734, 1.779, 1.774, 1.743, 1.694, 10.002
Atom 6, 0.272, 0.325, 0.326, 0.335, 1.730, 1.792, 1.776, 1.733, 1.709, 9.998
Atom 7, 0.282, 0.335, 0.333, 0.339, 1.743, 1.767, 1.776, 1.742, 1.694, 10.011
Atom 8, 0.278, 0.331, 0.330, 0.337, 1.744, 1.763, 1.788, 1.735, 1.697, 10.004
Atom 9, 0.317, 0.308, 0.306, 0.216, 1.731, 1.755, 1.808, 1.720, 1.764, 9.926
Atom 10, 0.330, 0.337, 0.367, 0.363, 1.774, 1.695, 1.876, 1.775, 1.679, 10.197
Atom 11, 0.396, 0.281, 0.294, 0.151, 1.722, 1.801, 1.789, 1.708, 1.763, 9.905
Atom 12, 0.330, 0.301, 0.313, 0.203, 1.728, 1.838, 1.753, 1.721, 1.736, 9.923
Atom 13, 1.345, 1.024, 0.972, 1.110, 0.004, 0.004, 0.010, 0.005, 0.004, 4.479
Atom 14, 0.791, 0.006, 0.004, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.807
Atom 15, 0.781, 0.008, 0.004, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.797
Atom 16, 0.854, 0.003, 0.005, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.865
Atom 17, 0.447, 0.304, 0.303, 0.169, 1.727, 1.809, 1.792, 1.728, 1.692, 9.972
Atom 18, 0.447, 0.304, 0.303, 0.170, 1.727, 1.813, 1.801, 1.728, 1.695, 9.986
Atom 19, 0.445, 0.305, 0.305, 0.167, 1.727, 1.792, 1.800, 1.726, 1.684, 9.949
Atom 20, 0.446, 0.303, 0.305, 0.169, 1.728, 1.790, 1.808, 1.727, 1.693, 9.968
total charge= 166.745

BAND CENTER:

Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.267, -4.032, -4.023, -4.163, -2.208, -1.992, -1.974, -2.208, -2.367, -2.329
Atom 2, -5.277, -4.023, -4.004, -4.154, -2.208, -1.983, -2.011, -2.217, -2.385, -2.348
Atom 3, -5.277, -4.013, -4.032, -4.135, -2.208, -1.964, -1.955, -2.189, -2.385, -2.339
Atom 4, -5.267, -4.032, -4.042, -4.070, -2.180, -1.936, -1.936, -2.180, -2.348, -2.329
Atom 5, -5.342, -4.042, -3.957, -4.070, -2.180, -1.843, -1.908, -2.123, -2.311, -2.283
Atom 6, -5.174, -3.901, -3.892, -3.826, -2.086, -1.674, -1.740, -2.067, -2.273, -2.180
Atom 7, -5.548, -4.051, -4.070, -4.154, -2.189, -1.974, -1.936, -2.189, -2.357, -2.339
Atom 8, -5.398, -3.892, -3.985, -4.079, -2.161, -1.918, -1.880, -2.198, -2.301, -2.311
Atom 9, -4.949, -3.106, -3.630, -3.639, -2.133, -1.646, -1.590, -2.170, -1.861, -2.002
Atom 10, -6.605, -3.097, -3.284, -4.537, -2.264, -2.984, -1.964, -2.254, -2.891, -2.563
Atom 11, -4.425, -3.396, -3.274, -2.685, -1.955, -1.553, -1.525, -1.946, -1.646, -1.824
Atom 12, -4.594, -3.817, -3.415, -4.257, -2.123, -1.581, -1.712, -2.105, -1.946, -2.011
Atom 13, -13.108, -6.895, -6.586, -5.875, -2.816, -2.713, -2.198, -3.284, -2.479, -6.811
Atom 14, -7.036, -6.848, -6.512, -7.064, -13.529, -13.529, -13.529, -13.529, -13.529, -13.529
Atom 15, -6.914, -7.859, -13.005, -6.942, -13.529, -13.529, -13.529, -13.529, -13.529, -13.529
Atom 16, -5.623, -2.320, -2.470, -5.688, -13.529, -13.529, -13.529, -13.529, -13.529, -13.529
Atom 17, -4.257, -3.190, -3.209, -1.890, -2.021, -1.590, -1.600, -2.021, -1.740, -1.852
Atom 18, -4.275, -3.199, -3.218, -1.880, -2.021, -1.590, -1.590, -2.030, -1.731, -1.843
Atom 19, -4.266, -3.181, -3.181, -1.899, -2.039, -1.590, -1.590, -2.039, -1.749, -1.871
Atom 20, -4.257, -3.218, -3.190, -1.890, -2.030, -1.590, -1.581, -2.021, -1.749, -1.852

CH2 to CH + H transition state between fcc and hcp sites on Ni111
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.41627	0.01861	4.11989
10 Ni	1.40223	2.54891	4.11787
11 Ni	3.58273	-1.22736	4.05448
12 Ni	3.58461	1.27452	4.12977
13 C	2.10800	1.31025	5.31310
14 H	1.19430	2.71129	5.58567
15 H	2.18937	1.15412	6.39509
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1511.5234871689

Total electrons from output= 166
Spin up from output= 88.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -4.3694150262
Fermi level down from output= -4.5603668152
# of atoms= 19

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total

Atom 1, 0.017, -0.012, -0.012, -0.015, 0.164, 0.132, 0.142, 0.168, 0.168, 0.753
Atom 2, 0.017, -0.012, -0.012, -0.016, 0.163, 0.149, 0.147, 0.167, 0.170, 0.773
Atom 3, 0.017, -0.012, -0.012, -0.016, 0.168, 0.154, 0.143, 0.162, 0.170, 0.774
Atom 4, 0.016, -0.012, -0.012, -0.017, 0.160, 0.149, 0.153, 0.160, 0.184, 0.781
Atom 5, 0.015, -0.012, -0.009, -0.011, 0.161, 0.106, 0.146, 0.153, 0.202, 0.749
Atom 6, 0.015, -0.008, -0.007, -0.008, 0.163, 0.084, 0.085, 0.157, 0.128, 0.609
Atom 7, 0.013, -0.011, -0.011, -0.011, 0.158, 0.136, 0.113, 0.157, 0.193, 0.736
Atom 8, 0.015, -0.010, -0.011, -0.011, 0.153, 0.143, 0.108, 0.160, 0.200, 0.745
Atom 9, 0.005, -0.008, -0.005, -0.007, 0.101, 0.079, 0.064, 0.091, 0.053, 0.372
Atom 10, -0.003, -0.010, -0.010, -0.005, 0.076, 0.023, 0.020, 0.082, 0.099, 0.274
Atom 11, 0.022, -0.003, -0.003, 0.002, 0.159, 0.132, 0.137, 0.161, 0.172, 0.779
Atom 12, 0.005, -0.004, -0.009, -0.006, 0.104, 0.069, 0.073, 0.088, 0.053, 0.373
Atom 13, 0.011, 0.013, 0.022, 0.009, -0.000, 0.000, 0.000, -0.000, -0.000, 0.055
Atom 14, 0.019, -0.000, -0.000, 0.019, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 16, 0.013, -0.013, -0.013, -0.011, 0.168, 0.107, 0.122, 0.167, 0.220, 0.761
Atom 17, 0.011, -0.012, -0.013, -0.013, 0.168, 0.108, 0.117, 0.167, 0.212, 0.746
Atom 18, 0.021, -0.014, -0.013, -0.009, 0.170, 0.130, 0.130, 0.170, 0.235, 0.820
Atom 19, 0.013, -0.014, -0.011, -0.011, 0.166, 0.124, 0.106, 0.169, 0.220, 0.761
total spin= 10.8603698568061

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.270, 0.332, 0.331, 0.337, 1.741, 1.780, 1.768, 1.738, 1.713, 10.010
Atom 2, 0.272, 0.333, 0.333, 0.337, 1.742, 1.769, 1.768, 1.740, 1.712, 10.007
Atom 3, 0.272, 0.333, 0.334, 0.337, 1.738, 1.761, 1.775, 1.744, 1.712, 10.006
Atom 4, 0.270, 0.333, 0.332, 0.335, 1.747, 1.772, 1.769, 1.746, 1.705, 10.009
Atom 5, 0.283, 0.323, 0.332, 0.332, 1.732, 1.785, 1.777, 1.746, 1.694, 10.004
Atom 6, 0.265, 0.318, 0.323, 0.318, 1.729, 1.797, 1.804, 1.733, 1.732, 10.018
Atom 7, 0.285, 0.330, 0.329, 0.332, 1.741, 1.776, 1.785, 1.738, 1.699, 10.014
Atom 8, 0.284, 0.327, 0.328, 0.332, 1.745, 1.774, 1.788, 1.734, 1.695, 10.006
Atom 9, 0.324, 0.303, 0.297, 0.215, 1.755, 1.690, 1.797, 1.753, 1.796, 9.931
Atom 10, 0.334, 0.356, 0.353, 0.364, 1.790, 1.750, 1.823, 1.786, 1.678, 10.233
Atom 11, 0.401, 0.272, 0.286, 0.149, 1.740, 1.796, 1.799, 1.734, 1.751, 9.928
Atom 12, 0.325, 0.298, 0.303, 0.215, 1.749, 1.826, 1.663, 1.757, 1.798, 9.933
Atom 13, 1.431, 0.933, 0.897, 1.066, 0.006, 0.005, 0.004, 0.004, 0.012, 4.358
Atom 14, 0.854, 0.004, 0.004, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.867
Atom 15, 0.814, 0.003, 0.003, 0.010, 0.000, 0.000, 0.000, 0.000, 0.000, 0.830
Atom 16, 0.442, 0.301, 0.301, 0.168, 1.726, 1.811, 1.797, 1.728, 1.703, 9.977
Atom 17, 0.441, 0.301, 0.301, 0.167, 1.726, 1.812, 1.803, 1.727, 1.709, 9.987
Atom 18, 0.445, 0.301, 0.301, 0.168, 1.727, 1.793, 1.793, 1.726, 1.693, 9.948
Atom 19, 0.442, 0.300, 0.302, 0.168, 1.728, 1.795, 1.813, 1.726, 1.703, 9.978
total charge= 166.044

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.232, -3.955, -3.964, -4.158, -2.142, -1.931, -1.931, -2.151, -2.301, -2.274
Atom 2, -5.232, -3.973, -3.973, -4.123, -2.151, -1.949, -1.940, -2.151, -2.336, -2.292
Atom 3, -5.232, -3.964, -3.955, -4.123, -2.160, -1.949, -1.949, -2.142, -2.336, -2.292
Atom 4, -5.223, -3.964, -3.973, -4.017, -2.134, -1.922, -1.922, -2.134, -2.301, -2.274
Atom 5, -5.293, -3.964, -3.859, -3.982, -2.134, -1.808, -1.817, -2.081, -2.257, -2.230
Atom 6, -5.117, -3.938, -3.859, -3.718, -1.975, -1.544, -1.509, -1.958, -2.125, -2.046
Atom 7, -5.320, -4.017, -4.008, -4.087, -2.098, -1.817, -1.773, -2.107, -2.248, -2.230
Atom 8, -5.302, -3.885, -3.911, -3.991, -2.081, -1.834, -1.790, -2.125, -2.257, -2.222
Atom 9, -4.721, -3.287, -3.383, -3.155, -2.081, -1.922, -1.641, -2.151, -1.905, -2.063
Atom 10, -6.297, -3.383, -3.304, -4.043, -2.257, -2.811, -2.301, -2.283, -3.146, -2.697

Atom 11, -4.528, -3.295, -3.181, -2.697, -1.808, -1.430, -1.350, -1.808, -1.579, -1.702
Atom 12, -4.730, -3.436, -3.331, -3.163, -2.142, -1.500, -2.204, -2.107, -1.887, -2.063
Atom 13, -12.264, -3.982, -4.202, -6.789, -2.371, -3.093, -3.251, -2.002, -2.715, -6.376
Atom 14, -5.716, -3.111, -3.181, -5.760, -12.695, -12.695, -12.695, -12.695, -12.695, -12.695
Atom 15, -6.939, -3.445, -3.647, -6.957, -12.695, -12.695, -12.695, -12.695, -12.695, -12.695
Atom 16, -4.228, -3.216, -3.216, -1.861, -1.984, -1.535, -1.544, -1.984, -1.685, -1.799
Atom 17, -4.272, -3.216, -3.207, -1.861, -1.984, -1.544, -1.553, -1.984, -1.667, -1.790
Atom 18, -4.237, -3.225, -3.216, -1.843, -1.993, -1.553, -1.553, -1.993, -1.694, -1.834
Atom 19, -4.228, -3.243, -3.207, -1.861, -1.984, -1.544, -1.544, -1.975, -1.685, -1.799

CH to C + H transition state between two hcp sites on Ni111
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	2.03458
2 Ni	0.00000	2.49184	2.03458
3 Ni	2.15800	-1.24592	2.03458
4 Ni	2.15800	1.24592	2.03458
5 Ni	0.71933	1.24592	0.00000
6 Ni	0.71933	3.73777	0.00000
7 Ni	2.87733	0.00000	0.00000
8 Ni	2.87733	2.49184	0.00000
9 Ni	1.42459	-0.05872	4.10259
10 Ni	1.42388	2.53015	4.10131
11 Ni	3.61096	-1.26766	4.07491
12 Ni	3.59785	1.22525	4.14546
13 C	2.11234	1.24960	5.16898
14 H	0.65014	0.75672	5.28280
15 Ni	1.43867	0.00000	-2.03458
16 Ni	1.43867	2.49184	-2.03458
17 Ni	3.59667	-1.24592	-2.03458
18 Ni	3.59667	1.24592	-2.03458

FINAL RELAXED ENERGY (Rydberg) = -1510.2693185479

Total electrons from output= 165
Spin up from output= 87.5000000000
Spin down from output= 77.5000000000
Fermi level up from output= -5.1390588988
Fermi level down from output= -5.2597251914
# of atoms= 18

