

Raney Nickel-Catalyzed Reductive *N*-methylation of Amines with Paraformaldehyde: Theoretical and Experimental Study

Xin Ge, Chenxi Luo, Chao Qian*, Zhiping Yu, Xinzhi Chen

Key Laboratory of Biomass Chemical Engineering of Ministry of Education, Department of Chemical and Biological Engineering, Zhejiang University, P.R China

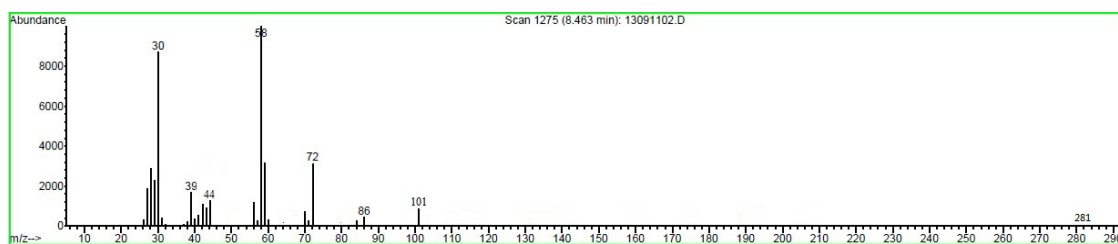
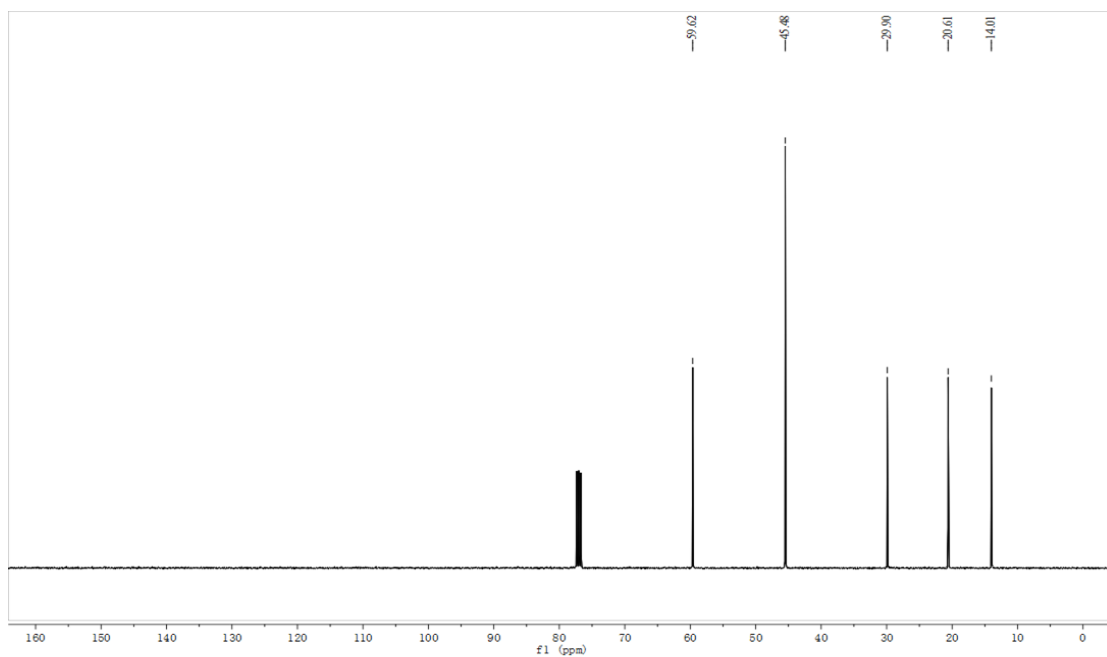
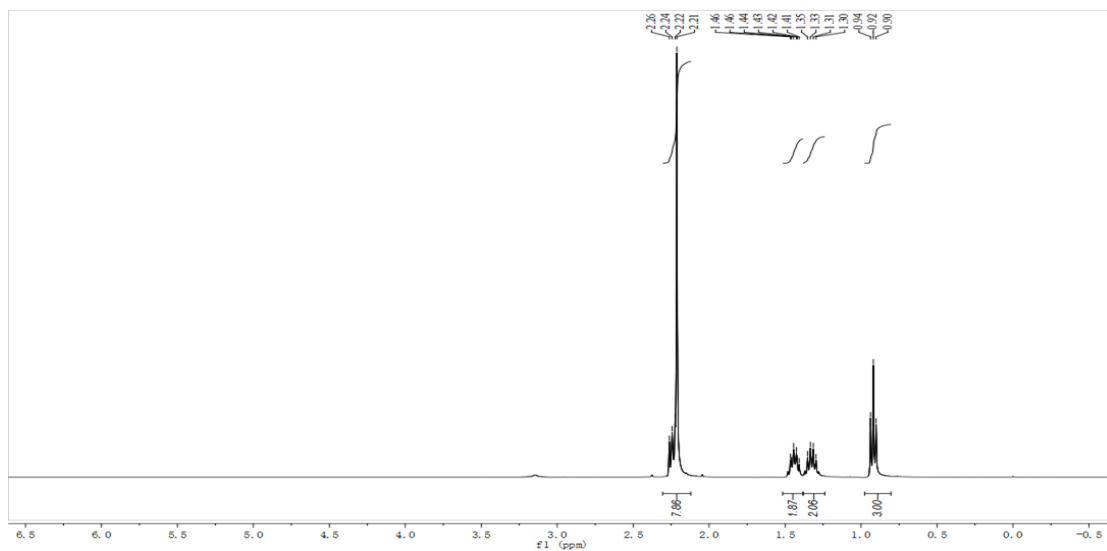
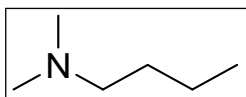
*Corresponding author. Tel: +86-571-87951615, Fax: +86-571-87951615,