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.014, -0.012, -0.011, -0.009, 0.155, 0.122, 0.106, 0.152, 0.187, 0.705
Atom 2, 0.013, -0.011, -0.010, -0.009, 0.151, 0.120, 0.113, 0.151, 0.172, 0.689
Atom 3, 0.013, -0.010, -0.012, -0.007, 0.145, 0.107, 0.101, 0.151, 0.164, 0.652
Atom 4, 0.016, -0.011, -0.010, -0.004, 0.165, 0.113, 0.111, 0.163, 0.202, 0.743
Atom 5, 0.017, -0.012, -0.013, -0.016, 0.160, 0.136, 0.146, 0.163, 0.170, 0.751
Atom 6, 0.016, -0.012, -0.012, -0.016, 0.159, 0.155, 0.155, 0.158, 0.163, 0.767
Atom 7, 0.017, -0.013, -0.012, -0.017, 0.163, 0.143, 0.139, 0.160, 0.168, 0.749
Atom 8, 0.017, -0.013, -0.012, -0.016, 0.163, 0.137, 0.139, 0.161, 0.167, 0.744
Atom 9, 0.002, -0.008, -0.005, -0.007, 0.037, 0.031, 0.031, 0.026, 0.023, 0.129
Atom 10, 0.001, -0.010, -0.005, -0.009, 0.057, 0.034, 0.039, 0.033, 0.033, 0.173
Atom 11, 0.016, 0.001, -0.003, -0.001, 0.118, 0.116, 0.097, 0.096, 0.078, 0.518
Atom 12, 0.001, -0.002, -0.010, -0.007, 0.033, 0.035, 0.055, 0.058, 0.038, 0.203
Atom 13, 0.016, 0.005, -0.008, 0.021, -0.000, -0.000, -0.000, -0.000, -0.000, 0.034

Atom 14, 0.006, -0.000, -0.000, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 15, 0.013, -0.014, -0.013, -0.013, 0.166, 0.114, 0.113, 0.166, 0.217, 0.751
Atom 16, 0.014, -0.014, -0.013, -0.012, 0.166, 0.112, 0.114, 0.166, 0.222, 0.756
Atom 17, 0.015, -0.014, -0.014, -0.012, 0.167, 0.119, 0.118, 0.166, 0.222, 0.768
Atom 18, 0.015, -0.014, -0.013, -0.012, 0.167, 0.116, 0.112, 0.166, 0.223, 0.761
total spin= 9.8935497628018

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.281, 0.327, 0.329, 0.332, 1.741, 1.778, 1.796, 1.743, 1.701, 10.028
Atom 2, 0.279, 0.327, 0.330, 0.331, 1.743, 1.781, 1.789, 1.742, 1.709, 10.031
Atom 3, 0.267, 0.328, 0.327, 0.332, 1.744, 1.794, 1.781, 1.742, 1.714, 10.029
Atom 4, 0.277, 0.322, 0.323, 0.307, 1.730, 1.796, 1.800, 1.734, 1.690, 9.979
Atom 5, 0.271, 0.333, 0.332, 0.336, 1.745, 1.779, 1.768, 1.742, 1.715, 10.019
Atom 6, 0.272, 0.332, 0.332, 0.338, 1.746, 1.762, 1.760, 1.747, 1.721, 10.010
Atom 7, 0.271, 0.332, 0.333, 0.336, 1.742, 1.770, 1.775, 1.744, 1.715, 10.017
Atom 8, 0.271, 0.332, 0.333, 0.336, 1.742, 1.773, 1.775, 1.743, 1.715, 10.019
Atom 9, 0.353, 0.362, 0.372, 0.269, 1.772, 1.752, 1.780, 1.784, 1.784, 10.228
Atom 10, 0.310, 0.319, 0.321, 0.225, 1.765, 1.726, 1.818, 1.775, 1.754, 10.013
Atom 11, 0.387, 0.297, 0.298, 0.179, 1.745, 1.798, 1.795, 1.771, 1.813, 10.081
Atom 12, 0.324, 0.352, 0.296, 0.220, 1.782, 1.858, 1.696, 1.734, 1.766, 10.027
Atom 13, 1.618, 0.825, 0.802, 0.810, 0.007, 0.007, 0.007, 0.007, 0.007, 4.092
Atom 14, 0.714, 0.007, 0.004, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.730
Atom 15, 0.443, 0.300, 0.302, 0.169, 1.728, 1.806, 1.805, 1.728, 1.703, 9.984
Atom 16, 0.443, 0.300, 0.302, 0.169, 1.729, 1.807, 1.804, 1.729, 1.701, 9.985
Atom 17, 0.443, 0.300, 0.301, 0.169, 1.729, 1.802, 1.804, 1.728, 1.703, 9.979
Atom 18, 0.443, 0.301, 0.301, 0.169, 1.728, 1.803, 1.807, 1.728, 1.699, 9.978
total charge= 165.229

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.231, -3.953, -3.867, -3.945, -2.054, -1.744, -1.744, -2.037, -2.218, -2.167
Atom 2, -5.283, -3.979, -3.902, -3.945, -2.037, -1.744, -1.735, -2.029, -2.210, -2.158
Atom 3, -5.378, -3.807, -3.945, -3.876, -2.029, -1.709, -1.744, -2.020, -2.193, -2.149
Atom 4, -5.265, -3.824, -3.798, -3.971, -1.977, -1.640, -1.632, -1.977, -2.141, -2.106
Atom 5, -5.240, -3.902, -3.902, -4.040, -2.115, -1.899, -1.916, -2.115, -2.296, -2.244
Atom 6, -5.231, -3.953, -3.953, -4.057, -2.106, -1.916, -1.925, -2.089, -2.270, -2.244
Atom 7, -5.214, -3.919, -3.919, -4.066, -2.115, -1.916, -1.882, -2.115, -2.288, -2.244
Atom 8, -5.240, -3.919, -3.910, -4.057, -2.115, -1.890, -1.882, -2.115, -2.296, -2.244
Atom 9, -5.334, -3.824, -3.764, -4.212, -2.339, -2.236, -2.201, -2.443, -2.408, -2.460
Atom 10, -4.842, -3.461, -3.418, -3.341, -2.167, -2.244, -1.692, -2.227, -2.253, -2.218
Atom 11, -4.739, -3.513, -3.410, -3.289, -1.735, -1.243, -1.312, -1.701, -1.381, -1.632
Atom 12, -4.851, -4.359, -4.350, -3.608, -2.072, -1.433, -2.201, -2.305, -2.072, -2.149
Atom 13, -11.989, -6.198, -4.644, -3.720, -2.288, -4.040, -2.978, -2.374, -4.299, -5.032
Atom 14, -6.612, -4.333, -4.575, -6.646, -12.499, -12.499, -12.499, -12.499, -12.499, -12.499
Atom 15, -4.212, -3.194, -3.177, -1.796, -1.942, -1.511, -1.519, -1.942, -1.640, -1.761
Atom 16, -4.221, -3.211, -3.177, -1.787, -1.942, -1.511, -1.519, -1.942, -1.649, -1.761
Atom 17, -4.204, -3.228, -3.211, -1.796, -1.942, -1.511, -1.502, -1.942, -1.649, -1.761
Atom 18, -4.221, -3.185, -3.185, -1.796, -1.951, -1.519, -1.511, -1.942, -1.649, -1.770

3. Relaxed geometries and energies for reference species

Atomic hydrogen gas (doublet)
1 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 H 2.24945 1.32402 0.30526

FINAL RELAXED ENERGY (Rydberg) = -0.9991775296

Atomic carbon gas (triplet)
1 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 C 2.24945 1.32402 0.30526

FINAL RELAXED ENERGY (Rydberg) = -10.8232305385

Methylidyne Gas (doublet)
2 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 C 2.24945 1.32402 0.30526
2 H 1.17166 1.67523 0.38448

FINAL RELAXED ENERGY (Rydberg) = -12.0875884948

Methylene gas (triplet)
3 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 C 2.16031 1.22018 1.25018
2 H 2.11215 1.83620 0.35843
3 H 1.96071 1.39765 2.30161

FINAL RELAXED ENERGY (Rydberg) = -13.4537857543

Methyl gas (doublet)
4 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 C -2.13131 3.76054 1.48021
2 H -2.59020 4.63214 1.93944
3 H -1.64098 3.01353 2.09818
4 H -2.12938 3.65395 0.39924

FINAL RELAXED ENERGY (Rydberg) = -14.8149116835

Diatomic hydrogen gas (singlet)
2 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 H 2.24906 1.24594 5.13305
2 H 2.24902 1.24595 4.38251

FINAL RELAXED ENERGY (Rydberg) = -2.3311760070

Graphite (singlet)
16 4.92800 4.92800 6.71100 90.00000 90.00000 90.00000

1 C 0.00000 0.00000 0.00000
2 C 0.00000 2.46400 0.00000
3 C 1.42259 0.00000 0.00000
4 C 1.42259 2.46400 0.00000
5 C 2.13389 -1.23200 0.00000
6 C 2.13389 1.23200 0.00000
7 C 3.55648 -1.23200 0.00000
8 C 3.55648 1.23200 0.00000

 9 C 0.00000 0.00000 3.35550
10 C 0.00000 2.46400 3.35550
11 C 0.71130 1.23200 3.35550
12 C 0.71130 3.69600 3.35550
13 C 2.13389 -1.23200 3.35550
14 C 2.13389 1.23200 3.35550
15 C 2.84518 0.00000 3.35550
16 C 2.84518 2.46400 3.35550

FINAL RELAXED ENERGY (Rydberg) = -182.3852989615

Methane gas (singlet)
5 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 C 2.24532 1.15017 2.13400
 2 H 2.53005 2.14222 2.50061
 3 H 1.24151 0.90280 2.49678
 4 H 2.96000 0.40462 2.49968
 5 H 2.24600 1.15087 1.03881

FINAL RELAXED ENERGY (Rydberg) = -16.1600067313

Bulk fcc nickel (nine unpaired electrons)
12 4.98369 4.98369 6.10375 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43867 0.00000 -2.03458
10 Ni 1.43867 2.49184 -2.03458
11 Ni 3.59667 -1.24592 -2.03458
12 Ni 3.59667 1.24592 -2.03458

FINAL RELAXED ENERGY (Rydberg) = -1123.6710850447

4. NudgedElastic Band Pathways

NEB Pathways: Note that full pathways are included for pathways where carbon is bonded at an fcc site, but only transition states and endpoints where found for cases where carbon is bonded at an hcp site.

CH3_CH2-H fcc, fcc Pathway
INITIAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458

 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44291 0.00080 4.09402
10 Ni 1.44279 2.49067 4.09422
11 Ni 3.60006 -1.24607 4.01003
12 Ni 3.59971 1.24581 4.09355
13 C 2.16958 1.24569 5.72089
14 H 1.65613 0.35422 6.14245
15 H 3.19959 1.24526 6.14032
16 H 1.65637 2.13688 6.14341
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7625335663

IMAGE 1
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43544 -0.07110 4.07020
10 Ni 1.43817 2.42138 4.10629
11 Ni 3.59781 -1.29819 4.00771
12 Ni 3.59173 1.20013 4.09232
13 C 2.13093 1.01074 5.71966
14 H 1.78046 -0.02349 5.99141
15 H 3.15337 1.08643 6.14245
16 H 1.48624 1.72800 6.25749
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7572624709

IMAGE 2
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43259 -0.05996 4.02435
10 Ni 1.46039 2.44102 4.12386
11 Ni 3.61179 -1.26669 4.00576
12 Ni 3.61372 1.23806 4.06469
13 C 2.09806 0.95402 5.60371

14 H 1.87004 -0.23116 5.64923
15 H 3.11715 1.00123 6.04724
16 H 1.40782 1.45361 6.30100
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7394148392

IMAGE 3
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.43534 -0.04601 4.05556
10 Ni 1.46432 2.45827 4.13552
11 Ni 3.60999 -1.25545 4.01378
12 Ni 3.62044 1.25296 4.06359
13 C 2.09473 1.00038 5.56698
14 H 1.86651 -0.34893 5.56040
15 H 3.10388 0.99027 6.03695
16 H 1.40157 1.42958 6.30879
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7215769467

IMAGE 4
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.44262 -0.03195 4.09013
10 Ni 1.46766 2.47171 4.14214
11 Ni 3.60808 -1.25029 4.01981
12 Ni 3.62458 1.25833 4.06484
13 C 2.09957 1.07041 5.54099
14 H 1.85598 -0.47176 5.50911
15 H 3.09842 0.99330 6.03102
16 H 1.40078 1.43020 6.31308
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458

20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7074419482

IMAGE 5 (TRANSITION STATE)
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.45672 0.01039 4.14515
10 Ni 1.45624 2.48272 4.14470
11 Ni 3.60570 -1.24539 4.04171
12 Ni 3.63109 1.24637 4.06900
13 C 2.09288 1.24743 5.48530
14 H 2.08165 -1.24557 5.03897
15 H 3.12857 1.25082 5.93784
16 H 1.40941 1.24487 6.34935
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7040395200

IMAGE 6
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.45398 0.00799 4.13261
 0 Ni 1.47730 2.50917 4.15977
11 Ni 3.61044 -1.23493 4.02998
12 Ni 3.63213 1.26933 4.06792
13 C 2.10941 1.18371 5.50978
14 H 1.83666 -0.72933 5.40021
15 H 3.09615 1.01602 6.01193
16 H 1.40290 1.43518 6.31692
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7081518371

IMAGE 7
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.45446 0.04608 4.14593
10 Ni 1.48234 2.54312 4.18003
11 Ni 3.61093 -1.21591 4.03722
12 Ni 3.63296 1.28173 4.07253
13 C 2.11033 1.24199 5.50210
14 H 1.83724 -0.99609 5.24819
15 H 3.10010 1.05536 5.99765
16 H 1.40369 1.43393 6.32554
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7241529969

FINAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44784 -0.01853 4.11820
10 Ni 1.46964 2.48535 4.14769
11 Ni 3.60730 -1.24657 4.02363
12 Ni 3.62644 1.26083 4.06759
13 C 2.10339 1.13209 5.52269
14 H 1.81513 -0.58599 5.47631
15 H 3.09302 0.99616 6.02418
16 H 1.40096 1.43765 6.31443
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7335680709

CH3_CH2-H fcc, hcp Pathway
INITIAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458

 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44291 0.00080 4.09402
10 Ni 1.44279 2.49067 4.09422
11 Ni 3.60006 -1.24607 4.01003
12 Ni 3.59971 1.24581 4.09355
13 C 2.16958 1.24569 5.72089
14 H 1.65613 0.35422 6.14245
15 H 3.19959 1.24526 6.14032
16 H 1.65637 2.13688 6.14341
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7625335663

IMAGE 1
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.45038 0.02400 4.11985
10 Ni 1.42172 2.52866 4.02803
11 Ni 3.59803 -1.23912 4.00433
12 Ni 3.58973 1.24972 4.08811
13 C 2.03059 1.45039 5.66681
14 H 1.42538 0.76417 6.28329
15 H 3.03730 1.53944 6.12373
16 H 1.54691 2.48261 5.80641
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7531301384

IMAGE 2
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.46844 -0.01699 4.11094
10 Ni 1.43815 2.49786 4.09571
11 Ni 3.61357 -1.26953 4.01100

12 Ni 3.61472 1.21258 4.08580
13 C 2.04491 1.37762 5.56026
14 H 1.41914 0.81259 6.27158
15 H 3.03274 1.52680 6.05820
16 H 1.38920 2.73030 5.62738
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7139030774

IMAGE 3
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73776 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.46955 -0.03257 4.11462
10 Ni 1.44483 2.48062 4.12892
11 Ni 3.61126 -1.27114 4.01263
12 Ni 3.61913 1.20513 4.09255
13 C 2.07967 1.30461 5.52439
14 H 1.41670 0.82514 6.26422
15 H 3.02092 1.55046 6.06646
16 H 1.32652 2.85662 5.58020
17 Ni 1.43866 0.00000 -2.03458
18 Ni 1.43866 2.49184 -2.03458
19 Ni 3.59666 -1.24592 -2.03458
20 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7043844929

IMAGE 4 (TRANSITION STATE)
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.46011 -0.01338 4.13031
10 Ni 1.43560 2.50028 4.13255
11 Ni 3.60206 -1.25374 4.01454
12 Ni 3.60861 1.22265 4.08574
13 C 2.08423 1.33289 5.52096
14 H 1.38376 0.90633 6.25967
15 H 3.01789 1.56662 6.07990
16 H 1.48440 3.02828 5.53723
17 Ni 1.43867 0.00000 -2.03458

18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7040166043

IMAGE 5
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73776 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.47332 -0.05030 4.11918
10 Ni 1.45241 2.46196 4.15196
11 Ni 3.61434 -1.27908 4.01548
12 Ni 3.62739 1.19577 4.09778
13 C 2.10464 1.25226 5.50641
14 H 1.42516 0.82419 6.26210
15 H 3.02987 1.53791 6.05949
16 H 1.26136 2.99003 5.53251
17 Ni 1.43866 0.00000 -2.03458
18 Ni 1.43866 2.49184 -2.03458
19 Ni 3.59666 -1.24592 -2.03458
20 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7043956896

IMAGE 6
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73776 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.48012 -0.07291 4.13139
10 Ni 1.46406 2.43754 4.16227
11 Ni 3.62074 -1.29025 4.01761
12 Ni 3.63776 1.18276 4.10580
13 C 2.12281 1.21602 5.49947
14 H 1.43236 0.82452 6.26564
15 H 3.04102 1.52432 6.05522
16 H 1.19517 3.12322 5.46365
17 Ni 1.43866 0.00000 -2.03458
18 Ni 1.43866 2.49184 -2.03458
19 Ni 3.59666 -1.24592 -2.03458
20 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7090050251

IMAGE 7

20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000
 5 Ni   0.71933 1.24592 2.03458
 6 Ni   0.71933 3.73777 2.03458
 7 Ni   2.87733 0.00000 2.03458
 8 Ni   2.87733 2.49184 2.03458
 9 Ni   1.48912 -0.09720 4.14050
 0 Ni   1.47782 2.41328 4.17683
11 Ni   3.63068 -1.30482 4.02112
12 Ni   3.65447 1.16663 4.11327
13 C   2.14111 1.17548 5.49852
14 H   1.45533 0.81944 6.28424
15 H   3.07413 1.47513 6.03656
16 H   1.12383 3.24430 5.39438
17 Ni   1.43867 0.00000 -2.03458
18 Ni   1.43867 2.49184 -2.03458
19 Ni   3.59667 -1.24592 -2.03458
20 Ni   3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7153078072

IMAGE 8
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000
 5 Ni   0.71933 1.24592 2.03458
 6 Ni   0.71933 3.73777 2.03458
 7 Ni   2.87733 0.00000 2.03458
 8 Ni   2.87733 2.49184 2.03458
 9 Ni   1.50476 -0.10745 4.15841
10 Ni   1.49562 2.38934 4.16062
11 Ni   3.64196 -1.32234 4.02149
12 Ni   3.66906 1.15035 4.13402
13 C   2.14554 1.17220 5.51005
14 H   1.44900 0.85366 6.30075
15 H   3.09320 1.44061 6.04118
16 H   0.99794 3.49451 5.19146
17 Ni   1.43867 0.00000 -2.03458
18 Ni   1.43867 2.49184 -2.03458
19 Ni   3.59667 -1.24592 -2.03458
20 Ni   3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1512.7297419044

FINAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000

 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.47984 0.00242 4.13478
10 Ni 1.47952 2.48998 4.13466
11 Ni 3.61759 -1.24565 4.01951
12 Ni 3.63370 1.24611 4.12740
13 C 2.07041 1.24679 5.50411
14 H 1.35783 1.24406 6.34129
15 H 3.08429 1.25012 5.99222
16 H 0.81878 3.73766 5.04484
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7363863174

CH3_CH2-H hcp, fcc Pathway
INITIAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.44465 0.00654 4.09953
10 Ni 1.44456 2.48526 4.09977
11 Ni 3.59882 -1.24592 4.00688
12 Ni 3.59194 1.24594 4.09905
13 C 2.16546 1.24566 5.73032
14 H 1.65173 0.35427 6.15117
15 H 3.19602 1.24555 6.14815
16 H 1.65202 2.13714 6.15153
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7612933603

TRANSITION STATE
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.45261 0.00236 4.14025

10 Ni 1.42457 2.51268 4.13502
11 Ni 3.59368 -1.24352 4.00781
12 Ni 3.59280 1.23478 4.09281
13 C 2.07609 1.35029 5.52734
14 H 1.37826 0.92561 6.26934
15 H 3.01359 1.58525 6.08108
16 H 1.48013 3.04780 5.53694
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7019221788

FINAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 2.03458
2 Ni 0.00000 2.49184 2.03458
3 Ni 2.15800 -1.24592 2.03458
4 Ni 2.15800 1.24592 2.03458
5 Ni 0.71933 1.24592 0.00000
6 Ni 0.71933 3.73777 0.00000
7 Ni 2.87733 0.00000 0.00000
8 Ni 2.87733 2.49184 0.00000
9 Ni 1.46218 -0.00009 4.14173
10 Ni 1.46192 2.49239 4.14174
11 Ni 3.60341 -1.24574 4.01421
12 Ni 3.60281 1.24605 4.13317
13 C 2.03779 1.24649 5.51558
14 H 1.31581 1.24454 6.34525
15 H 3.04657 1.24859 6.01178
16 H 0.78732 3.73777 5.05010
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7332797227

CH3_CH2-H hcp, hcp Pathway
INITIAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 2.03458
Ni 0.00000 2.49184 2.03458
Ni 2.15800 -1.24592 2.03458
Ni 2.15800 1.24592 2.03458
Ni 0.71933 1.24592 0.00000
Ni 0.71933 3.73777 0.00000
Ni 2.87733 0.00000 0.00000
Ni 2.87733 2.49184 0.00000
Ni 1.44465 0.00654 4.09953
Ni 1.44456 2.48526 4.09977
Ni 3.59882 -1.24592 4.00688
Ni 3.59194 1.24594 4.09905
C 2.16546 1.24566 5.73032
H 1.65173 0.35427 6.15117

H 3.19602 1.24555 6.14815
H 1.65202 2.13714 6.15153
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 -1.24592 -2.03458
Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7019056239

TRANSITION STATE
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 2.03458
Ni 0.00000 2.49184 2.03458
Ni 2.15800 -1.24592 2.03458
Ni 2.15800 1.24592 2.03458
Ni 0.71933 1.24592 0.00000
Ni 0.71933 3.73777 0.00000
Ni 2.87733 0.00000 0.00000
Ni 2.87733 2.49184 0.00000
Ni 1.43460 -0.01996 4.13030
Ni 1.46292 2.48561 4.15309
Ni 3.60096 -1.24854 4.01160
Ni 3.60643 1.25728 4.08252
C 2.09682 1.13152 5.52923
H 1.66341 -0.59239 5.50713
H 3.06345 0.93900 6.05332
H 1.39698 1.49396 6.30026
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 -1.24592 -2.03458
Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) =

FINAL ENDPOINT
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 2.03458
Ni 0.00000 2.49184 2.03458
Ni 2.15800 -1.24592 2.03458
Ni 2.15800 1.24592 2.03458
Ni 0.71933 1.24592 0.00000
Ni 0.71933 3.73777 0.00000
Ni 2.87733 0.00000 0.00000
Ni 2.87733 2.49184 0.00000
Ni 1.44322 0.00750 4.15767
Ni 1.44286 2.48558 4.15750
Ni 3.59504 -1.24549 4.03610
Ni 3.61201 1.24627 4.07443
C 2.09145 1.24715 5.49182
H 2.07080 -1.24555 5.04924
H 3.13094 1.24990 5.93942
H 1.41550 1.24467 6.36157
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 -1.24592 -2.03458
Ni 3.59667 1.24592 -2.03458

GEOMETRY RELAXED ENERGY (Rydbergs) =
CH2_CH-H fcc, fcc Pathway
INITIAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.46811	-0.00945	4.11644
10 Ni	1.46808	2.50157	4.11642
11 Ni	3.61165	-1.24579	4.03476
12 Ni	3.64450	1.24607	4.08550
13 C	2.13363	1.24613	5.42999
14 H	3.18264	1.24607	5.88175
15 H	1.46435	1.24614	6.30358
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5497755462

IMAGE 1
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.41663	0.01306	4.12071
10 Ni	1.41544	2.54319	4.08520
11 Ni	3.58083	-1.23000	4.03490
12 Ni	3.57706	1.28695	4.10774
13 C	2.12221	1.22963	5.42811
14 H	2.68710	0.83429	6.28594
15 H	1.39437	1.97782	5.88135
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1511.5484868871

IMAGE 2
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000

 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.38694 0.01365 4.10968
10 Ni 1.37034 2.57305 4.05915
11 Ni 3.55114 -1.22334 4.04205
12 Ni 3.52167 1.29487 4.13455
13 C 2.00387 1.28808 5.39635
14 H 2.37513 1.01100 6.39105
15 H 1.13127 2.03199 5.67028
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5430669978

IMAGE 3
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.40381 0.00485 4.09970
10 Ni 1.38611 2.58287 4.04507
11 Ni 3.56867 -1.22405 4.04961
12 Ni 3.52723 1.29316 4.14217
13 C 1.97357 1.30755 5.36922
14 H 2.26100 1.09927 6.40591
15 H 0.99199 2.00284 5.55041
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5365723525

IMAGE 4
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42298 -0.00475 4.09832
10 Ni 1.40634 2.57117 4.06762
11 Ni 3.58872 -1.22488 4.06924

12 Ni 3.55445 1.28468 4.14135
13 C 2.00554 1.30482 5.33801
14 H 2.19207 1.14489 6.40563
15 H 0.84799 2.03234 5.45004
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5266792132

IMAGE 5 (TRANSITION STATE)
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.43066 -0.01031 4.09868
10 Ni 1.41860 2.54579 4.10253
11 Ni 3.59896 -1.22448 4.08601
12 Ni 3.57994 1.27763 4.13433
13 C 2.08267 1.27247 5.31260
14 H 2.17274 1.15026 6.39823
15 H 0.72149 2.10218 5.40255
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5216755012

IMAGE 6
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.43937 -0.01342 4.10083
10 Ni 1.43759 2.52562 4.12605
11 Ni 3.61047 -1.22423 4.09918
12 Ni 3.60248 1.26974 4.13484
13 C 2.13554 1.24921 5.30153
14 H 2.16410 1.15568 6.39381
15 H 0.58969 2.16610 5.35171
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1511.5261352410

IMAGE 7
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.45842	-0.02418	4.10195
10 Ni	1.48314	2.49141	4.14419
11 Ni	3.63000	-1.24215	4.10746
12 Ni	3.65043	1.23737	4.15591
13 C	2.19313	1.21297	5.29503
14 H	2.15685	1.15167	6.38990
15 H	0.33905	2.33756	5.21236
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1511.5452759402

FINAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.43501	-0.01304	4.09822
10 Ni	1.45967	2.50775	4.14423
11 Ni	3.60944	-1.23002	4.09129
12 Ni	3.60839	1.26844	4.14081
13 C	2.15381	1.22280	5.29088
14 H	2.12463	1.15724	6.38584
15 H	0.09917	2.65689	5.07567
16 Ni	1.43867	0.00000	-2.03458
17 Ni	1.43867	2.49184	-2.03458
18 Ni	3.59667	-1.24592	-2.03458
19 Ni	3.59667	1.24592	-2.03458

GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5588069285

CH2_CH-H fcc, hcp Pathway
INITIAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000