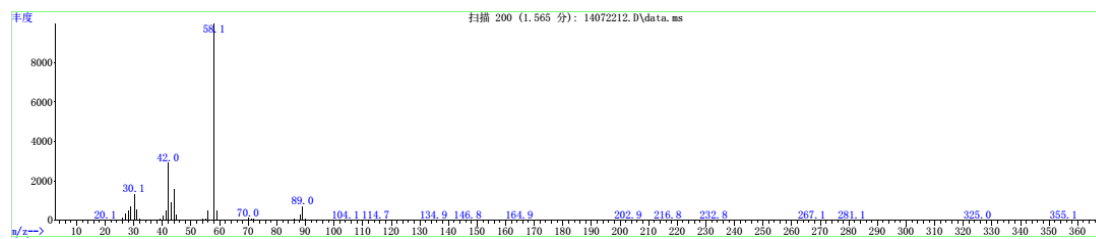
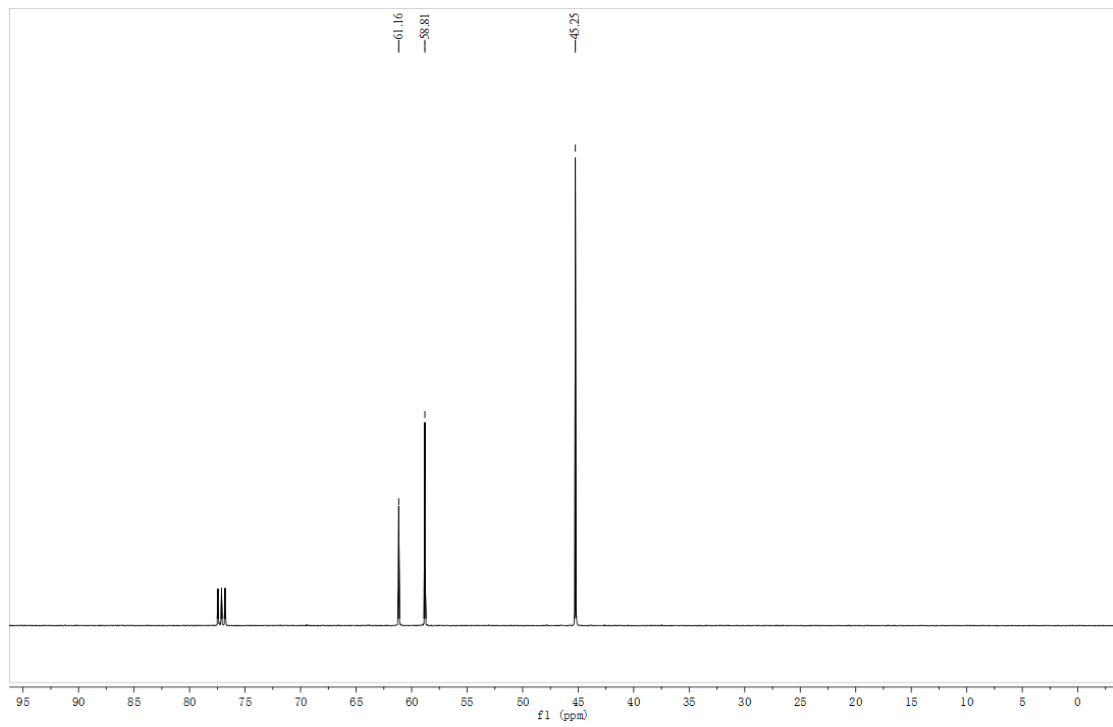
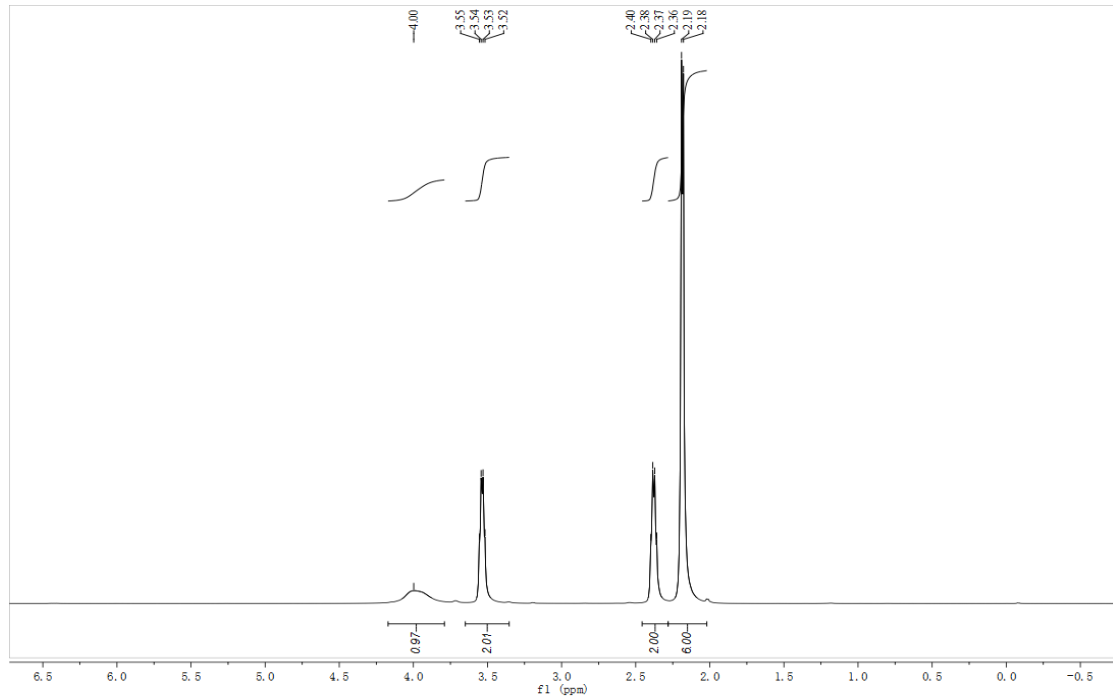
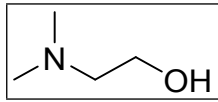
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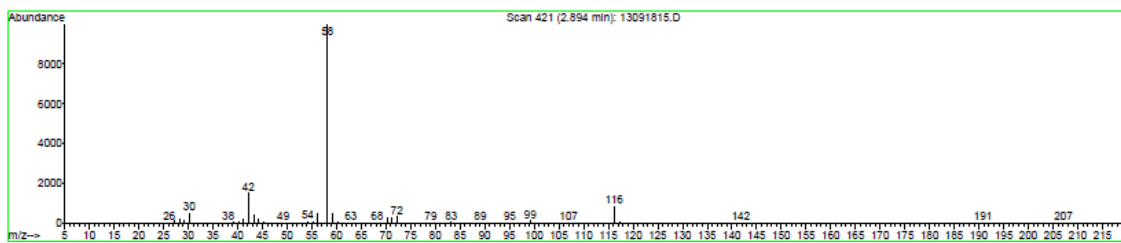
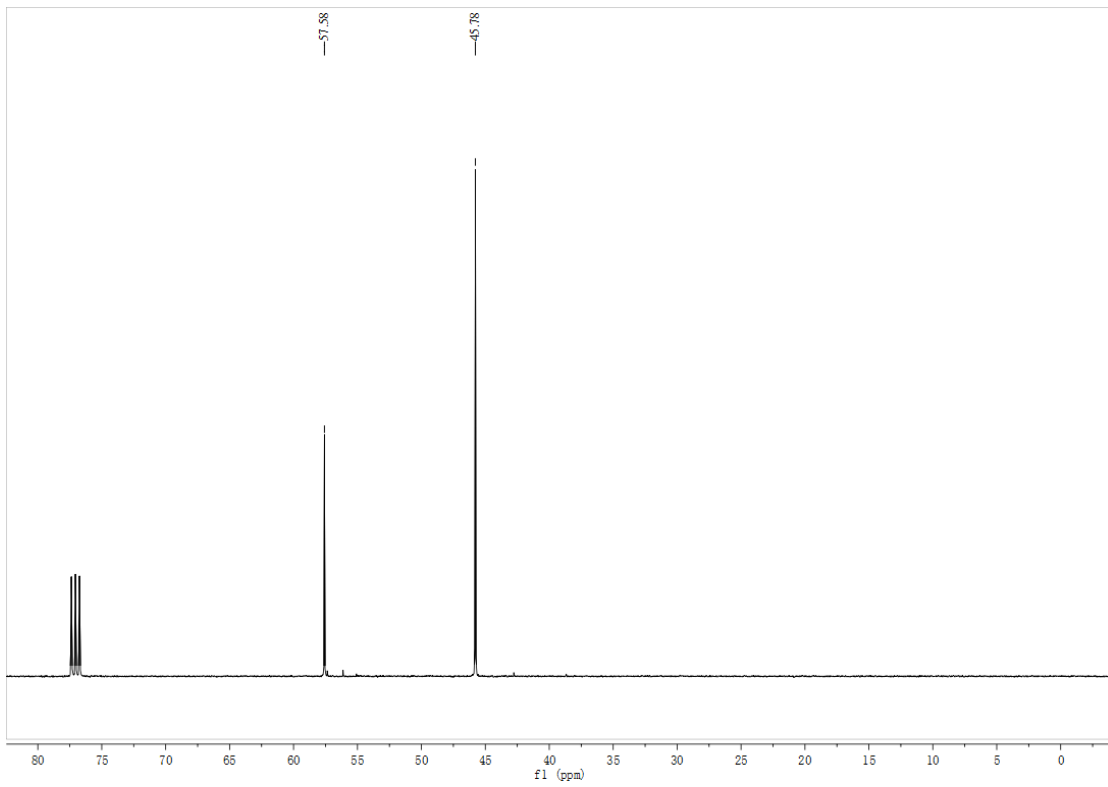
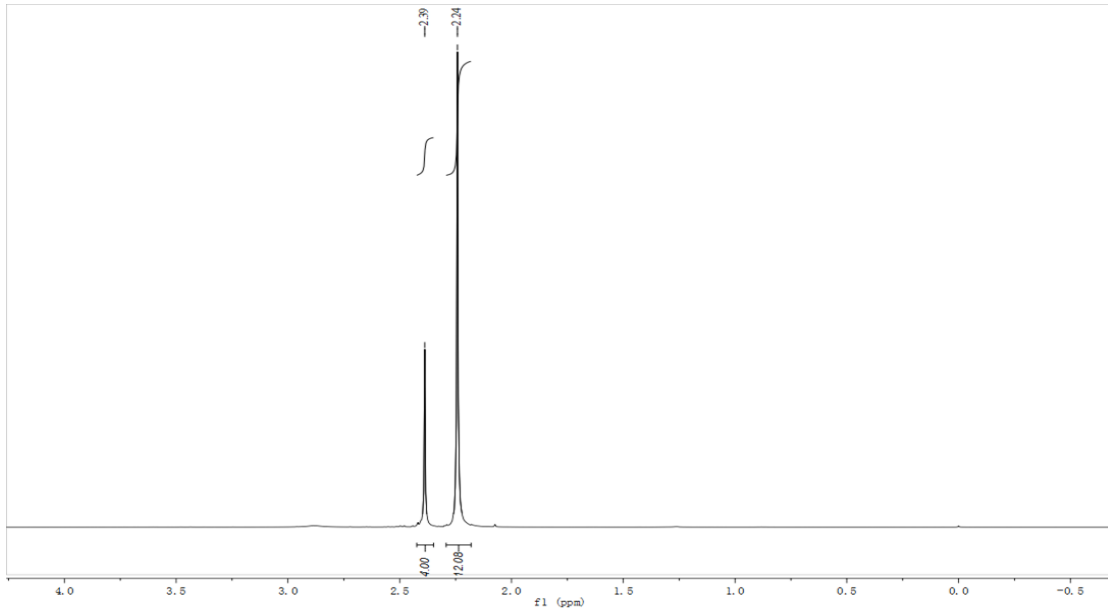
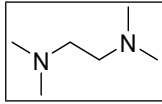
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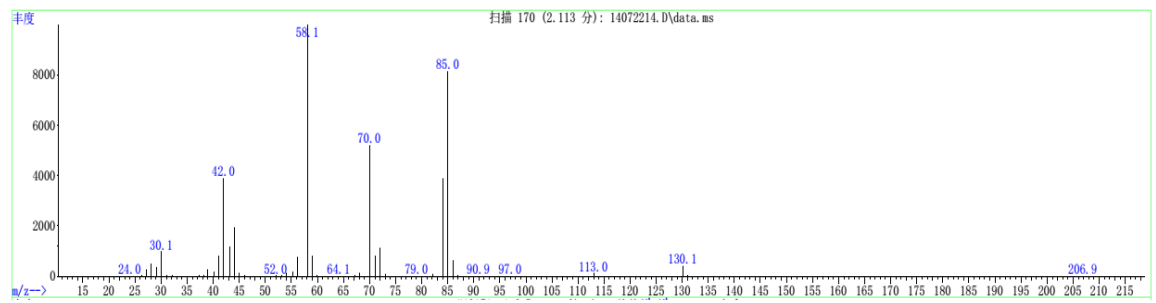
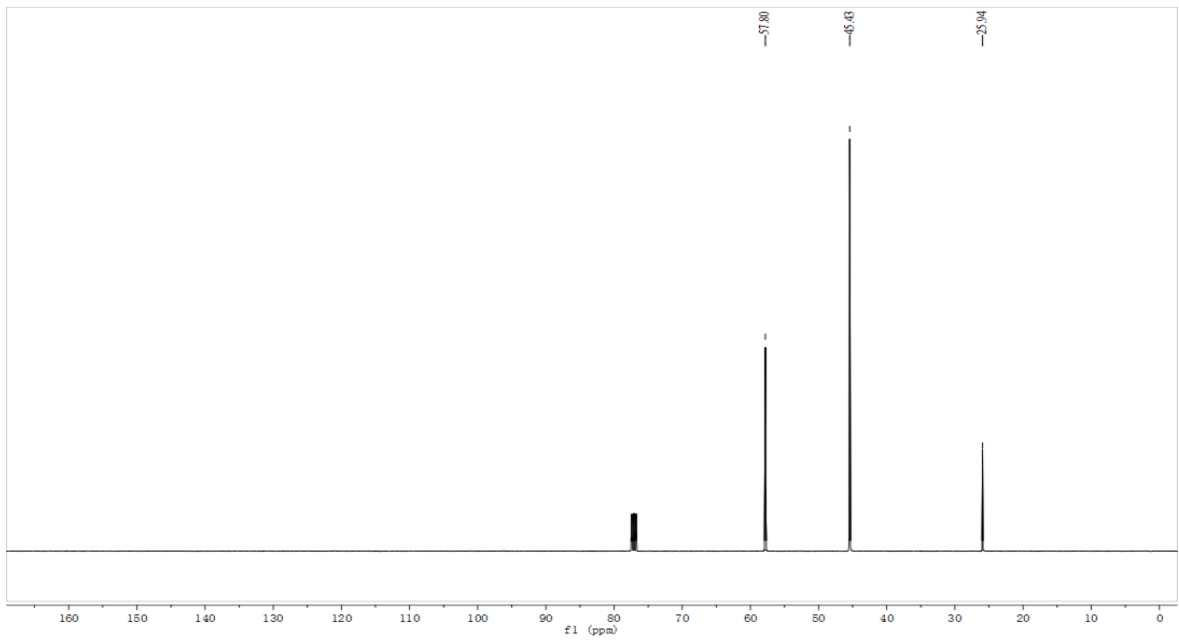
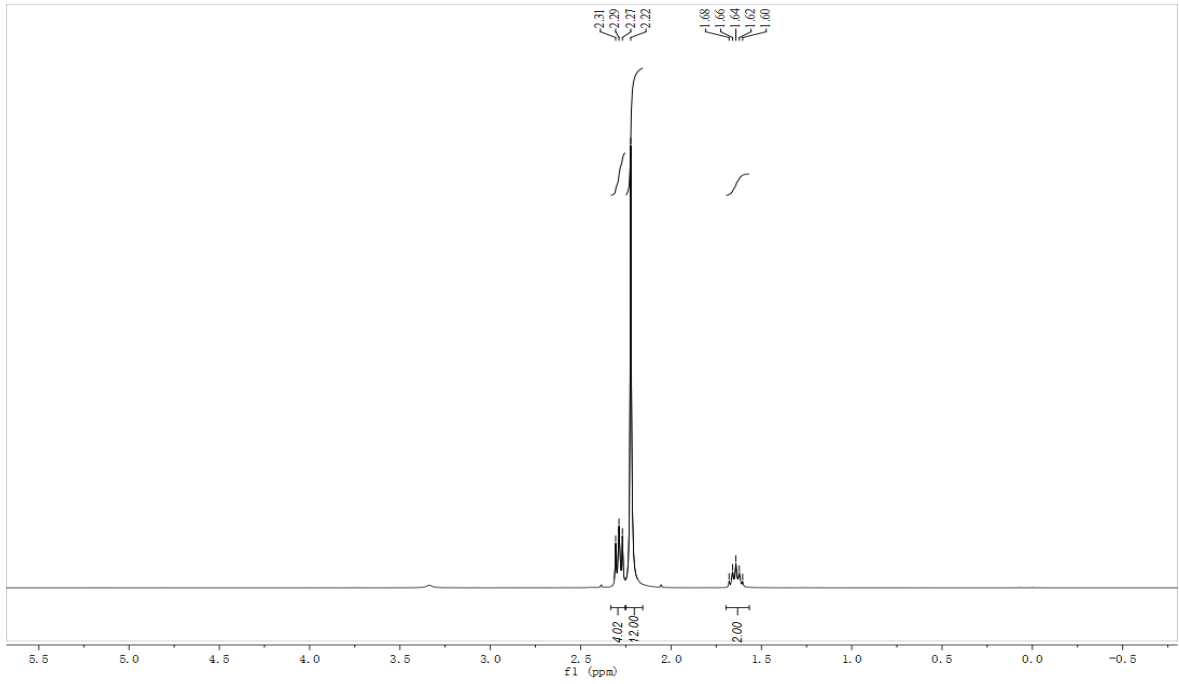
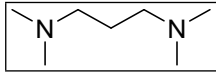
| | |
|---|-----|
| NMR and MS for Products..... | S3 |
| The Dissociation of H ₂ in the Ni(111) Surface | S14 |
| The Cartesian components | S15 |