 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.41278 0.02812 4.11874
10 Ni 1.41043 2.54196 4.08413
11 Ni 3.58588 -1.22681 4.03522
12 Ni 3.58569 1.28318 4.11766
13 C 2.16215 1.23926 5.42994
14 H 1.63038 2.14865 5.87447
15 H 2.49946 0.67340 6.31122
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5498153189

IMAGE 1
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.40311 0.04550 4.12216
10 Ni 1.39415 2.56683 4.07519
11 Ni 3.57377 -1.21196 4.03675
12 Ni 3.56867 1.30122 4.11924
13 C 2.12609 1.28636 5.41812
14 H 1.54964 2.20008 5.82428
15 H 2.46789 0.78698 6.33513
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5495837663

IMAGE 2
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.40925 0.04547 4.12913
10 Ni 1.38169 2.58492 4.05700

11 Ni 3.57460 -1.21708 4.04912
12 Ni 3.55777 1.29511 4.14080
13 C 2.04175 1.39452 5.35642
14 H 1.27717 2.49591 5.60954
15 H 2.20413 1.14256 6.40993
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5328059561

IMAGE 3
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73776 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.41559 0.02686 4.12191
10 Ni 1.39537 2.56107 4.09698
11 Ni 3.58082 -1.22472 4.05274
12 Ni 3.57583 1.28138 4.13431
13 C 2.08478 1.34014 5.32546
14 H 1.19790 2.61831 5.58890
15 H 2.19121 1.15407 6.40013
16 Ni 1.43866 0.00000 -2.03458
17 Ni 1.43866 2.49184 -2.03458
18 Ni 3.59666 -1.24592 -2.03458
19 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5242869850

IMAGE 4 (TRANSITION STATE)
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.41627 0.01861 4.11989
10 Ni 1.40223 2.54891 4.11787
11 Ni 3.58273 -1.22736 4.05448
12 Ni 3.58461 1.27452 4.12977
13 C 2.10800 1.31025 5.31310
14 H 1.19430 2.71129 5.58567
15 H 2.18937 1.15412 6.39509
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458

19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5234871689

IMAGE 5
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73776 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42065 0.01034 4.11897
10 Ni 1.41036 2.53719 4.12856
11 Ni 3.58627 -1.23133 4.05597
12 Ni 3.59382 1.26877 4.13285
13 C 2.12254 1.28961 5.30698
14 H 1.10999 2.74206 5.56802
15 H 2.18709 1.15867 6.39349
16 Ni 1.43866 0.00000 -2.03458
17 Ni 1.43866 2.49184 -2.03458
18 Ni 3.59666 -1.24592 -2.03458
19 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5244617670

IMAGE 6
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73776 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42889 -0.00591 4.12080
10 Ni 1.42868 2.51369 4.14235
11 Ni 3.59444 -1.24083 4.05757
12 Ni 3.61362 1.25366 4.14098
13 C 2.14737 1.25753 5.29931
14 H 1.00155 2.86473 5.51970
15 H 2.18184 1.16584 6.39138
16 Ni 1.43866 0.00000 -2.03458
17 Ni 1.43866 2.49184 -2.03458
18 Ni 3.59666 -1.24592 -2.03458
19 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5302264914

IMAGE 7
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000

 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43953 -0.01924 4.12564
10 Ni 1.45092 2.49084 4.14369
11 Ni 3.60455 -1.25211 4.05769
12 Ni 3.63699 1.23630 4.15970
13 C 2.16789 1.23344 5.30033
14 H 0.89028 2.97738 5.44704
15 H 2.17380 1.17964 6.39525
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5386777691

IMAGE 8
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.45880 -0.04839 4.14286
10 Ni 1.47925 2.45572 4.13871
11 Ni 3.62297 -1.27825 4.05374
12 Ni 3.66056 1.20631 4.18518
13 C 2.18603 1.20929 5.31161
14 H 0.68895 3.21969 5.27208
15 H 2.16463 1.18298 6.40767
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1511.5581031913

FINAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44462 -0.00416 4.14850
10 Ni 1.44435 2.49596 4.14861

11 Ni 3.60387 -1.24603 4.04678
12 Ni 3.61329 1.24596 4.14507
13 C 2.17299 1.24584 5.31838
14 H 0.72938 3.73803 5.09777
15 H 2.17829 1.24579 6.41556
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5703939857

CH2_CH-H hcp, fcc Pathway
INITIAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 2.03458
2 Ni 0.00000 2.49184 2.03458
3 Ni 2.15800 -1.24592 2.03458
4 Ni 2.15800 1.24592 2.03458
5 Ni 0.71933 1.24592 0.00000
6 Ni 0.71933 3.73777 0.00000
7 Ni 2.87733 0.00000 0.00000
8 Ni 2.87733 2.49184 0.00000
9 Ni 1.45414 -0.01182 4.13148
10 Ni 1.45933 2.50317 4.12242
11 Ni 3.60550 -1.24589 4.02175
12 Ni 3.62885 1.25005 4.08986
13 C 2.13552 1.24108 5.43491
14 H 1.47292 1.33480 6.30857
15 H 3.18409 1.17233 5.88540
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5474444852

TRANSITION STATE
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 2.03458
2 Ni 0.00000 2.49184 2.03458
3 Ni 2.15800 -1.24592 2.03458
4 Ni 2.15800 1.24592 2.03458
5 Ni 0.71933 1.24592 0.00000
6 Ni 0.71933 3.73777 0.00000
7 Ni 2.87733 0.00000 0.00000
8 Ni 2.87733 2.49184 0.00000
9 Ni 1.42138 0.00248 4.12981
10 Ni 1.41187 2.53561 4.11454
11 Ni 3.58868 -1.23608 4.03645
12 Ni 3.59610 1.26112 4.13817
13 C 2.11352 1.30280 5.31239
14 H 1.21516 2.69213 5.58620
15 H 2.20172 1.14631 6.39431
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458

18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5225824476

FINAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.44097 -0.00833 4.15245
10 Ni 1.44097 2.50019 4.15254
11 Ni 3.60297 -1.24591 4.03186
12 Ni 3.61776 1.24592 4.14951
13 C 2.17215 1.24587 5.31147
14 H 0.72847 3.73790 5.10992
15 H 2.17498 1.24583 6.40979
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5697062136

CH2_CH-H hcp, hcp Pathway
INITIAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.45644 -0.01168 4.12654
10 Ni 1.45644 2.50371 4.12650
11 Ni 3.60503 -1.24585 4.02196
12 Ni 3.62820 1.24600 4.09013
13 C 2.13339 1.24605 5.43393
14 H 3.18472 1.24593 5.88470
15 H 1.46697 1.24617 6.30968
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5475496736

TRANSITION STATE
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.41955 -0.00791 4.12479
10 Ni 1.41311 2.52703 4.11465
11 Ni 3.58846 -1.24221 4.03686
12 Ni 3.59441 1.25414 4.14242
13 C 2.10644 1.28747 5.31233
14 H 2.18854 1.12621 6.39397
15 H 1.16225 2.64701 5.58231
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5225064976

FINAL ENDPOINT
19 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.42978 -0.02152 4.10149
10 Ni 1.45344 2.51003 4.15263
11 Ni 3.60836 -1.23145 4.07132
12 Ni 3.61347 1.26410 4.14952
13 C 2.14983 1.21744 5.28520
14 H 2.12044 1.15372 6.38116
15 H 0.09928 2.65705 5.08549
16 Ni 1.43867 0.00000 -2.03458
17 Ni 1.43867 2.49184 -2.03458
18 Ni 3.59667 -1.24592 -2.03458
19 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1511.5583718441
CH_C-H fcc, fcc Pathway
INITIAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458

 9 Ni 1.36892 -0.09847 4.01156
10 Ni 1.38808 2.49240 4.09944
11 Ni 3.56877 -1.27342 4.04943
12 Ni 3.51895 1.20593 4.19135
13 C 1.94461 1.15040 5.21410
14 H 1.33477 0.65634 5.99829
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3707241823

IMAGE 1
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.35811 -0.08537 4.04928
10 Ni 1.37095 2.47740 4.12198
11 Ni 3.55315 -1.27615 4.06563
12 Ni 3.51443 1.20846 4.18262
13 C 1.96309 1.14204 5.25937
14 H 1.68550 0.90823 6.29558
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.3604353205

IMAGE 2
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.36892 -0.09847 4.01156
10 Ni 1.38808 2.49240 4.09944
11 Ni 3.56877 -1.27342 4.04943
12 Ni 3.51895 1.20593 4.19135
13 C 1.94461 1.15040 5.21410
14 H 1.33477 0.65634 5.99829
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1510.3321985663

IMAGE 3
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.39426	-0.09981	4.03277
10 Ni	1.41814	2.49770	4.10080
11 Ni	3.58921	-1.27228	4.04633
12 Ni	3.54274	1.20424	4.18998
13 C	1.97630	1.16643	5.21674
14 H	1.04971	0.51088	5.62116
15 Ni	1.43867	0.00000	-2.03458
16 Ni	1.43867	2.49184	-2.03458
17 Ni	3.59667	-1.24592	-2.03458
18 Ni	3.59667	1.24592	-2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1510.2949042457

IMAGE 4
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458
6 Ni	0.71933	3.73777	2.03458
7 Ni	2.87733	0.00000	2.03458
8 Ni	2.87733	2.49184	2.03458
9 Ni	1.40721	-0.08982	4.06171
10 Ni	1.43275	2.50136	4.10621
11 Ni	3.60315	-1.27338	4.05732
12 Ni	3.56791	1.20532	4.18045
13 C	2.01968	1.18527	5.20658
14 H	0.88935	0.44220	5.48799
15 Ni	1.43867	0.00000	-2.03458
16 Ni	1.43867	2.49184	-2.03458
17 Ni	3.59667	-1.24592	-2.03458
18 Ni	3.59667	1.24592	-2.03458

SCF CONVERGED ENERGY (Rydbergs) = -1510.2739345033

IMAGE 5 (TRANSITION STATE)
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni	0.00000	0.00000	0.00000
2 Ni	0.00000	2.49184	0.00000
3 Ni	2.15800	-1.24592	0.00000
4 Ni	2.15800	1.24592	0.00000
5 Ni	0.71933	1.24592	2.03458

 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.43096 -0.06180 4.10915
10 Ni 1.44434 2.51600 4.10539
11 Ni 3.61889 -1.27636 4.08742
12 Ni 3.60200 1.20868 4.14919
13 C 2.12265 1.24152 5.18633
14 H 0.65906 0.70616 5.29867
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2663200950

IMAGE 6
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.44791 -0.04315 4.13014
10 Ni 1.44717 2.50819 4.11288
11 Ni 3.62655 -1.27586 4.08066
12 Ni 3.62811 1.21694 4.16673
13 C 2.15661 1.26060 5.17824
14 H 0.57434 0.27976 5.35327
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.2730224396

IMAGE 7
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.48154 -0.02328 4.14513
10 Ni 1.45919 2.51385 4.11585
11 Ni 3.64060 -1.26661 4.08455
12 Ni 3.65979 1.23722 4.18015
13 C 2.18974 1.28430 5.17710
14 H 0.41440 0.18453 5.26040
15 Ni 1.43867 0.00000 -2.03458

16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.2874613449

FINAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.45804 -0.02767 4.15876
10 Ni 1.42905 2.51095 4.11718
11 Ni 3.60797 -1.26325 4.06295
12 Ni 3.61363 1.21683 4.15890
13 C 2.13955 1.28088 5.17648
14 H 0.04453 -0.07435 5.02819
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3090542240

CH_C-H fcc, hcp Pathway
INITIAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.43770 -0.01410 4.12172
10 Ni 1.43766 2.50589 4.12168
11 Ni 3.60335 -1.24593 4.07130
12 Ni 3.62372 1.24588 4.11850
13 C 2.17152 1.24588 5.27424
14 H 2.17494 1.24585 6.37312
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3707241823

IMAGE 1
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000

 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.40307 0.07098 4.16390
10 Ni 1.37481 2.60762 4.04493
11 Ni 3.56640 -1.18932 4.06601
12 Ni 3.55993 1.31431 4.15764
13 C 2.05837 1.43699 5.26672
14 H 1.86387 1.78806 6.28981
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.3589546959

IMAGE 2
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.40647 0.07270 4.16649
10 Ni 1.36633 2.62013 4.00872
11 Ni 3.56960 -1.19604 4.04882
12 Ni 3.55548 1.31138 4.16183
13 C 2.04452 1.45668 5.23856
14 H 1.62526 2.20299 5.96808
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.3278539638

IMAGE 3
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 0.00000
 2 Ni 0.00000 2.49184 0.00000
 3 Ni 2.15800 -1.24592 0.00000
 4 Ni 2.15800 1.24592 0.00000
 5 Ni 0.71933 1.24592 2.03458
 6 Ni 0.71933 3.73777 2.03458
 7 Ni 2.87733 0.00000 2.03458
 8 Ni 2.87733 2.49184 2.03458
 9 Ni 1.42114 0.03916 4.16716
10 Ni 1.38393 2.58696 4.04488
11 Ni 3.58435 -1.22327 4.03759

12 Ni 3.57362 1.28105 4.16172
13 C 2.07220 1.40452 5.23048
14 H 1.41697 2.57865 5.62795
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.2786446501

IMAGE 4 (TRANSITION STATE)
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.41545 0.01094 4.15209
10 Ni 1.40233 2.55469 4.11243
11 Ni 3.58589 -1.22768 4.03773
12 Ni 3.59896 1.27071 4.14929
13 C 2.13140 1.29514 5.18830
14 H 1.29437 2.79021 5.59090
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2656040480

IMAGE 5
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73776 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.42165 -0.01537 4.16132
10 Ni 1.41939 2.52404 4.12488
11 Ni 3.59427 -1.24270 4.03628
12 Ni 3.61726 1.25228 4.15670
13 C 2.15345 1.25687 5.17949
14 H 1.21681 2.94201 5.54096
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43866 2.49184 -2.03458
17 Ni 3.59666 -1.24592 -2.03458
18 Ni 3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.2707712997