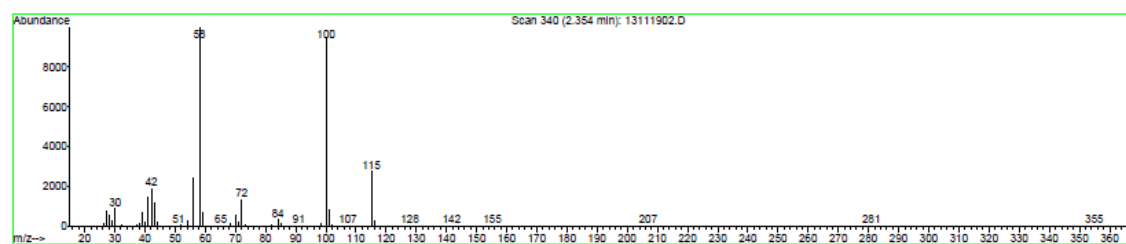
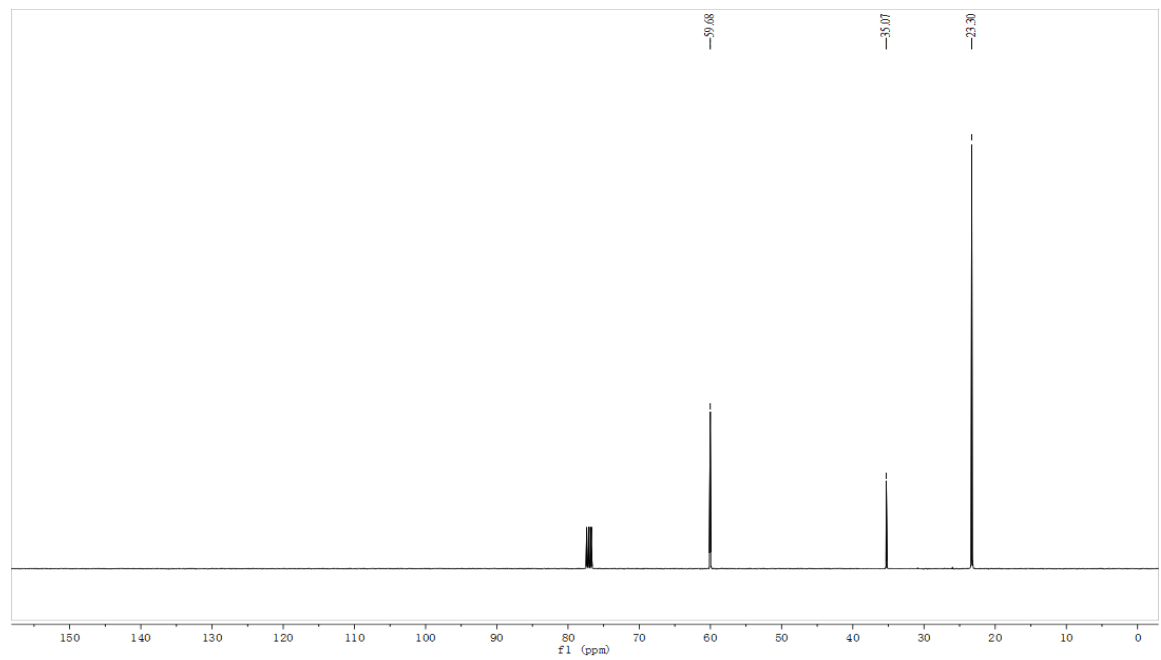
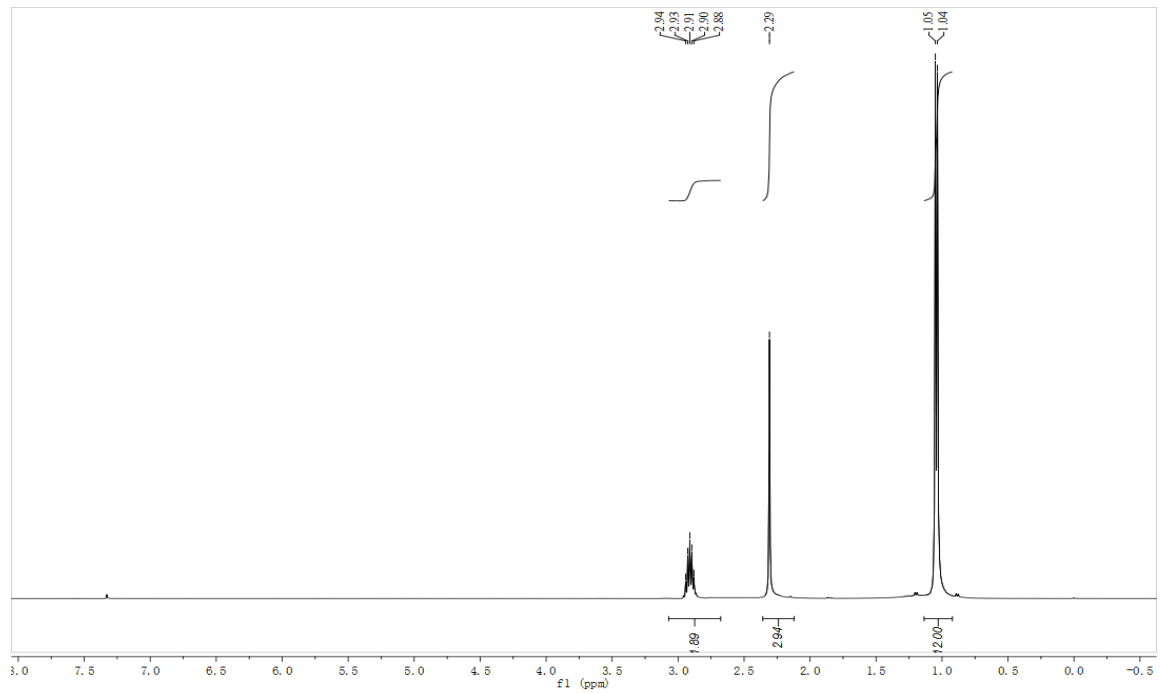
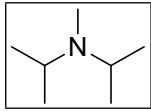
NMR and MS for Products

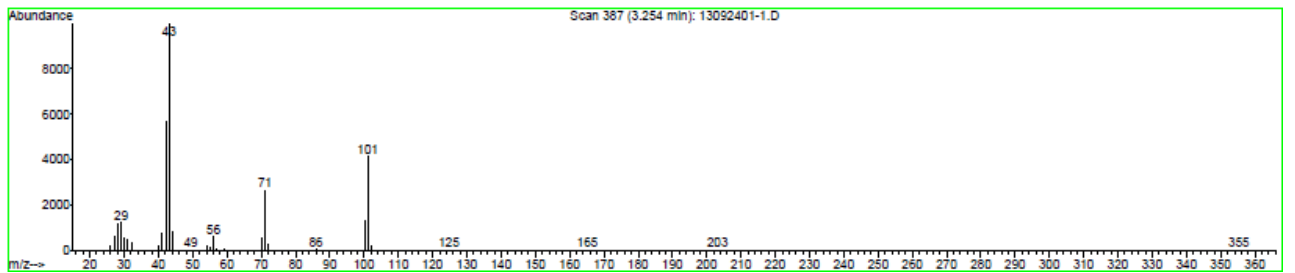
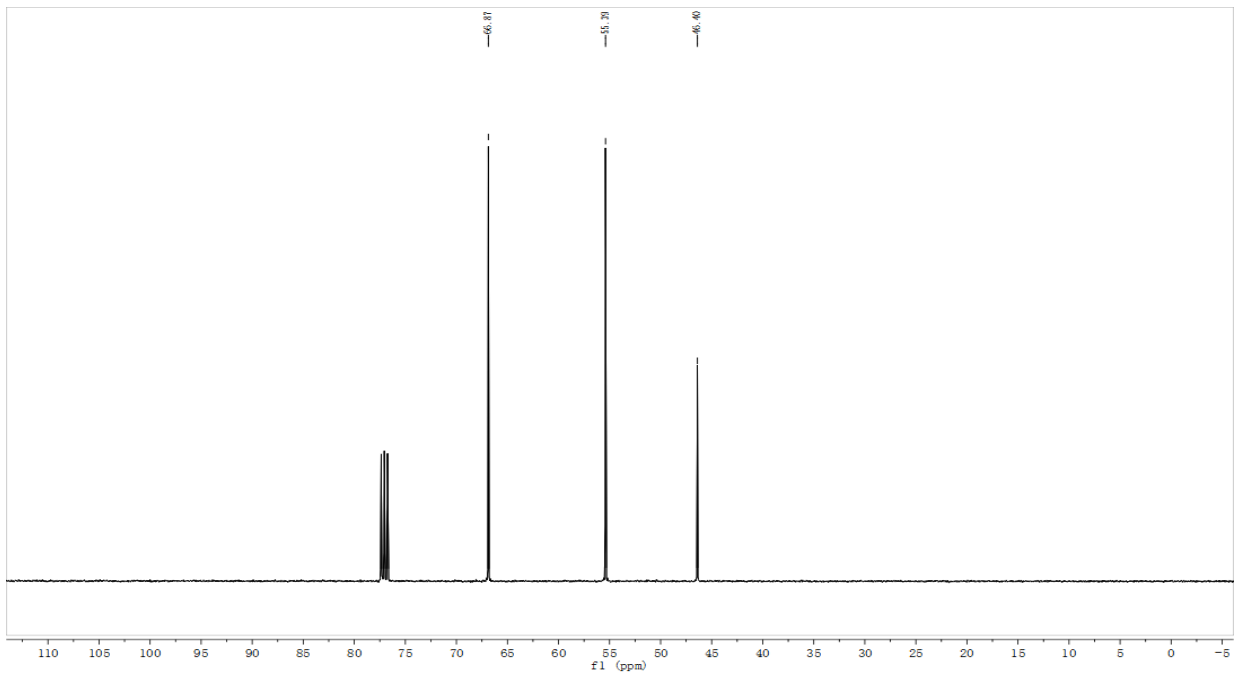
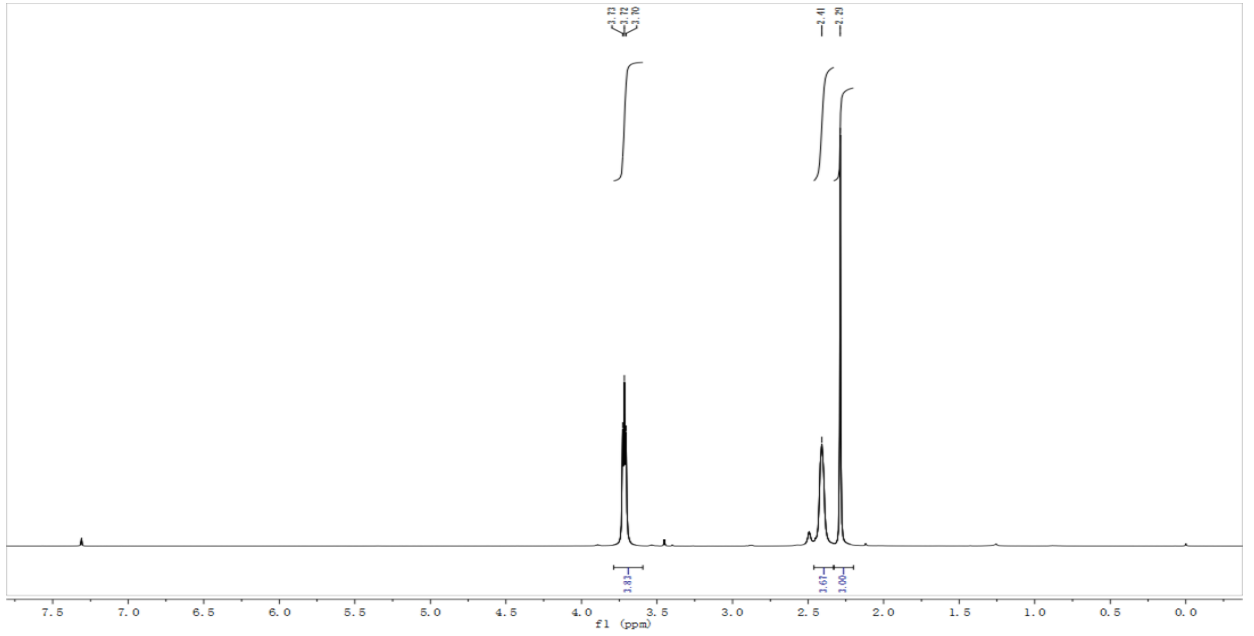
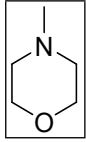


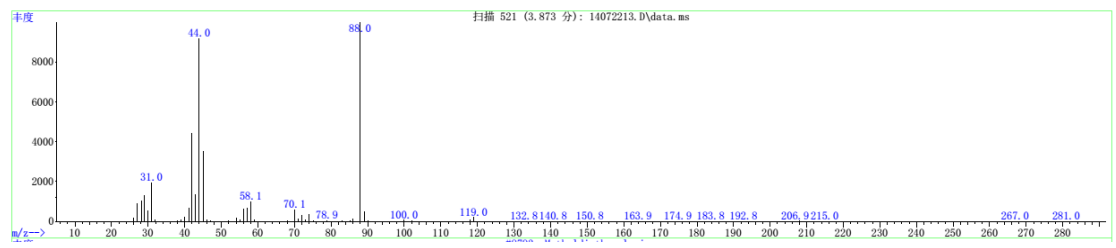
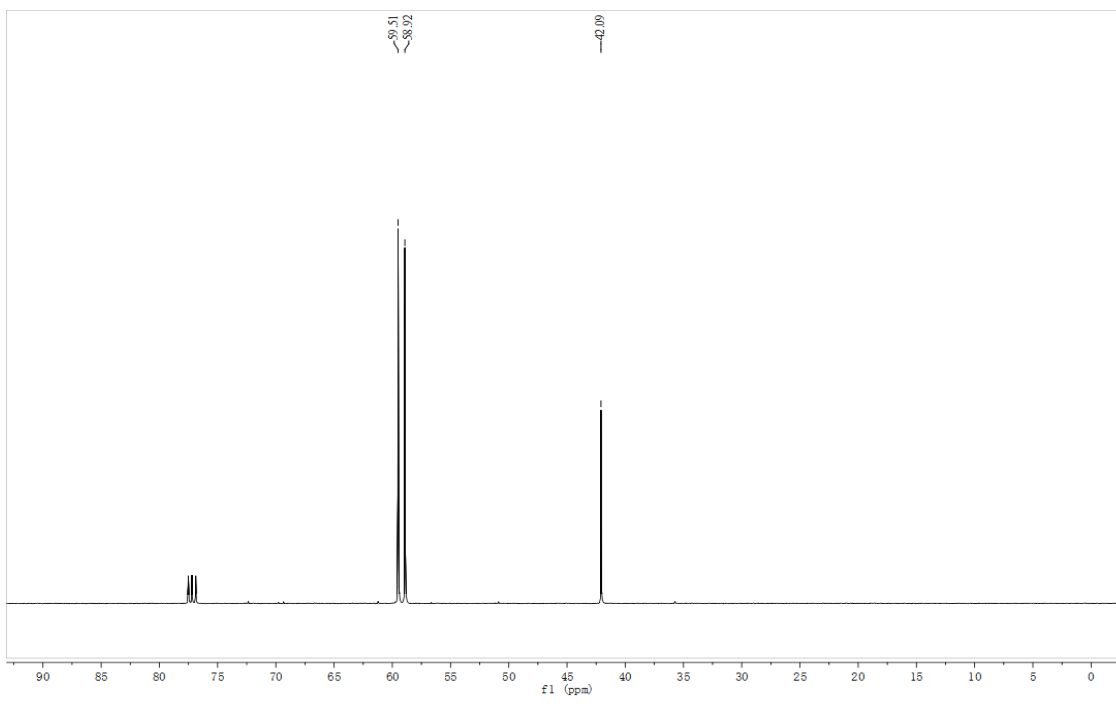
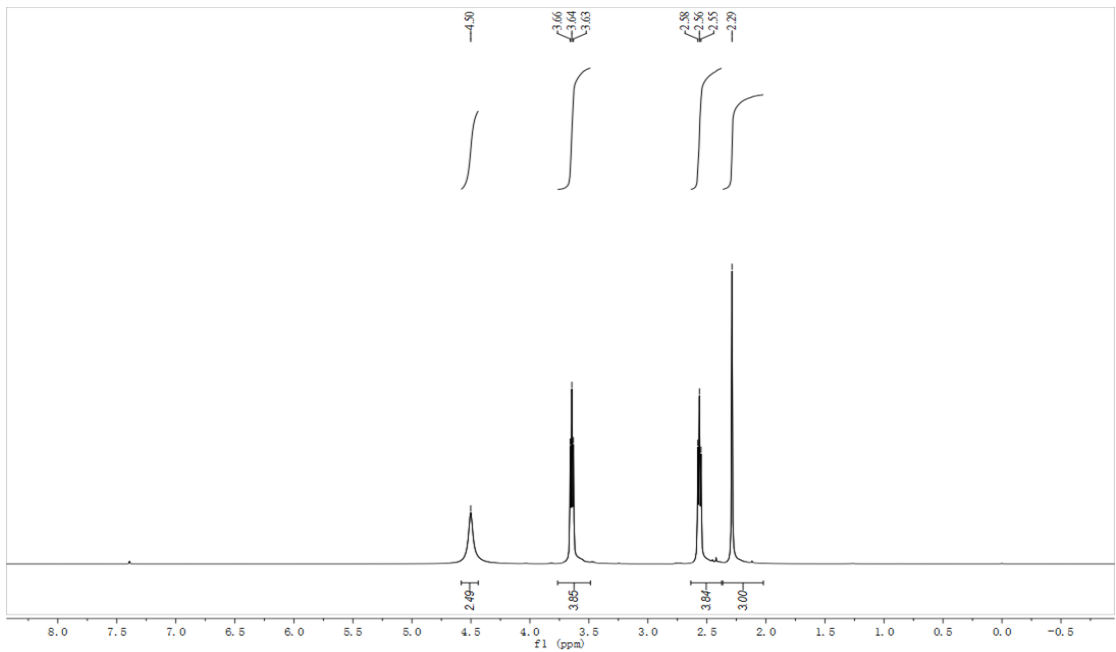
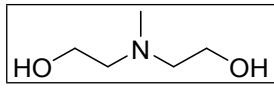