IMAGE 6

18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000
 5 Ni   0.71933 1.24592 2.03458
 6 Ni   0.71933 3.73776 2.03458
 7 Ni   2.87733 0.00000 2.03458
 8 Ni   2.87733 2.49184 2.03458
 9 Ni   1.42925 -0.04919 4.17652
10 Ni   1.44010 2.48567 4.13560
11 Ni   3.60420 -1.26022 4.03260
12 Ni   3.63931 1.22959 4.16931
13 C   2.17549 1.21675 5.17522
14 H   1.11292 3.13113 5.45578
15 Ni   1.43866 0.00000 -2.03458
16 Ni   1.43866 2.49184 -2.03458
17 Ni   3.59666 -1.24592 -2.03458
18 Ni   3.59666 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.2839394983

IMAGE 7
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000
 5 Ni   0.71933 1.24592 2.03458
 6 Ni   0.71933 3.73777 2.03458
 7 Ni   2.87733 0.00000 2.03458
 8 Ni   2.87733 2.49184 2.03458
 9 Ni   1.44135 -0.07693 4.19640
10 Ni   1.45942 2.45174 4.13702
11 Ni   3.61529 -1.27951 4.02735
12 Ni   3.65770 1.20558 4.18911
13 C   2.18732 1.19643 5.18359
14 H   1.00464 3.31017 5.33690
15 Ni   1.43867 0.00000 -2.03458
16 Ni   1.43867 2.49184 -2.03458
17 Ni   3.59667 -1.24592 -2.03458
18 Ni   3.59667 1.24592 -2.03458
SCF CONVERGED ENERGY (Rydbergs) = -1510.3005140227

FINAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni   0.00000 0.00000 0.00000
 2 Ni   0.00000 2.49184 0.00000
 3 Ni   2.15800 -1.24592 0.00000
 4 Ni   2.15800 1.24592 0.00000
 5 Ni   0.71933 1.24592 2.03458
 6 Ni   0.71933 3.73777 2.03458
 7 Ni   2.87733 0.00000 2.03458
 8 Ni   2.87733 2.49184 2.03458

 9 Ni 1.43673 -0.01272 4.16585
10 Ni 1.43700 2.50418 4.16593
11 Ni 3.60201 -1.24605 4.01991
12 Ni 3.61914 1.24576 4.16712
13 C 2.16509 1.24573 5.19304
14 H 0.72715 3.73775 5.10334
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3219230322

CH_C-H hcp, fcc Pathway
INITIAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.43301 -0.01992 4.12597
10 Ni 1.43303 2.51168 4.12600
11 Ni 3.60166 -1.24593 4.04911
12 Ni 3.62923 1.24590 4.12320
13 C 2.16949 1.24586 5.26453
14 H 2.17169 1.24585 6.36450
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3737014133

IMAGE 1 (TRANSITION STATE)
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.41968 -0.00488 4.15147
10 Ni 1.40801 2.54510 4.09606
11 Ni 3.59060 -1.23562 4.02640
12 Ni 3.61067 1.25999 4.14891
13 C 2.13285 1.29268 5.17353
14 H 1.29736 2.77041 5.57943
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458

18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2687432582

FINAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.43230 -0.01846 4.15205
10 Ni 1.43232 2.51021 4.15205
11 Ni 3.60039 -1.24597 4.01426
12 Ni 3.62367 1.24585 4.15321
13 C 2.16273 1.24587 5.16499
14 H 0.72584 3.73779 5.10183
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.3251982730

CH_C-H hcp, hcp Pathway
INITIAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.43301 -0.01992 4.12597
10 Ni 1.43303 2.51168 4.12600
11 Ni 3.60166 -1.24593 4.04911
12 Ni 3.62923 1.24590 4.12320
13 C 2.16949 1.24586 5.26453
14 H 2.17169 1.24585 6.36450
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2739345033

IMAGE 1 (TRANSITION STATE)
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458

 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.42459 -0.05872 4.10259
10 Ni 1.42388 2.53015 4.10131
11 Ni 3.61096 -1.26766 4.07491
12 Ni 3.59785 1.22525 4.14546
13 C 2.11234 1.24960 5.16898
14 H 0.65014 0.75672 5.28280
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2693185479

FINAL ENDPOINT
18 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

 1 Ni 0.00000 0.00000 2.03458
 2 Ni 0.00000 2.49184 2.03458
 3 Ni 2.15800 -1.24592 2.03458
 4 Ni 2.15800 1.24592 2.03458
 5 Ni 0.71933 1.24592 0.00000
 6 Ni 0.71933 3.73777 0.00000
 7 Ni 2.87733 0.00000 0.00000
 8 Ni 2.87733 2.49184 0.00000
 9 Ni 1.44389 -0.02512 4.15139
10 Ni 1.42110 2.52349 4.10606
11 Ni 3.60251 -1.25483 4.05717
12 Ni 3.61748 1.22917 4.15144
13 C 2.13613 1.28568 5.15215
14 H 0.03904 -0.06604 5.03525
15 Ni 1.43867 0.00000 -2.03458
16 Ni 1.43867 2.49184 -2.03458
17 Ni 3.59667 -1.24592 -2.03458
18 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1510.2730224396

CH3_fcc rotation (staggered)
Transition State (note that starting and ending point are CH_3 bindind to fcc site)
20 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

1 Ni 0.00000 0.00000 0.00000
2 Ni 0.00000 2.49184 0.00000
3 Ni 2.15800 -1.24592 0.00000
4 Ni 2.15800 1.24592 0.00000
5 Ni 0.71933 1.24592 2.03458
6 Ni 0.71933 3.73777 2.03458
7 Ni 2.87733 0.00000 2.03458
8 Ni 2.87733 2.49184 2.03458
9 Ni 1.43134 0.00220 4.08427
10 Ni 1.43097 2.49003 4.08376
11 Ni 3.58887 -1.24590 4.00563
12 Ni 3.57522 1.24600 4.10270

13 C 2.18646 1.24543 5.85017
14 H 2.67965 0.35892 6.27721
15 H 2.67971 2.13277 6.27527
16 H 1.14842 1.24605 6.22182
17 Ni 1.43867 0.00000 -2.03458
18 Ni 1.43867 2.49184 -2.03458
19 Ni 3.59667 -1.24592 -2.03458
20 Ni 3.59667 1.24592 -2.03458
GEOMETRY RELAXED ENERGY (Rydbergs) = -1512.7377261822

5. Spin State Optimization Inputs, Parameters & Results

Energies for 3 adjacent spin states are listed. Then A & B parameters for $E = AS^2 + BS + C$ fit are listed, followed by the lowest energy value for S, based on this fit.

Ni	8	-1123.6697857862	0.00941914
bulk	9	-1123.6710850447	0.161424633
	10	-1123.6535460238	**8.569**
Ni	11	-1497.8071503539	0.002438025
slab	12	-1497.8114218081	0.060346028
	13	-1497.8108172124	**12.376**
H	11	-1499.0159685393	0.007247881
fcc	12	-1499.0198844722	0.170617192
	13	-1499.0093046434	**11.770**
H	11	-1499.0152746528	0.007024697
hcp	12	-1499.0191911430	0.165484512
	13	-1499.0090582400	**11.779**
H	11	-1499.0060407593	0.006816619
2f	12	-1499.0101030521	0.160844527
	13	-1499.0005321071	**11.798**
H	11	-1498.9742269886	0.005117885
top	12	-1498.9786106543	0.12209501
	13	-1498.9727585509	**11.928**
CH3	11	-1512.7621096323	0.004977343
fcc	12	-1512.7625335663	0.11490283
	13	-1512.7530028137	**11.543**
CH3	11	-1512.7602698840	0.00461727
hcp	12	-1512.7612103534	0.107137672
	13	-1512.7529162834	**11.602**
CH3	11	-1512.7497846356	0.004853178
2f	12	-1512.7516166861	0.11345515
	13	-1512.7437423801	**11.689**
CH3	11	-1512.7422237416	0.004652728
top	12	-1512.7450415316	0.109830531
	13	-1512.7385538659	**11.803**
CH2	10	-1511.5465108710	0.00423546
fcc	11	-1511.5497755462	0.092209327
	12	-1511.5445693022	**10.885**
CH2	10	-1511.5451452574	0.004414227

hcp	11	-1511.5475193241	0.09507283
	12	-1511.5410649372	**10.769**
CH2	11	-1511.5371101010	0.004989114
2f	12	-1511.5325021468	0.110141663
	13	-1511.5179159650	**11.038**
CH2	11	-1511.4744653232	0.003875434
top	12	-1511.4754297562	0.090099416
	13	-1511.4686433211	**11.624**
CH	9	-1510.3646333763	0.004139527
fcc	10	-1510.3707241823	0.084741811
	11	-1510.3685359351	**10.236**
CH	9	-1510.3679351196	0.005079133
hcp	10	-1510.3736719006	0.102240302
	11	-1510.3692504162	**10.065**
CH	9	-1510.3366178216	0.003723735
2f	10	-1510.3434645597	0.077597695
	11	-1510.3428638286	**10.419**
CH	10	-1510.2101598969	0.007224748
top	11	-1510.2161610433	0.157720852
	12	-1510.2077126939	**10.915**
C	9	-1509.1195662333	0.004633359
fcc	10	-1509.1229796738	0.091447252
	11	-1509.1171263973	**9.868**
C	9	-1509.1244451626	0.005453604
hcp	10	-1509.1279669723	0.107140292
	11	-1509.1205815733	**9.823**
C	9	-1509.0861051121	0.004190673
bridge	10	-1509.0905929832	0.084110657
	11	-1509.0866995084	**10.035**
C	10	-1508.9606563014	0.004528125
top	11	-1508.9648238294	0.099258146
	12	-1508.9599351081	**10.960**
C_H	8	-1510.3075881817	0.003218104
hcp-hcp	9	-1510.3130751329	0.060194713
	10	-1510.3121258768	**9.353**
CH_H	9	-1511.5753896622	0.005067569
fcc_hcp	10	-1511.5779593931	0.098853545
	11	-1511.5703939857	**9.754**
CH2_H	9	-1512.7398587438	0.003376131
fcc_hcp	10	-1512.7459668220	0.070254563
	11	-1512.7453226386	**10.405**
C---H	9	-1510.2682634778	0.003499519
hcp-hcp	10	-1510.2693267789	0.067554168
TS	11	-1510.2633910414	**9.652**
CH---H	10	-1511.5254801385	0.003735648
fcc_hcp	11	-1511.5234906540	0.076459128
TS	12	-1511.5140298731	**10.234**
CH2--H	11	-1512.7083603348	0.004501415

fcc_hcp	12	-1512.7040234740	0.099195693
TS	13	-1512.6906837824	**11.018**

6. Frequencies and thermodynamic data from cluster calculations

Geometry is given, followed by forces, forces cancelling out ignored atoms in cluster, frequencies, and finally thermodynamic data.

Hydrogen

```
                                  angstroms
  atom               x                   y                   z
  ni1           0.7193335041        1.2459221485       -0.0000000147
  ni2           2.8773339614       -0.0000000080       -0.0000000021
  ni3           2.8773339588        2.4918442978       -0.0000000020
  ni4          -0.6964946252        1.2452165418        2.0447600530
  ni5           3.6195062992        3.7370608401        2.0447600557
  ni6           3.6195063003       -1.2466277535        2.0447600588
  ni7           1.4502816125       -0.0061781655        2.0448054493
  ni8           1.4505954168        2.4967741892        2.0448150202
  ni9           3.6108637762        1.2452202806        2.0147772388
  h10           2.1333998098        1.2569796802        3.0658466593

forces (hartrees/bohr

atom  label           x             y             z
 ---- --------   -------------  -------------  -------------
    1 ni1         1.539535E-04   8.847185E-04   4.717794E-03
    2 ni2         2.419357E-03  -5.281464E-03   4.418782E-03
    3 ni3         3.958383E-03   3.950282E-03   7.395311E-03
    4 ni4         7.038866E-03   2.195210E-03   1.029699E-03
    5 ni5        -4.244322E-03  -7.224781E-03  -1.129825E-02
    6 ni6        -3.800141E-03   6.717397E-03  -1.099310E-02
    7 ni7        -7.656262E-03  -9.625317E-03  -3.635824E-03
    8 ni8        -1.239012E-02   7.887262E-03  -2.530472E-03
    9 ni9         1.487214E-02  -8.261615E-04  -1.979569E-03
   10 h10        -1.078564E-03  -1.706557E-05   2.314773E-04
 -------------   -------------  -------------  -------------
     total       -7.267024E-04  -1.339920E-03  -1.264415E-02

  end of program der1b

  start of program nude

  forces (hartrees/bohr) : numerical

 atom  label           x             y             z
 ---- --------   -------------  -------------  -------------
    1 ni1         0.000000E+00   0.000000E+00   0.000000E+00
    2 ni2         0.000000E+00   0.000000E+00   0.000000E+00
    3 ni3         0.000000E+00   0.000000E+00   0.000000E+00
    4 ni4         0.000000E+00   0.000000E+00   0.000000E+00
    5 ni5         0.000000E+00   0.000000E+00   0.000000E+00
    6 ni6         0.000000E+00   0.000000E+00   0.000000E+00
    7 ni7        -1.183832E-02  -1.632503E-02   4.061194E-03
    8 ni8        -1.423560E-02   1.380255E-02   4.249672E-03
```