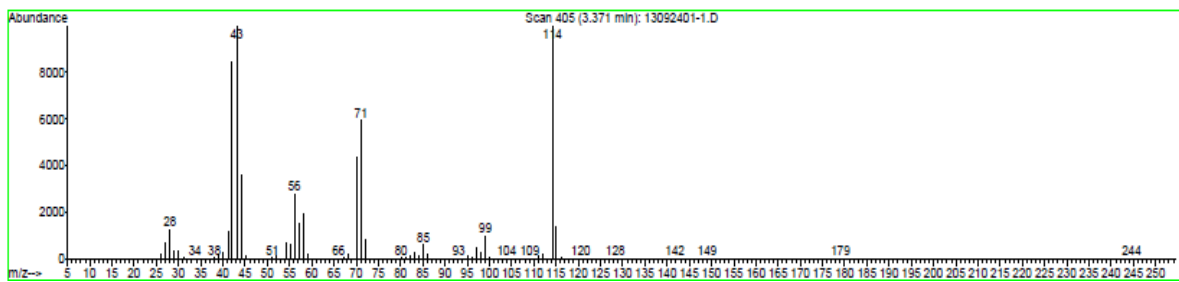
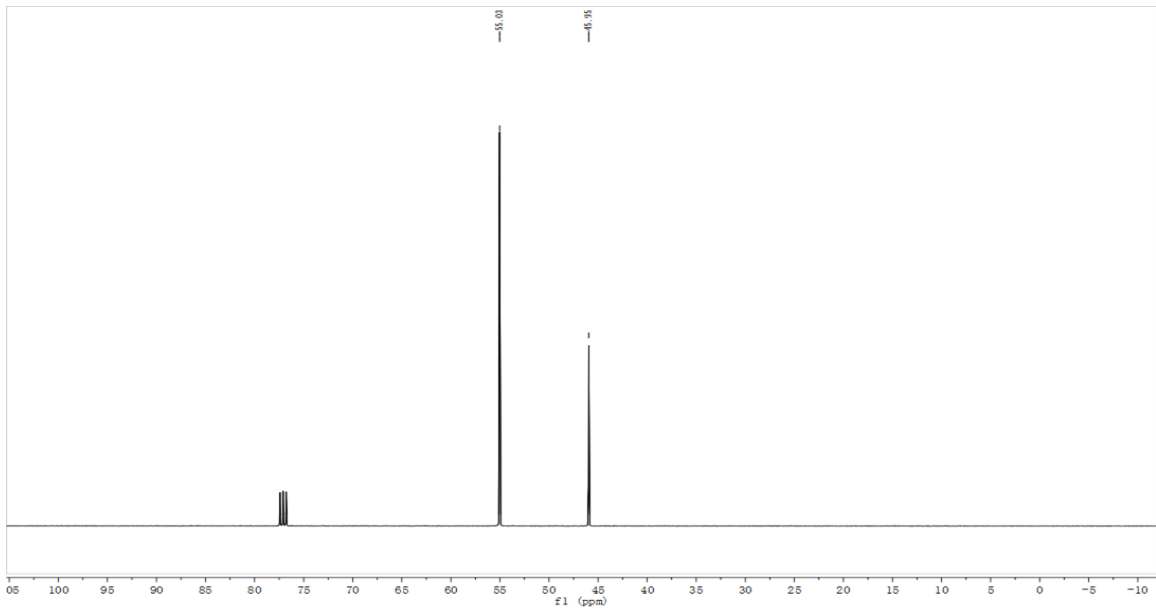
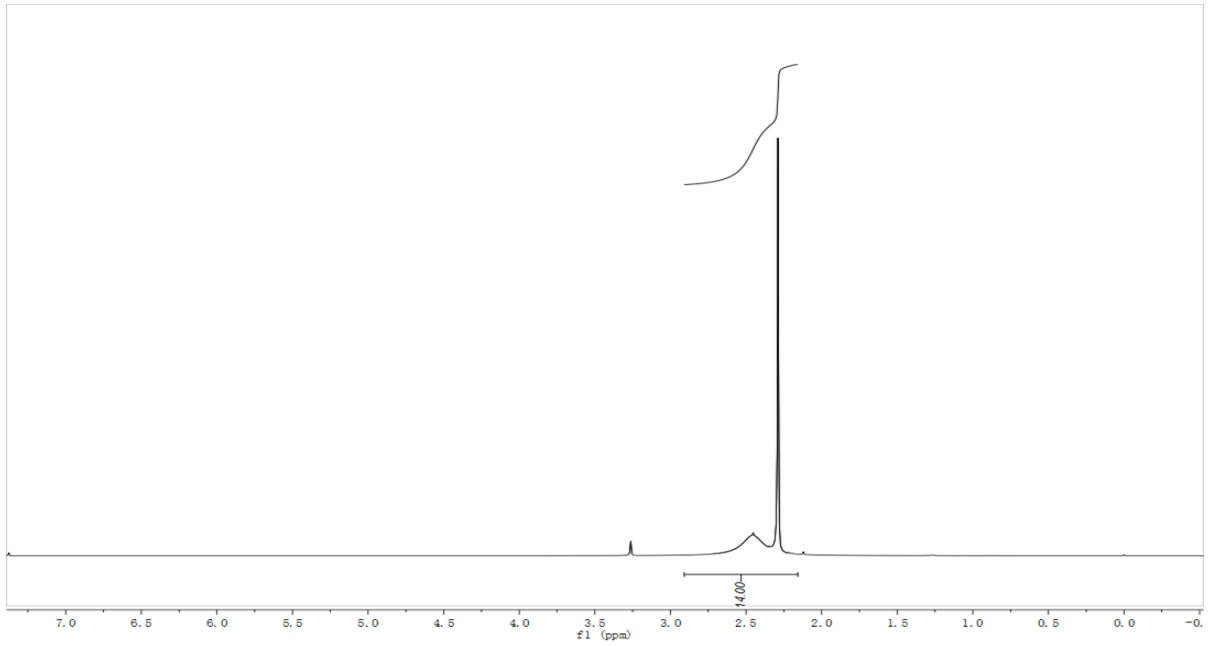
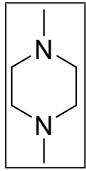