9 ni9	1.945478E-02	-2.724574E-03	1.975691E-03
10 h10	-2.694165E-03	6.478826E-04	1.950023E-03
total	-9.313310E-03	-4.599176E-03	1.223658E-02

largest asymmetry in numerical hessian: 21 19 5.560E-02
end of program nude

start of program freq

harmonic frequencies in cm**-1, reduced masses in amu,
force constants in mDyne/A, and
normal modes in cartesian coordinates:

frequencies		181.82	190.58	245.61	824.94	981.75	1134.18
reduc. mass		21.32	19.47	21.21	0.99	0.99	0.99
force const		0.42	0.42	0.75	0.40	0.56	0.75
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	0.08206	-0.00959	-0.01840	0.00608	-0.00118	-0.00280
ni7	Y	0.02348	0.07089	-0.06694	-0.00092	-0.00540	-0.00442
ni7	Z	-0.00133	0.00020	0.00058	0.00323	-0.00731	-0.00604
ni8	X	-0.03469	-0.06406	-0.04277	0.00750	0.00170	-0.00396
ni8	Y	0.04391	-0.03938	0.08083	0.00045	-0.00802	0.00564
ni8	Z	0.00058	0.00100	0.00123	0.00287	0.00680	-0.00687
ni9	X	-0.04739	0.07404	0.06150	0.00340	-0.00029	0.00389
ni9	Y	-0.06774	-0.03156	-0.01425	0.00085	-0.00377	-0.00040
ni9	Z	0.00063	-0.00122	-0.00065	-0.00898	-0.00039	-0.00406
h10	X	0.00134	-0.02233	-0.01932	-0.97589	-0.01301	0.16527
h10	Y	0.02012	0.00318	0.02054	-0.02166	0.98854	-0.04739
h10	Z	0.00690	0.00148	-0.06694	0.16604	0.05172	0.97557

Thermochemical properties at 1.0000 atm

rotational symmetry number: 1

rotational temperatures (K): 0.000111 0.000111 0.000078

vibrational temperatures:

```
     mode:      1        2        3        4        5        6
 temp. (K):   261.59   274.19   353.38  1186.91  1412.51  1631.83


 Thermodynamic properties calculated assuming an ideal gas

 In the table below, the units for temperature
 are kelvins, the units for U, H, and G are
 kcal/mol and the units for Cv and S are cal/(mol K)

 The zero point energy (ZPE):      5.088 kcal/mol
 is not included in U, H, or G in the table below


 T =   298.15 K

            U         Cv         S          H          G
         ---------  ---------  ---------  ---------  ---------
 trans.      0.889      2.981     58.795      1.481    -16.048
   rot.      0.889      2.981     48.593      0.889    -13.599
   vib.      1.124      6.748      6.637      1.124     -0.855
  elec.      0.000      0.000      4.576      0.000     -1.364
  total      2.901     12.709    118.600      3.494    -31.867

 Total internal energy, Utot (SCFE + ZPE + U):   -1524.310353 hartrees
            Total enthalpy, Htot (Utot + pV):   -1524.309409 hartrees
   Total Gibbs free energy, Gtot (Htot - T*S):   -1524.365760 hartrees
```

Carbon

```
                              angstroms
 atom              x                 y                 z
 ni1         -1.0207907723      1.4606120673      0.0000000000
 ni2         -1.0207907447     -0.6973884096      1.2459221615
 ni3         -1.0207907447     -0.6973884096     -1.2459221615
 ni4          1.0137916345     -1.4607441430      2.4918323168
 ni5          1.0137916345     -1.4607441430     -2.4918323168
 ni6          1.0137916361      2.8552567764      0.0000000000
 ni7          1.0784786931      0.7350993246      1.2657906151
 ni8          1.0784786931      0.7350993246     -1.2657906151
 ni9          0.9949643839     -1.4321141971      0.0000000000
 c10          2.2804901085      0.1463481785      0.0000000000

atom  label          x             y             z
 ---- --------   -------------  -------------  -------------
    1 ni1         2.537163E-03  -4.840771E-03   0.000000E+00
    2 ni2        -2.210081E-03   4.359478E-03   1.008618E-02
    3 ni3        -2.210081E-03   4.359478E-03  -1.008618E-02
    4 ni4        -2.791700E-03   6.444920E-03  -5.591805E-03
    5 ni5        -2.791700E-03   6.444920E-03   5.591805E-03
    6 ni6         4.168446E-03  -2.709936E-03   0.000000E+00
    7 ni7         1.302192E-02  -1.742688E-02  -1.477352E-03
    8 ni8         1.302192E-02  -1.742688E-02   1.477352E-03
    9 ni9         1.147832E-02  -6.577841E-04   0.000000E+00
   10 c10        -3.290552E-02   2.131742E-02   0.000000E+00
 -------------   -------------  -------------  -------------
```

```
    total        1.318688E-03  -1.360272E-04   0.000000E+00

 end of program der1b


 start of program nude

 forces (hartrees/bohr) : numerical

atom  label           x             y             z
---- --------   -------------  -------------  -------------
   1 ni1         0.000000E+00   0.000000E+00   0.000000E+00
   2 ni2         0.000000E+00   0.000000E+00   0.000000E+00
   3 ni3         0.000000E+00   0.000000E+00   0.000000E+00
   4 ni4         0.000000E+00   0.000000E+00   0.000000E+00
   5 ni5         0.000000E+00   0.000000E+00   0.000000E+00
   6 ni6         0.000000E+00   0.000000E+00   0.000000E+00
   7 ni7         7.300894E-03  -1.052942E-02  -1.202080E-03
   8 ni8         7.300894E-03  -1.052942E-02   1.202080E-03
   9 ni9         1.442562E-02   4.001172E-03   0.000000E+00
  10 c10        -1.944238E-02   3.544647E-03   0.000000E+00
-------------   -------------  -------------  -------------
    total        9.585026E-03  -1.351301E-02   0.000000E+00

  largest asymmetry in numerical hessian:   20  19   4.678E-03
 end of program nude


 start of program freq

 harmonic frequencies in cm**-1, reduced masses in amu,
 force constants in mDyne/A, and
 normal modes in cartesian coordinates:

 frequencies       -13.94    14.26    17.20   268.62   366.56   510.46
 symmetries       App      Ap       Ap       Ap       App      Ap
 reduc. mass      3320.53  3355.17  3355.16    11.98    11.97    11.98
 force const         0.38     0.40     0.58     0.51     0.95     1.84
   ni1      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni1      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni1      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni2      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni2      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni2      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni3      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni3      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni3      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni4      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni4      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni4      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni5      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni5      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni5      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni6      X     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni6      Y     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni6      Z     0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   ni7      X    -0.00020 -0.00010  0.00012 -0.00007 -0.00016 -0.00014
```

ni7	Y	-0.00499	-0.00262	0.00308	0.00006	0.00022	0.00007
ni7	Z	-0.00277	0.00534	0.00471	0.00008	0.00025	0.00013
ni8	X	0.00020	-0.00011	0.00012	-0.00007	0.00016	-0.00014
ni8	Y	0.00493	-0.00280	0.00302	0.00006	-0.00022	0.00007
ni8	Z	-0.00302	-0.00524	-0.00467	-0.00008	0.00025	-0.00013
ni9	X	0.00000	0.00021	-0.00023	0.00022	0.00000	-0.00005
ni9	Y	0.00006	0.00541	-0.00611	0.00022	0.00000	-0.00005
ni9	Z	0.00580	-0.00010	-0.00004	0.00000	-0.00016	0.00000
c10	X	-0.00005	-0.00099	-0.00564	-0.06800	0.00000	0.28043
c10	Y	0.00010	0.00539	0.00047	-0.28037	0.00000	-0.06794
c10	Z	-0.01294	0.00023	0.00008	0.00000	-0.28825	0.00000

Thermochemical properties at 1.0000 atm

rotational symmetry number: 1

rotational temperatures (K): 0.000090 0.000089 0.000065

1 vibrational frequencies below 10.0 cm-1 not included in zero-point energy or thermochemical analysis. Set opt403 to change the frequency cutoff value.

vibrational temperatures:

mode:	2	3	4	5	6
temp. (K):	20.52	24.74	386.48	527.39	734.44

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 1.683 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	59.995	1.481	-16.406
rot.	0.889	2.981	49.209	0.889	-13.783
vib.	1.781	8.471	17.572	1.781	-3.458
elec.	0.000	0.000	4.366	0.000	-1.302
total	3.559	14.433	131.142	4.151	-34.949

Total internal energy, Utot (SCFE + ZPE + U): -1561.765101 hartrees
Total enthalpy, Htot (Utot + pV): -1561.764157 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1561.826467 hartrees

CH

	angstroms		
atom	x	y	z
ni1	1.4486124823	-1.0208978950	0.0000000000

ni2	-0.7093879885	-1.0208978891	-1.2459221509
ni3	-0.7093879885	-1.0208978891	1.2459221509
ni4	2.8674776441	1.0136831892	0.0000000000
ni5	-1.4485232781	1.0136831900	2.4918442944
ni6	-1.4485232781	1.0136831900	-2.4918442944
ni7	0.7124779467	1.0648959226	-1.2560400198
ni8	0.7124779467	1.0648959226	1.2560400198
ni9	-1.4728853450	1.0568687524	0.0000000000
c10	0.0110994352	2.3618466433	0.0000000000
h11	-0.0320671697	3.4515825205	0.0000000000

atom	label	x	y	z
1	ni1	3.397865E-03	3.635057E-03	0.000000E+00
2	ni2	-7.552239E-04	3.709090E-03	5.530268E-04
3	ni3	-7.552239E-04	3.709090E-03	-5.530268E-04
4	ni4	-2.067199E-04	-5.759745E-05	0.000000E+00
5	ni5	5.645060E-04	4.206869E-04	8.600235E-05
6	ni6	5.645060E-04	4.206869E-04	-8.600235E-05
7	ni7	-3.224168E-04	-6.109164E-04	-3.309080E-03
8	ni8	-3.224168E-04	-6.109164E-04	3.309080E-03
9	ni9	5.967963E-03	-4.218506E-03	0.000000E+00
10	c10	-2.205412E-03	-6.475756E-03	0.000000E+00
11	h11	8.701126E-05	-5.281760E-04	0.000000E+00
	total	6.014438E-03	-6.072579E-04	0.000000E+00

end of program der1b

start of program nude

forces (hartrees/bohr) : numerical

atom	label	x	y	z
1	ni1	0.000000E+00	0.000000E+00	0.000000E+00
2	ni2	0.000000E+00	0.000000E+00	0.000000E+00
3	ni3	0.000000E+00	0.000000E+00	0.000000E+00
4	ni4	0.000000E+00	0.000000E+00	0.000000E+00
5	ni5	0.000000E+00	0.000000E+00	0.000000E+00
6	ni6	0.000000E+00	0.000000E+00	0.000000E+00
7	ni7	-1.513289E-03	-4.133286E-03	-3.277098E-03
8	ni8	-1.513289E-03	-4.133286E-03	3.277098E-03
9	ni9	6.222227E-03	-6.437448E-03	0.000000E+00
10	c10	-3.828717E-03	-5.289931E-03	0.000000E+00
11	h11	4.804238E-04	-2.058875E-04	0.000000E+00
	total	-1.526440E-04	-2.019984E-02	0.000000E+00

largest asymmetry in numerical hessian: 20 19 4.664E-03
end of program nude

start of program freq

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and
normal modes in cartesian coordinates:

frequencies		13.09	13.85	16.03	259.75	297.86	534.47
symmetries		Ap	App	Ap	Ap	App	Ap
reduc. mass		3441.49	3370.13	3484.64	10.99	10.80	10.06
force const		0.35	0.38	0.53	0.44	0.56	1.69
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	0.00206	0.00572	0.00219	-0.00003	-0.00012	-0.00005
ni7	Y	0.00000	-0.00003	-0.00001	-0.00010	-0.00020	-0.00013
ni7	Z	-0.00480	0.00212	0.00554	-0.00014	-0.00019	-0.00010
ni8	X	0.00429	-0.00404	0.00266	-0.00003	0.00012	-0.00005
ni8	Y	-0.00001	0.00002	-0.00001	-0.00010	0.00020	-0.00013
ni8	Z	0.00352	0.00348	-0.00581	0.00014	-0.00019	0.00010
ni9	X	-0.00634	-0.00168	-0.00486	-0.00030	0.00000	0.00008
ni9	Y	0.00002	0.00000	0.00002	0.00023	0.00000	-0.00010
ni9	Z	0.00128	-0.00561	0.00027	0.00000	0.00002	0.00000
c10	X	-0.00803	-0.00178	0.00113	0.28159	0.00000	0.01559
c10	Y	0.00062	0.00039	0.00503	-0.01887	0.00000	0.27572
c10	Z	-0.00145	0.00635	-0.00031	0.00000	0.28107	0.00000
h11	X	-0.00737	-0.00163	0.00118	0.20397	0.00000	0.06862
h11	Y	0.00060	0.00038	0.00495	-0.01583	0.00000	0.28055
h11	Z	-0.00155	0.00680	-0.00033	0.00000	0.22325	0.00000

frequencies		572.01	600.81	3159.46
symmetries		App	Ap	Ap
reduc. mass		0.94	0.94	0.93
force const		0.18	0.20	5.47
ni1	X	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000

ni5	X	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000
ni7	X	-0.00001	0.00000	0.00000
ni7	Y	-0.00005	-0.00003	0.00000
ni7	Z	-0.00001	0.00000	0.00000
ni8	X	0.00001	0.00000	0.00000
ni8	Y	0.00005	-0.00003	0.00000
ni8	Z	-0.00001	0.00000	0.00000
ni9	X	0.00000	-0.00002	0.00000
ni9	Y	0.00000	0.00007	0.00000
ni9	Z	0.00000	0.00000	0.00000
c10	X	0.00000	-0.06028	-0.00327
c10	Y	0.00000	-0.01235	-0.08213
c10	Z	-0.06483	0.00000	0.00000
h11	X	0.00000	0.97173	0.03734
h11	Y	0.00000	-0.05316	0.95415
h11	Z	0.97063	0.00000	0.00000

Thermochemical properties at 1.0000 atm

rotational symmetry number: 1

rotational temperatures (K): 0.000089 0.000089 0.000065

vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	18.84	19.93	23.06	373.72	428.55	768.98

mode:	7	8	9
temp. (K):	823.00	864.43	4545.75

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 7.816 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	59.995	1.481	-16.406
rot.	0.889	2.981	49.212	0.889	-13.784
vib.	2.615	12.679	26.532	2.615	-5.296
elec.	0.000	0.000	4.132	0.000	-1.232
total	4.392	18.641	139.872	4.985	-36.718

```
 Total internal energy, Utot (SCFE + ZPE + U):   -1562.418852 hartrees
            Total enthalpy, Htot (Utot + pV):   -1562.417907 hartrees
   Total Gibbs free energy, Gtot (Htot - T*S):   -1562.484365 hartrees
```

CH_2

```
                                 angstroms
 atom              x                 y                 z
 ni1          0.7193334723      1.2459221513     -0.0000000185
 ni2          2.8773339596     -0.0000000076     -0.0000000184
 ni3          2.8773339534      2.4918443045     -0.0000000112
 ni4          3.6045278532     -1.2453980573      1.9981465623
 ni5         -0.7114730663      1.2464462328      1.9981465615
 ni6          3.6045278534      3.7382905282      1.9981465627
 ni7          1.4609339550     -0.0077161955      2.0767683910
 ni8          1.4606005041      2.5011440219      2.0763203655
 ni9          3.6303425743      1.2463394397      2.0517489121
 c10          2.1322523889      1.2114026024      3.6031540825
 h11          3.0715721957      1.1799834999      4.1793795384
 h12          1.3174569776      1.2767646696      4.3302510845

 forces (hartrees/bohr) : total

atom  label          x             y             z
---- --------   -------------  -------------  -------------
   1 ni1        -1.931579E-04  -7.183607E-04  -2.203347E-04
   2 ni2         1.850079E-04   2.145742E-03  -3.593445E-03
   3 ni3         2.060085E-05  -2.210145E-03  -3.661617E-03
   4 ni4        -1.278479E-04   1.571163E-03   1.654925E-03
   5 ni5         2.007117E-03   1.299195E-04  -1.165827E-03
   6 ni6        -3.327229E-04  -1.575204E-03   1.857372E-03
   7 ni7         2.253287E-03   6.799409E-03   3.941389E-03
   8 ni8         2.625759E-03  -6.246058E-03   3.849355E-03
   9 ni9        -7.516444E-03   2.898874E-04  -1.095333E-03
  10 c10         1.040467E-04  -2.860079E-04  -1.032037E-04
  11 h11         1.704554E-05  -6.820520E-05   5.032204E-08
  12 h12        -9.249370E-05   1.123918E-04  -7.233765E-05
-------------  -------------  -------------  -------------
    total       -1.049803E-03  -5.546808E-05   1.390993E-03

 end of program der1b


 start of program nude

 forces (hartrees/bohr) : numerical

atom  label          x             y             z
---- --------   -------------  -------------  -------------
   1 ni1         0.000000E+00   0.000000E+00   0.000000E+00
   2 ni2         0.000000E+00   0.000000E+00   0.000000E+00
   3 ni3         0.000000E+00   0.000000E+00   0.000000E+00
   4 ni4         0.000000E+00   0.000000E+00   0.000000E+00
   5 ni5         0.000000E+00   0.000000E+00   0.000000E+00
   6 ni6         0.000000E+00   0.000000E+00   0.000000E+00
   7 ni7         1.756096E-03   3.799474E-03   7.912860E-03
```

8 ni8	1.654693E-03	-3.697864E-03	7.595211E-03
9 ni9	-1.626354E-03	7.051842E-05	1.868116E-03
10 c10	-4.912984E-03	5.120345E-05	-1.785999E-03
11 h11	1.462258E-03	-7.134469E-04	5.433608E-06
12 h12	1.763274E-03	2.783695E-04	3.334509E-03
total	9.698295E-05	-2.117451E-04	1.893013E-02

largest asymmetry in numerical hessian: 28 21 1.134E-02
end of program nude

start of program freq

harmonic frequencies in cm**-1, reduced masses in amu,
force constants in mDyne/A, and
normal modes in cartesian coordinates:

frequencies		12.88	13.43	14.60	130.53	177.57	310.48
reduc. mass		4051.30	3371.21	4084.28	9.38	8.15	0.59
force const		0.40	0.36	0.51	0.09	0.15	0.03
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	-0.00244	-0.00573	-0.00167	-0.00014	0.00020	-0.00001
ni7	Y	0.00346	-0.00209	-0.00648	-0.00026	0.00001	0.00004
ni7	Z	0.00003	0.00007	0.00002	-0.00023	0.00013	0.00007
ni8	X	-0.00481	0.00397	-0.00163	0.00019	0.00017	0.00004
ni8	Y	-0.00209	-0.00351	0.00645	-0.00017	0.00000	0.00003
ni8	Z	0.00006	-0.00005	0.00002	0.00023	0.00014	-0.00005
ni9	X	0.00726	0.00176	0.00331	-0.00005	0.00000	-0.00001
ni9	Y	-0.00137	0.00561	0.00003	0.00007	-0.00001	0.00000
ni9	Z	-0.00009	-0.00002	-0.00004	0.00000	-0.00029	-0.00001
c10	X	-0.00368	-0.00168	-0.00228	0.00068	-0.26127	-0.01429
c10	Y	0.00421	-0.00801	-0.00118	0.27098	0.00231	-0.03699
c10	Z	-0.00121	-0.00033	-0.00337	-0.00703	0.01720	-0.00364
h11	X	-0.00146	-0.00142	-0.00177	0.00524	-0.28585	0.01897
h11	Y	0.00572	-0.01118	-0.00056	0.33230	-0.01963	0.51836
h11	Z	-0.00460	-0.00096	-0.00369	-0.00954	0.04895	-0.02423
h12	X	-0.00089	-0.00082	-0.00040	-0.00550	-0.29460	-0.04960
h12	Y	0.00003	-0.00229	-0.00073	0.06390	0.04785	-0.83689
h12	Z	0.00244	0.00017	-0.00113	0.00426	-0.02127	0.02720

frequencies		409.99	533.85	671.29	1388.41	3002.52	3118.60
reduc. mass		8.11	0.62	0.58	0.50	0.81	0.83
force const		0.80	0.10	0.15	0.57	4.32	4.77
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	-0.00006	-0.00002	0.00001	0.00000	0.00000	0.00000
ni7	Y	-0.00007	0.00002	0.00001	0.00001	0.00000	0.00000
ni7	Z	-0.00013	0.00006	0.00005	0.00000	0.00000	0.00000
ni8	X	-0.00005	-0.00002	-0.00001	0.00000	0.00000	0.00000
ni8	Y	0.00006	-0.00002	0.00001	-0.00001	0.00000	0.00000
ni8	Z	-0.00011	0.00006	-0.00004	0.00000	0.00000	0.00000
ni9	X	0.00009	0.00003	0.00000	0.00000	0.00000	0.00000
ni9	Y	0.00000	0.00000	0.00001	0.00000	0.00000	0.00000
ni9	Z	-0.00011	-0.00002	0.00000	-0.00001	0.00000	0.00000
c10	X	0.03872	0.07242	0.00305	-0.00585	-0.04904	0.07448
c10	Y	0.00740	-0.00366	0.09076	-0.00286	0.00104	-0.00503
c10	Z	0.25855	-0.07662	-0.00916	-0.07693	-0.05119	-0.03980
h11	X	-0.05448	-0.29576	-0.03987	-0.38224	0.79769	-0.18843
h11	Y	0.00574	0.03483	-0.78042	0.03456	-0.02925	0.00615
h11	Z	0.38903	0.48389	0.01047	0.59633	0.47613	-0.14547
h12	X	-0.12218	-0.40943	-0.02481	0.44023	-0.21837	-0.69145
h12	Y	-0.02415	-0.00345	-0.53049	-0.00854	0.01586	0.05404
h12	Z	0.08516	-0.60756	0.01433	0.47379	0.14349	0.60770

Thermochemical properties at 1.0000 atm

rotational symmetry number: 1

rotational temperatures (K): 0.000090 0.000090 0.000065

vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	18.53	19.33	21.00	187.80	255.48	446.72

mode:	7	8	9	10	11	12
temp. (K):	589.88	768.08	965.84	1997.61	4319.96	4486.97

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 13.987 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	59.995	1.481	-16.406
rot.	0.889	2.981	49.194	0.889	-13.778
vib.	3.172	15.025	30.711	3.172	-5.984
elec.	0.000	0.000	3.867	0.000	-1.153
total	4.949	20.987	143.766	5.542	-37.322

Total internal energy, Utot (SCFE + ZPE + U): -1563.042575 hartrees
Total enthalpy, Htot (Utot + pV): -1563.041631 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1563.109939 hartrees

CH_3

angstroms

atom	x	y	z
ni1	0.7193334766	1.2459221505	-0.0000000088
ni2	2.8773339585	-0.0000000065	-0.0000000090
ni3	2.8773339542	2.4918443030	-0.0000000054
ni4	3.6038156524	-1.2467575283	1.9682527215
ni5	-0.7121852719	1.2450867638	1.9682527219
ni6	3.6038156526	3.7369310611	1.9682527219
ni7	1.4482978198	0.0024332459	2.0563666279
ni8	1.4483701575	2.4876523504	2.0564022589
ni9	3.6020547643	1.2450395072	2.0541900711
c10	2.1915695579	1.2332092292	3.8244917685
h11	1.6867511953	0.3569495684	4.2617556125
h12	3.2079696579	1.2388898361	4.2497986148
h13	1.6849717801	2.1156522854	4.2480517928

forces (hartrees/bohr) : total

atom	label	x	y	z
1	ni1	2.236496E-03	-3.729039E-04	-2.660118E-03
2	ni2	-1.172290E-03	2.472268E-03	-3.613773E-03
3	ni3	-7.731563E-04	-2.360812E-03	-3.691295E-03
4	ni4	3.473250E-03	3.876965E-03	3.476454E-03
5	ni5	4.779107E-04	1.190166E-03	2.675428E-03
6	ni6	1.887455E-03	-3.647290E-03	4.713109E-03
7	ni7	2.233405E-03	4.992982E-03	3.990228E-03
8	ni8	2.869238E-03	-4.221464E-03	3.909954E-03
9	ni9	-7.302108E-03	-6.680823E-04	5.494472E-03
10	c10	-3.365949E-04	7.759664E-04	-1.483457E-04
11	h11	8.298099E-06	-5.334706E-05	3.813995E-05
12	h12	1.674680E-04	-1.099458E-04	6.204897E-05

13 h13	3.930328E-05	-1.578014E-04	3.059409E-04
total	3.808674E-03	1.716702E-03	1.455224E-02

end of program der1b

start of program nude

forces (hartrees/bohr) : numerical

atom	label	x	y	z
1	ni1	0.000000E+00	0.000000E+00	0.000000E+00
2	ni2	0.000000E+00	0.000000E+00	0.000000E+00
3	ni3	0.000000E+00	0.000000E+00	0.000000E+00
4	ni4	0.000000E+00	0.000000E+00	0.000000E+00
5	ni5	0.000000E+00	0.000000E+00	0.000000E+00
6	ni6	0.000000E+00	0.000000E+00	0.000000E+00
7	ni7	9.182000E-04	6.122696E-03	3.609237E-03
8	ni8	3.653174E-03	-7.717839E-03	6.892129E-03
9	ni9	-7.915788E-03	-8.426030E-04	-2.776463E-03
10	c10	2.872834E-04	1.775350E-03	-6.524059E-03
11	h11	-2.307776E-03	9.185533E-04	3.607669E-03
12	h12	8.810870E-04	-1.393687E-03	1.226218E-02
13	h13	-4.212592E-03	3.173721E-03	-2.545243E-03
total		-8.696411E-03	2.036191E-03	1.452545E-02

largest asymmetry in numerical hessian: 36 27 4.284E-02

end of program nude

start of program freq

harmonic frequencies in cm**-1, reduced masses in amu,
force constants in mDyne/A, and
normal modes in cartesian coordinates:

frequencies		12.32	12.40	14.95	123.78	151.09	316.93
reduc. mass		4989.50	3447.45	4998.20	6.69	6.84	0.33
force const		0.45	0.31	0.66	0.06	0.09	0.02
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	0.00161	-0.00395	0.00484	-0.00012	-0.00015	0.00006
ni7	Y	-0.00560	-0.00514	0.00064	-0.00003	-0.00031	-0.00001
ni7	Z	0.00001	0.00001	-0.00001	-0.00008	-0.00033	0.00002
ni8	X	-0.00189	0.00527	0.00320	-0.00018	-0.00005	-0.00005
ni8	Y	0.00763	-0.00018	0.00030	0.00015	0.00001	0.00000
ni8	Z	0.00000	-0.00001	0.00000	-0.00026	0.00023	-0.00001
ni9	X	0.00029	-0.00132	-0.00805	-0.00007	0.00008	-0.00002
ni9	Y	-0.00202	0.00532	-0.00095	0.00000	-0.00007	0.00003
ni9	Z	-0.00001	0.00000	0.00001	0.00031	0.00010	0.00003
c10	X	-0.00407	-0.00008	0.00260	0.23731	0.07709	0.01090
c10	Y	-0.00332	-0.00294	0.00329	-0.07427	0.23795	-0.01185
c10	Z	-0.00075	-0.00019	0.00118	0.01320	-0.00214	-0.02832
h11	X	-0.00613	-0.00225	0.00338	0.29535	0.06894	-0.48438
h11	Y	-0.00382	-0.00554	0.00344	-0.10891	0.27658	0.27086
h11	Z	-0.00327	-0.00746	0.00129	0.01018	0.05769	-0.03144
h12	X	-0.00740	-0.00116	0.00311	0.26339	0.08590	0.01149
h12	Y	-0.00285	-0.00706	0.00590	-0.06254	0.25138	-0.58294
h12	Z	0.00744	0.00248	-0.00081	-0.03942	-0.01940	-0.02161
h13	X	-0.00832	-0.00046	0.00105	0.24749	0.10382	0.50590
h13	Y	-0.00537	-0.00583	0.00436	-0.10251	0.27580	0.27132
h13	Z	-0.00092	0.00496	-0.00345	0.07570	-0.04336	-0.02386