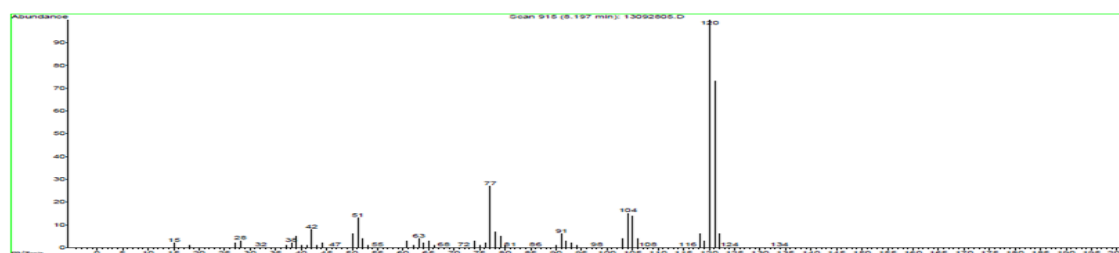
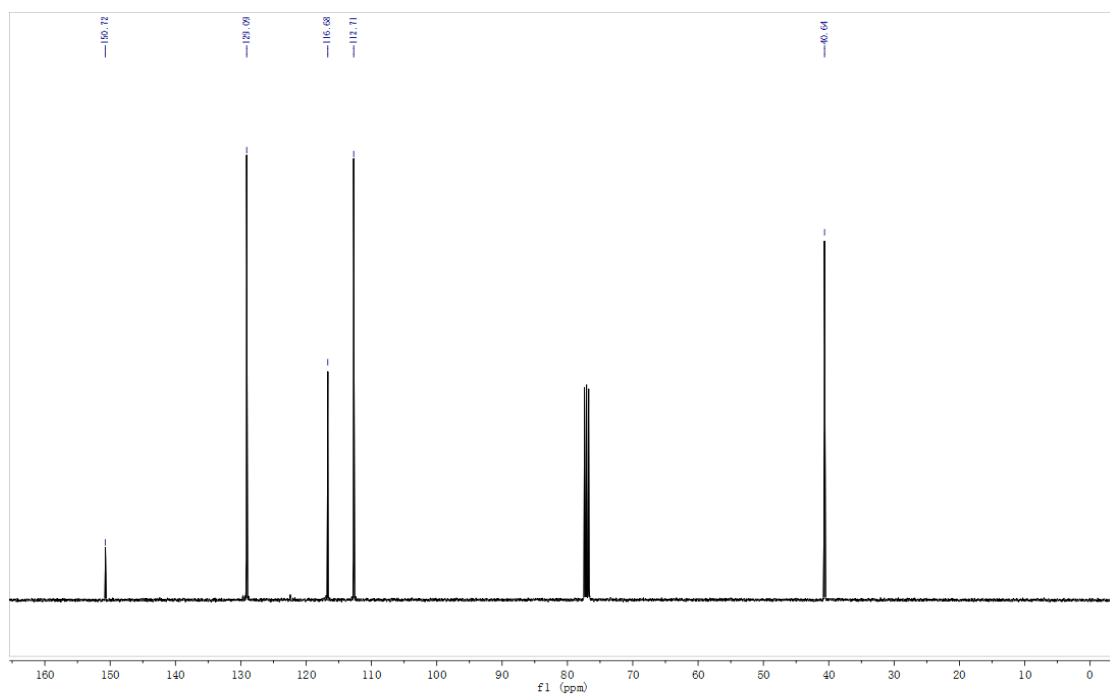
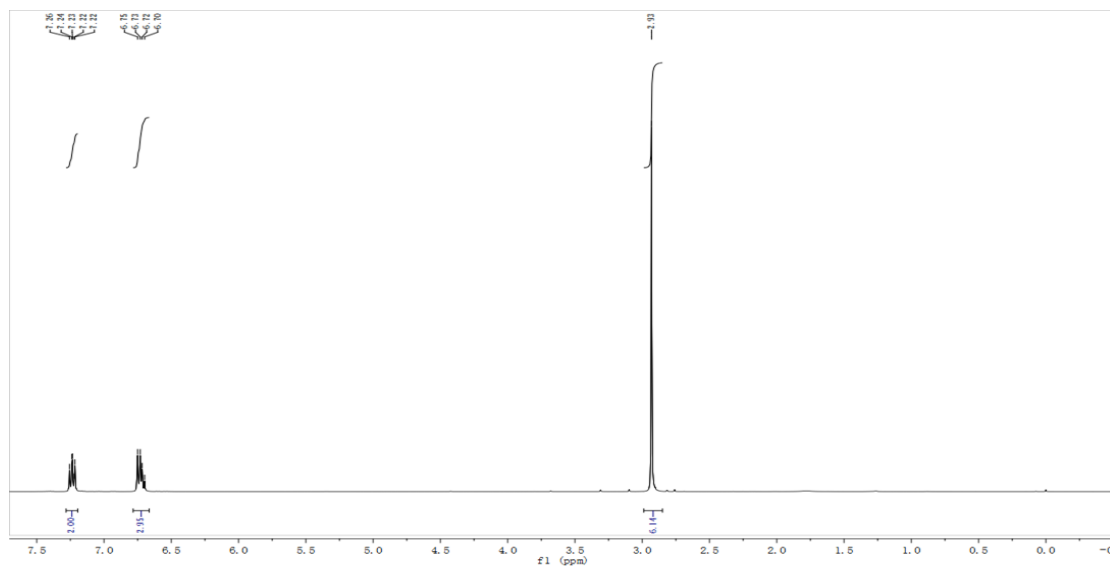
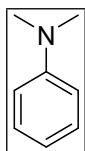


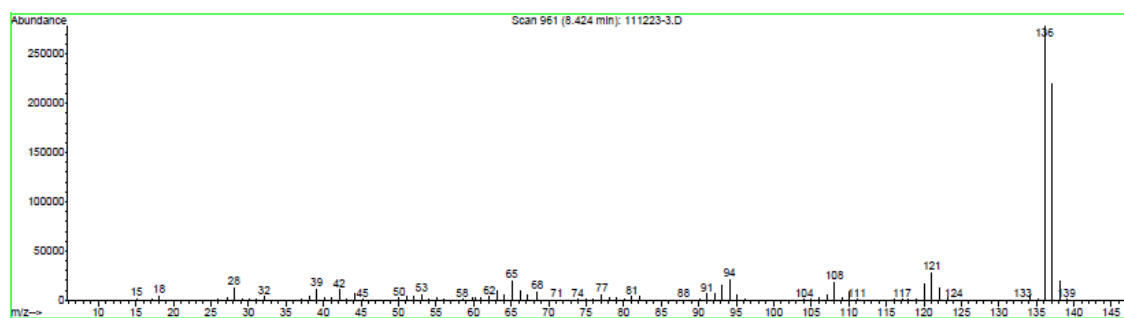
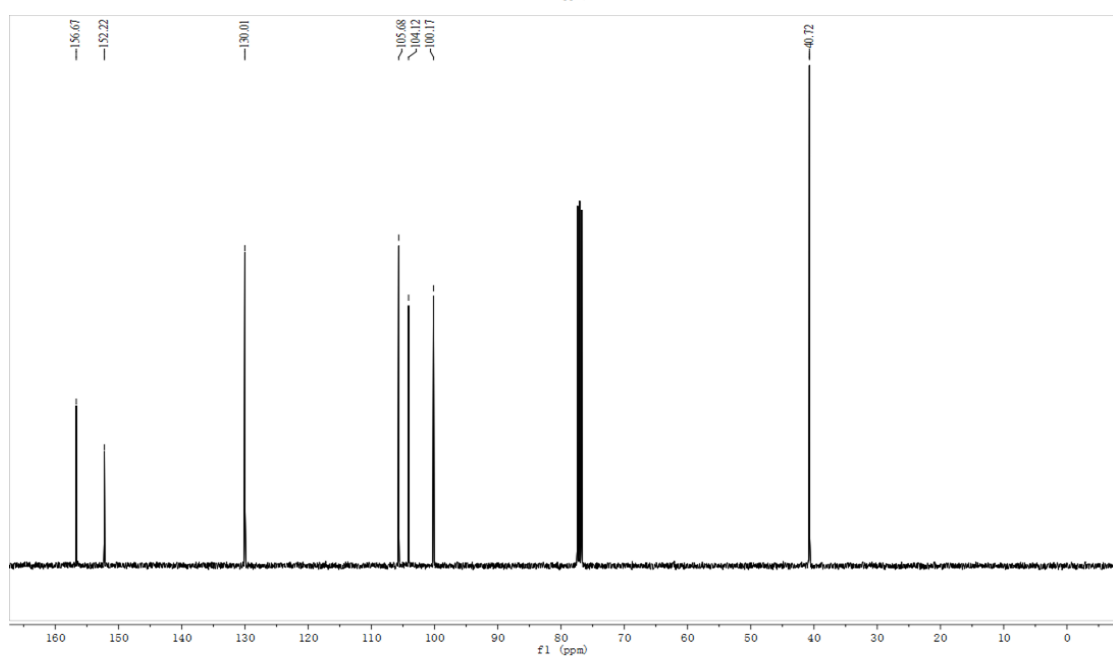
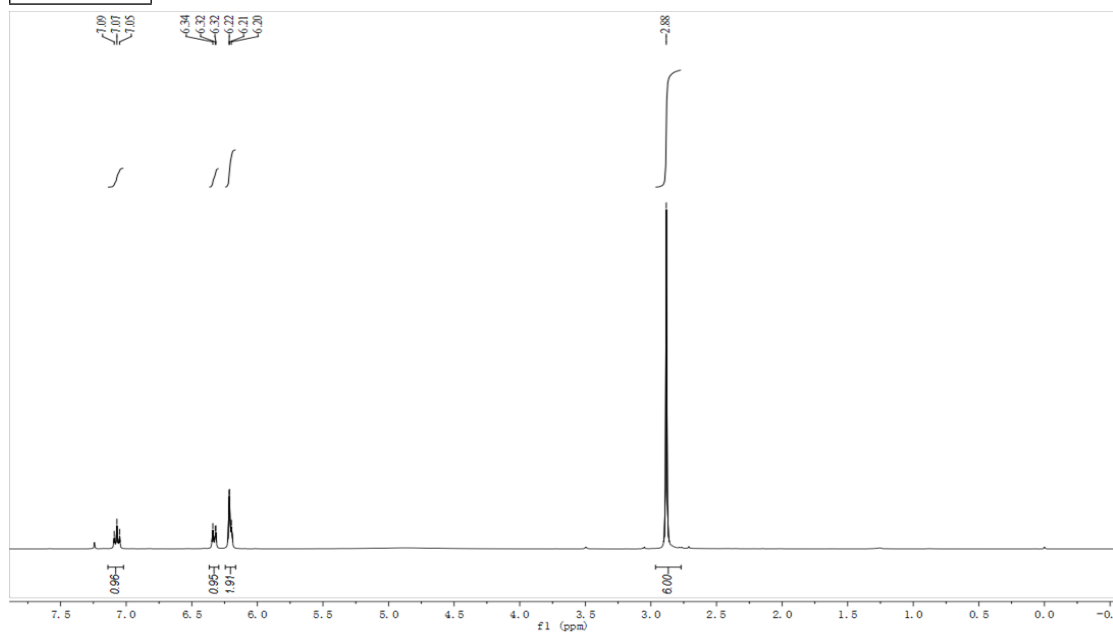
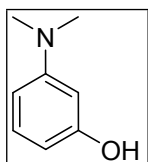


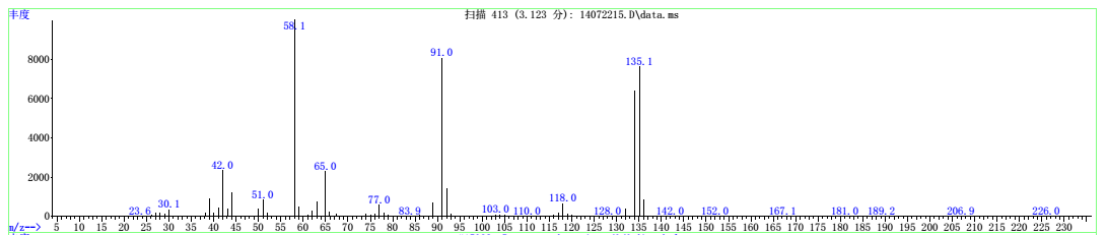
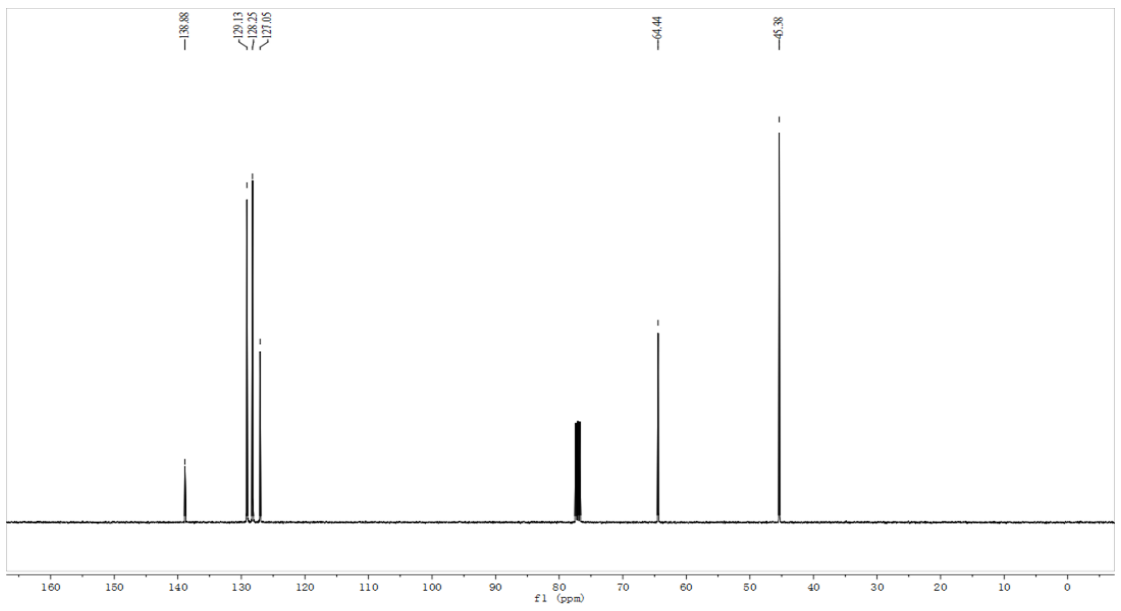
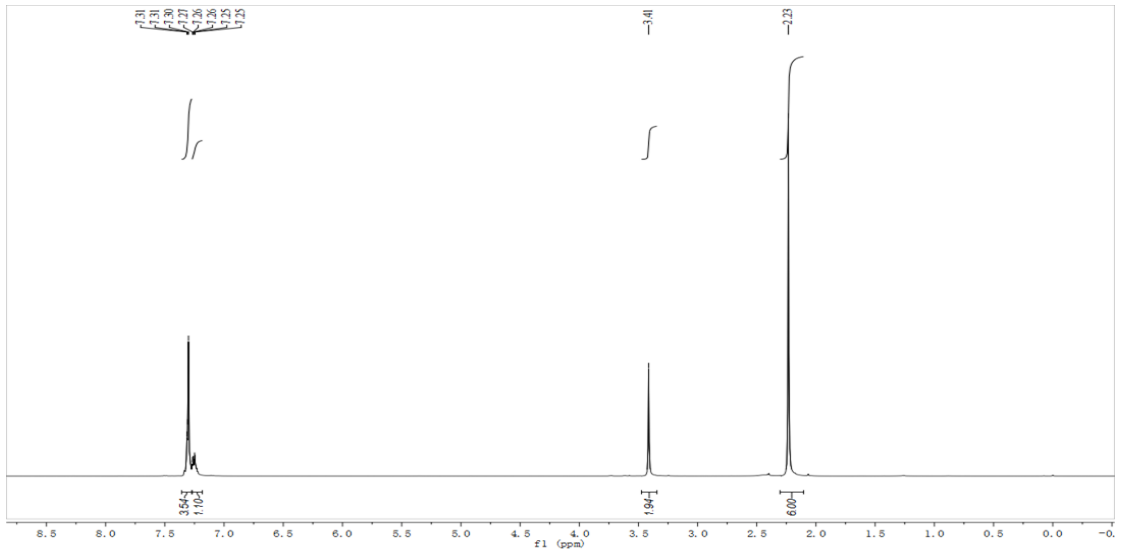
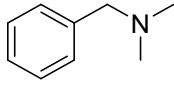




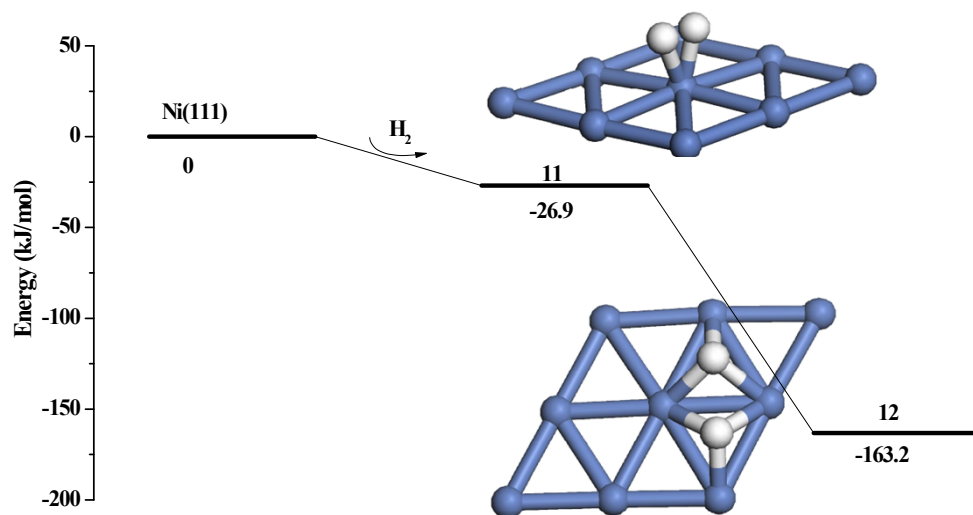








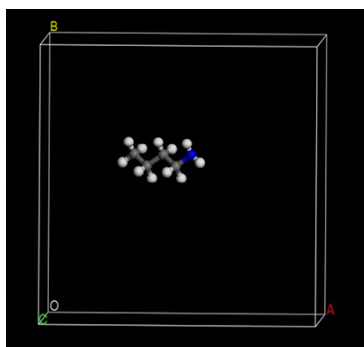
The Dissociation of H₂ in the Ni(111) Surface



11: H₂ located on top site of Ni(111).

12: H₂ located on hollow site of Ni(111).

The Cartesian components

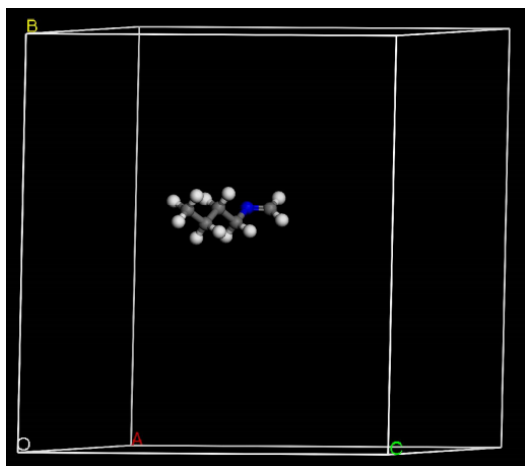


BFGS: Final Enthalpy = -1.06787546E+003 eV

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***** Forces *****
*
*                               Cartesian components (eV/A)                               *
* -----*
*           x           y           z           *
*
* H      1      -0.00092      -0.00709      -0.00202      *
* H      2       0.00284       0.00501      -0.00555      *
* H      3       0.00185       0.00611      -0.00391      *
* H      4       0.00346       0.00275       0.00344      *
* H      5      -0.00042      -0.00873      -0.00856      *
* H      6      -0.00416       0.00221      -0.00355      *
* H      7      -0.00033       0.00884      -0.00165      *
* H      8      -0.00588      -0.00313       0.00524      *
* H      9      -0.00367       0.00866       0.00235      *
* H     10      -0.00507      -0.01225      -0.01308      *
* H     11      -0.01356      -0.00093       0.01125      *
* C      1      -0.00570      -0.00292      -0.00147      *
* C      2       0.01134       0.00213       0.00956      *
* C      3       0.01513      -0.00156       0.00772      *
* C      4       0.00636       0.00037       0.00174      *
* N      1      -0.00126       0.00053      -0.00150      *
*
*****

```

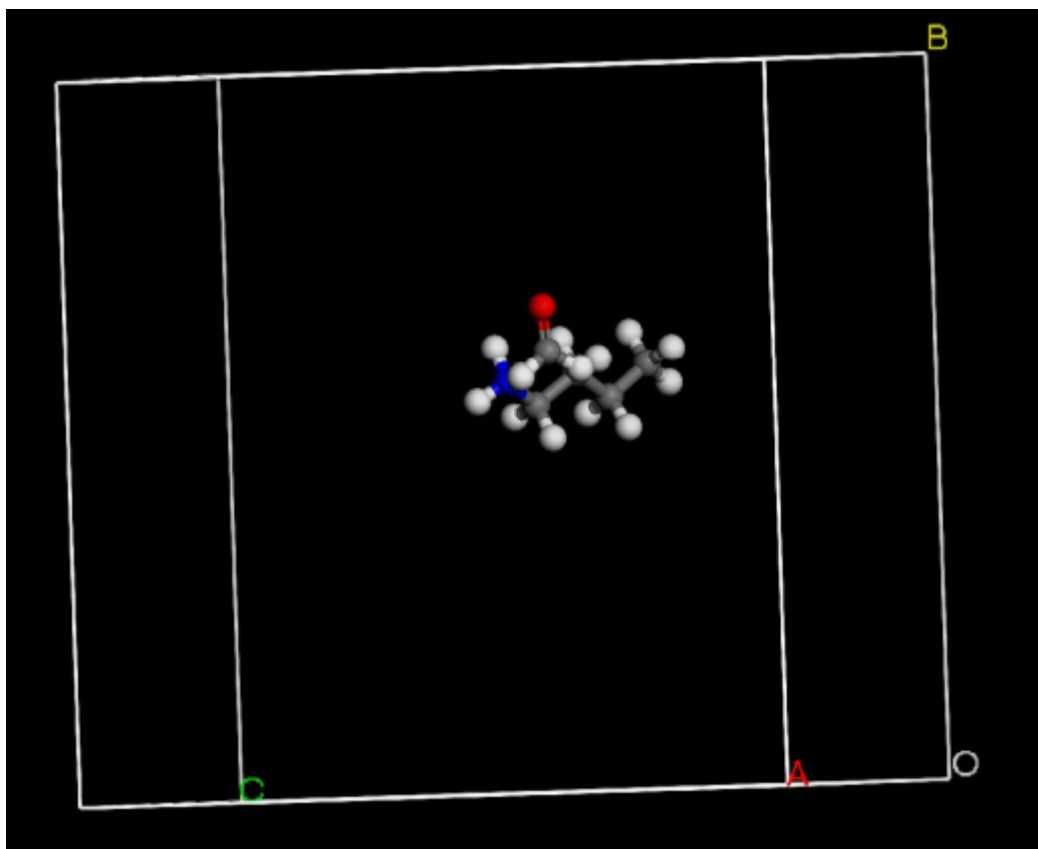


BFGS: Final Enthalpy = -1.22186255E+003 eV