frequencies		365.30	620.18	644.20	1253.61	1429.53	1437.72
reduc. mass		8.60	0.48	0.48	0.42	0.40	0.39
force const		0.68	0.11	0.12	0.39	0.48	0.47
ni1	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ni7	X	0.00000	0.00003	-0.00004	0.00001	0.00000	0.00000
ni7	Y	-0.00002	0.00006	0.00003	0.00002	0.00000	0.00000
ni7	Z	-0.00013	0.00004	0.00000	-0.00001	0.00000	0.00000
ni8	X	-0.00001	-0.00004	0.00000	0.00001	0.00000	0.00000
ni8	Y	0.00000	-0.00004	-0.00004	-0.00002	0.00000	0.00000
ni8	Z	-0.00011	-0.00001	0.00003	-0.00001	0.00000	-0.00001
ni9	X	0.00003	-0.00001	0.00000	-0.00003	0.00000	0.00000
ni9	Y	0.00001	-0.00005	0.00003	0.00000	0.00000	0.00000
ni9	Z	-0.00015	-0.00003	-0.00003	-0.00001	0.00001	0.00000
c10	X	-0.01021	0.03896	0.08332	0.00044	0.05229	0.04366
c10	Y	0.00444	0.08040	-0.04625	0.00421	0.04587	-0.05137

c10	Z	0.26530	0.00287	-0.00053	-0.09757	0.00211	-0.00138
h11	X	-0.07606	-0.12521	-0.24797	0.11106	-0.11281	-0.60204
h11	Y	0.02561	-0.19853	0.13969	0.20025	0.23958	0.29333
h11	Z	0.21987	-0.69905	-0.01145	0.48871	0.25561	-0.07285
h12	X	0.00495	-0.10452	-0.17898	-0.21949	0.13808	0.11148
h12	Y	-0.06106	-0.22066	0.14352	-0.03696	-0.47857	0.52992
h12	Z	0.21816	0.32865	0.58795	0.50190	-0.25107	-0.21067
h13	X	0.02925	-0.15223	-0.22363	0.07955	-0.62057	-0.03463
h13	Y	0.05085	-0.20902	0.07992	-0.19972	-0.31272	-0.21615
h13	Z	0.20642	0.34454	-0.59007	0.48960	-0.07137	0.31423

frequencies		2962.50	3034.01	3038.34
reduc. mass		0.33	0.52	0.55
force const		1.70	2.84	2.97
ni1	X	0.00000	0.00000	0.00000
ni1	Y	0.00000	0.00000	0.00000
ni1	Z	0.00000	0.00000	0.00000
ni2	X	0.00000	0.00000	0.00000
ni2	Y	0.00000	0.00000	0.00000
ni2	Z	0.00000	0.00000	0.00000
ni3	X	0.00000	0.00000	0.00000
ni3	Y	0.00000	0.00000	0.00000
ni3	Z	0.00000	0.00000	0.00000
ni4	X	0.00000	0.00000	0.00000
ni4	Y	0.00000	0.00000	0.00000
ni4	Z	0.00000	0.00000	0.00000
ni5	X	0.00000	0.00000	0.00000
ni5	Y	0.00000	0.00000	0.00000
ni5	Z	0.00000	0.00000	0.00000
ni6	X	0.00000	0.00000	0.00000
ni6	Y	0.00000	0.00000	0.00000
ni6	Z	0.00000	0.00000	0.00000
ni7	X	0.00000	0.00000	0.00000
ni7	Y	0.00000	0.00000	0.00000
ni7	Z	0.00000	0.00000	0.00000
ni8	X	0.00000	0.00000	0.00000
ni8	Y	0.00000	0.00000	0.00000
ni8	Z	0.00000	0.00000	0.00000
ni9	X	0.00000	0.00000	0.00000
ni9	Y	0.00000	0.00000	0.00000
ni9	Z	0.00000	0.00000	0.00000
c10	X	-0.00426	-0.06838	0.05385
c10	Y	-0.00170	0.05369	0.06800
c10	Z	-0.04885	0.00123	-0.00283
h11	X	-0.25082	-0.06901	-0.35669
h11	Y	-0.43575	-0.06424	-0.62700
h11	Z	0.19191	0.04298	0.31996
h12	X	0.56307	0.54543	-0.42179
h12	Y	0.00162	0.01975	0.01977
h12	Z	0.20977	0.23043	-0.17887
h13	X	-0.26324	0.32826	0.14239
h13	Y	0.45410	-0.59161	-0.19622
h13	Z	0.19338	-0.28769	-0.10368

Thermochemical properties at 1.0000 atm

```
 rotational symmetry number:  1

 rotational temperatures (K):   0.000091   0.000091   0.000065

 vibrational temperatures:
      mode:      1        2        3        4        5        6
 temp. (K):    17.73    17.83    21.52   178.09   217.39   455.99

      mode:      7        8        9       10       11       12
 temp. (K):   525.58   892.30   926.86  1803.66  2056.77  2068.55

      mode:     13       14       15
 temp. (K):  4262.36  4365.26  4371.49


 Thermodynamic properties calculated assuming an ideal gas

 In the table below, the units for temperature
 are kelvins, the units for U, H, and G are
 kcal/mol and the units for Cv and S are cal/(mol K)

 The zero point energy (ZPE):     22.040 kcal/mol
 is not included in U, H, or G in the table below


 T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
 trans.      0.889      2.981     59.995      1.481    -16.406
   rot.      0.889      2.981     49.175      0.889    -13.773
   vib.      3.220     15.266     31.377      3.220     -6.135
  elec.      0.000      0.000      4.576      0.000     -1.364
  total      4.998     21.227    145.123      5.590    -37.678

 Total internal energy, Utot (SCFE + ZPE + U):   -1563.678751 hartrees
            Total enthalpy, Htot (Utot + pV):   -1563.677807 hartrees
   Total Gibbs free energy, Gtot (Htot - T*S):   -1563.746760 hartrees
```

CH_4 (gas)

```
 C1           -0.0000324444      0.0000046782      0.0000000000
 H2            1.0836053304     -0.0000732163      0.0000000000
 H3           -0.3611341470      1.0217004941      0.0000000000
 H4           -0.3610424368     -0.5108414904      0.8847956974
 H5           -0.3610424368     -0.5108414904     -0.8847956974

 forces (hartrees/bohr) : total

atom  label          x             y             z
---- --------   -------------  -------------  -------------
   1 C1          0.000000E+00   0.000000E+00  -2.480473E-05
   2 H2          0.000000E+00   0.000000E+00   5.537882E-05
   3 H3          7.941175E-05  -4.336809E-18  -5.161634E-05
   4 H4         -3.970588E-05   6.877260E-05  -5.161634E-05
   5 H5         -3.970588E-05  -6.877260E-05  -5.161634E-05
-------------   -------------  -------------  -------------
```

```
    total        0.000000E+00   0.000000E+00  -1.242749E-04

 end of program der1b


 start of program nude

 forces (hartrees/bohr) : numerical

atom  label           x              y              z
---- --------   -------------  -------------  -------------
   1 C1          0.000000E+00   0.000000E+00  -5.333435E-04
   2 H2         -5.293956E-23  -9.169401E-23   4.876439E-04
   3 H3          4.081447E-04  -3.308722E-24  -1.606613E-05
   4 H4         -2.040723E-04   3.534637E-04  -1.606613E-05
   5 H5         -2.040723E-04  -3.534637E-04  -1.606613E-05
-------------   -------------  -------------  -------------
    total        0.000000E+00   0.000000E+00  -9.389793E-05

  largest asymmetry in numerical hessian:    9   7   3.977E-04
 end of program nude


 start of program freq

 harmonic frequencies in cm**-1, reduced masses in amu,
 force constants in mDyne/A, and
 normal modes in cartesian coordinates:

 frequencies      1355.81  1358.32  1358.32  1579.96  1579.96  3055.10
 symmetries       A1       E/App    E/Ap     E/App    E/Ap     A1
 reduc. mass         0.53     0.52     0.52     0.25     0.25     0.25
 force const         0.58     0.57     0.57     0.37     0.37     1.39
   C1       X     0.00000  0.00000 -0.11476  0.00000  0.00048  0.00000
   C1       Y     0.00000  0.11476  0.00000 -0.00048  0.00000  0.00000
   C1       Z     0.11480  0.00000  0.00000  0.00000  0.00000 -0.00050
   H2       X     0.00000 -0.00010  0.55834 -0.01899  0.49535  0.00000
   H2       Y     0.00000 -0.55834 -0.00010 -0.49535 -0.01899  0.00000
   H2       Z     0.08742  0.00000  0.00000  0.00000  0.00000 -0.49314
   H3       X    -0.20214 -0.00012 -0.01543 -0.00619  0.16603 -0.47118
   H3       Y     0.00000 -0.55416  0.00018  0.50008  0.01885  0.00000
   H3       Z    -0.48479 -0.00009  0.20442 -0.01790  0.46830  0.16636
   H4       X     0.10107 -0.24653  0.41189  0.30102 -0.32271  0.23559
   H4       Y    -0.17506 -0.12684  0.24660  0.01134 -0.28836 -0.40805
   H4       Z    -0.48479 -0.17699 -0.10229 -0.39661 -0.24965  0.16636
   H5       X     0.10107  0.24675  0.41163 -0.27584 -0.34439  0.23559
   H5       Y     0.17506 -0.12709 -0.24668 -0.01034  0.28850  0.40805
   H5       Z    -0.48479  0.17708 -0.10213  0.41451 -0.21865  0.16636

 frequencies      3173.41  3173.41  3173.79
 symmetries       E/App    E/Ap     A1
 reduc. mass         0.52     0.52     0.59
 force const         3.08     3.08     3.52
   C1       X     0.00000  0.08823  0.00000
   C1       Y     0.08823  0.00000  0.00000
   C1       Z     0.00000  0.00000  0.08818
   H2       X     0.00003  0.01667  0.00000
```

```
  H2       Y     0.01667 -0.00003  0.00000
  H2       Z     0.00000  0.00000 -0.82403
  H3       X     0.00012 -0.72798  0.26053
  H3       Y     0.01648  0.00013  0.00000
  H3       Z     0.00002  0.26321 -0.07529
  H4       X     0.32229 -0.16953 -0.13026
  H4       Y    -0.54197  0.32231  0.22562
  H4       Z     0.22794 -0.13163 -0.07529
  H5       X    -0.32243 -0.16975 -0.13026
  H5       Y    -0.54176 -0.32241 -0.22562
  H5       Z    -0.22796 -0.13158 -0.07529


 Thermochemical properties at    1.0000 atm

 rotational symmetry number:  3

 rotational temperatures (K):   7.568306   7.568306   7.567146

 vibrational temperatures:
      mode:      1        2        3        4        5        6
 temp. (K):  1950.70  1954.32  1954.32  2273.20  2273.20  4395.61

      mode:      7        8        9
 temp. (K):  4565.83  4565.83  4566.37


 Thermodynamic properties calculated assuming an ideal gas

 In the table below, the units for temperature
 are kelvins, the units for U, H, and G are
 kcal/mol and the units for Cv and S are cal/(mol K)

 The zero point energy (ZPE):     28.317 kcal/mol
 is not included in U, H, or G in the table below


 T =   298.15 K

            U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
 trans.      0.889      2.981     34.261      1.481     -8.734   14.74094
   rot.      0.889      2.981     12.886      0.889     -2.953    4.98427
   vib.      0.021      0.480      0.081      0.021     -0.003    0.00527
  elec.      0.000      0.000      0.000      0.000      0.000    0.00000
  total      1.799      6.442     47.228      2.391    -11.690   19.73048

 Total internal energy, Utot (SCFE + ZPE + U):     -40.475240 hartrees
            Total enthalpy, Htot (Utot + pV):     -40.474295 hartrees
   Total Gibbs free energy, Gtot (Htot - T*S):     -40.496735 hartrees
```

H_2 (gas)

```
atom               x                 y                 z
H1           0.0000000000      0.0000000000      0.3662957656
H2           0.0000000000      0.0000000000     -0.3662957656
```

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	2.465190E-32	0.000000E+00	7.500668E-05
2	H2	2.465190E-32	0.000000E+00	-7.500668E-05
	total	4.930381E-32	0.000000E+00	0.000000E+00

end of program der1b

start of program nude

forces (hartrees/bohr) : numerical

atom	label	x	y	z
1	H1	0.000000E+00	0.000000E+00	5.786333E-04
2	H2	0.000000E+00	0.000000E+00	-5.786333E-04
	total	0.000000E+00	0.000000E+00	0.000000E+00

largest asymmetry in numerical hessian: 0 0 0.000E+00
end of program nude

start of program freq

harmonic frequencies in cm**-1, reduced masses in amu,
force constants in mDyne/A, and
normal modes in cartesian coordinates:

frequencies		4482.80
symmetries		Sig_g+
reduc. mass		0.50
force const		5.97
H1	X	0.00000
H1	Y	0.00000
H1	Z	-0.70436
H2	X	0.00000
H2	Y	0.00000
H2	Z	0.70436

Thermochemical properties at 1.0000 atm

rotational symmetry number: 2

rotational temperatures (K): 87.250383 87.250383

vibrational temperatures:
mode: 1
temp. (K): 6449.74

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 6.408 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	28.080	1.481	-6.891	11.63054
rot.	0.592	1.987	3.052	0.592	-0.317	0.53567
vib.	0.000	0.000	0.000	0.000	0.000	0.00000
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.481	4.968	31.132	2.074	-7.208	12.16620

Total internal energy, Utot (SCFE + ZPE + U): -1.165966 hartrees
Total enthalpy, Htot (Utot + pV): -1.165022 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1.179813 hartrees