```

***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 -0.00381 0.01140 0.00266 *
* H 2 -0.00495 -0.01019 -0.00320 *
* H 3 -0.00094 0.00087 0.00118 *
* H 4 0.00013 0.00274 -0.00031 *
* H 5 -0.00375 -0.00293 -0.00125 *
* H 6 -0.00340 -0.00050 -0.00331 *
* H 7 0.01063 -0.00291 0.00256 *
* H 8 -0.00087 -0.00363 -0.00545 *
* H 9 -0.00283 0.00109 -0.00411 *
* H 10 -0.00280 0.00583 0.00309 *
* H 11 0.00387 0.00631 0.00442 *
* C 1 0.00304 0.00061 0.00339 *
* C 2 0.00074 -0.00208 0.00710 *
* C 3 0.00389 -0.00193 0.00169 *
* C 4 0.00065 -0.00197 -0.00306 *
* C 5 0.00273 -0.00245 -0.00081 *
* N 1 -0.00233 -0.00026 -0.00459 *
*
*****

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BFGS: Final Enthalpy = -1.69106809E+003 eV

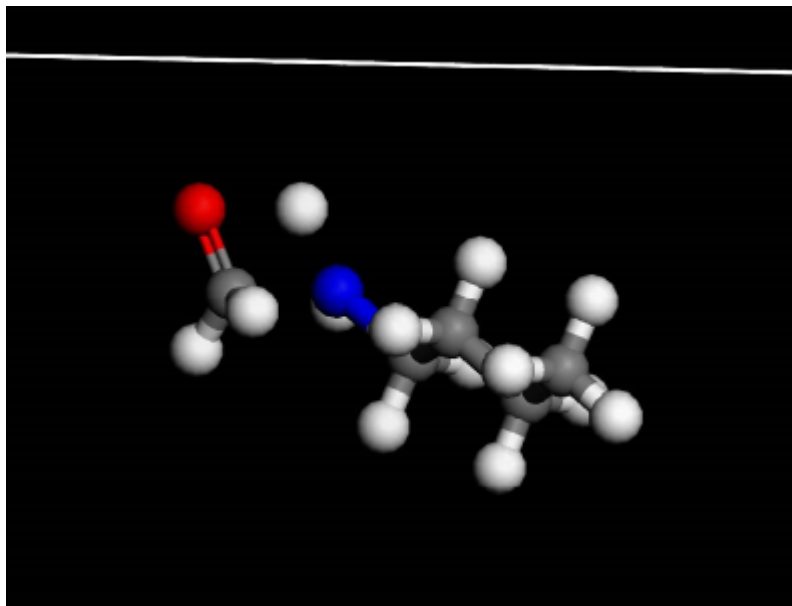
***** Forces *****

| | | Cartesian components (eV/A) | | | |
|-----|----|-----------------------------|----------|----------|---|
| | | x | y | z | |
| * H | 1 | 0.00125 | -0.00390 | -0.00238 | * |
| * H | 2 | -0.01285 | -0.00260 | 0.00076 | * |
| * H | 3 | -0.00485 | 0.00802 | 0.00146 | * |
| * H | 4 | 0.00461 | -0.00080 | -0.00478 | * |
| * H | 5 | 0.00345 | -0.00029 | 0.00101 | * |
| * H | 6 | 0.00435 | 0.00059 | 0.00623 | * |
| * H | 7 | -0.00481 | 0.00098 | -0.00431 | * |
| * H | 8 | 0.00681 | -0.00494 | 0.00079 | * |
| * H | 9 | -0.00280 | 0.00528 | -0.00160 | * |
| * H | 10 | -0.00003 | -0.00478 | -0.00270 | * |
| * H | 11 | 0.00133 | 0.00203 | -0.00570 | * |
| * H | 12 | 0.00181 | 0.00078 | 0.00410 | * |
| * H | 13 | 0.00318 | 0.00301 | 0.00116 | * |
| * C | 1 | -0.00553 | 0.00117 | 0.00222 | * |
| * C | 2 | -0.00049 | -0.00077 | -0.00199 | * |
| * C | 3 | -0.00041 | -0.00009 | 0.00044 | * |

```

* C      4      0.00236      -0.00364      -0.00344      *
* C      5      0.00410           0.00035      -0.00377      *
* N      1      0.00139      -0.00329           0.00645      *
* O      1     -0.00290           0.00289           0.00606      *
*
*****

```



Final energy = -1689.249869908 eV

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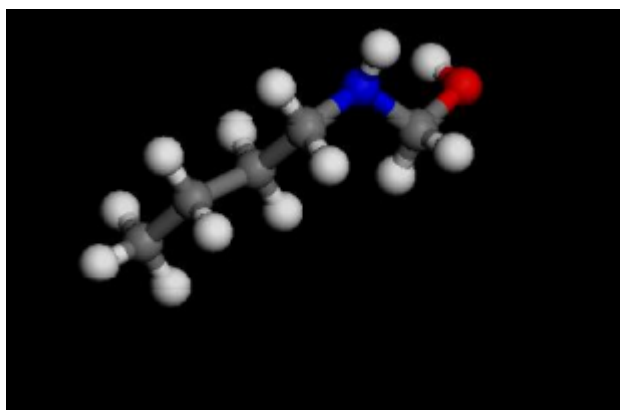
***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H  1  0.06185 -0.02460  0.05245 *
* H  2  0.01837  0.00657  0.00407 *
* H  3  0.02066  0.00713  0.01239 *
* H  4  0.07323  0.02276  0.04053 *
* H  5  0.05197 -0.00684  0.07406 *
* H  6 -0.07389  0.20133 -0.04978 *
* H  7  0.03238  0.14140 -0.07800 *
* H  8  0.30273  0.45483  0.26704 *
* H  9  0.30730  0.37180  0.30577 *
* H 10  0.30399  1.28503 -1.23550 *
* H 11 -1.41826 -1.29793 -0.83647 *
* H 12  0.11370 -0.27223  0.19628 *
* H 13  0.24308 -0.36111 -0.07370 *
* C  1  0.02294 -0.03982  0.03630 *

```

```

* C      2      0.10750      0.09522      0.05223      *
* C      3     -0.00544     -0.01082     0.13227      *
* C      4      0.18026      0.64464     -0.18832      *
* C      5     -0.59510     -0.68356     -0.75894      *
* N      1      0.91553     -0.67191     0.77378      *
* O      1     -0.66279      0.13809     1.27353      *
*

```



BFGS: Final Enthalpy = -1.69164755E+003 eV

***** Forces *****

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*
* Cartesian components (eV/A)
* -----

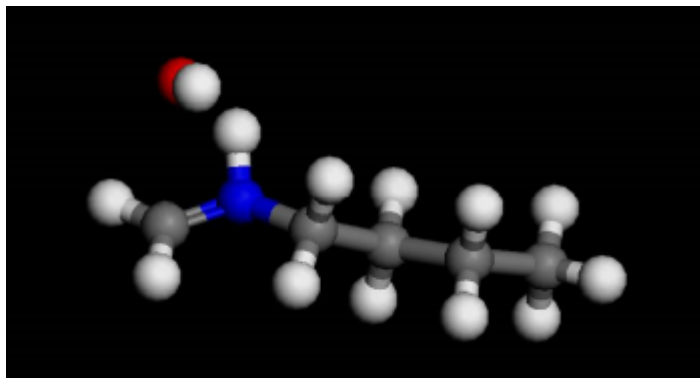
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| | x | y | z |
|--------|----------|----------|----------|
| * H 1 | 0.00656 | -0.00561 | 0.00592 |
| * H 2 | 0.00383 | -0.00818 | 0.00563 |
| * H 3 | -0.00335 | 0.00563 | -0.00737 |
| * H 4 | 0.00674 | 0.00201 | -0.00784 |
| * H 5 | 0.00648 | -0.00529 | -0.01026 |
| * H 6 | -0.01091 | -0.00332 | 0.00147 |
| * H 7 | 0.00497 | 0.00258 | 0.00249 |
| * H 8 | -0.01415 | 0.01116 | -0.01317 |
| * H 9 | -0.00503 | -0.01092 | 0.00246 |
| * H 10 | 0.00183 | 0.00109 | -0.00318 |
| * H 11 | -0.00697 | 0.00180 | -0.00436 |
| * H 12 | -0.00581 | -0.00363 | 0.00677 |
| * H 13 | -0.00059 | 0.00445 | 0.00536 |
| * C 1 | 0.00095 | -0.00204 | 0.00706 |
| * C 2 | 0.00865 | -0.00134 | -0.00063 |
| * C 3 | -0.00004 | 0.00032 | 0.00115 |
| * C 4 | -0.00196 | -0.00201 | 0.00427 |
| * C 5 | 0.00433 | 0.00165 | 0.00028 |

```

* N      1      0.00335      0.00382      0.00171      *
* O      1      0.00113      0.00781      0.00222      *
*
*****

```



Final energy = -1689.451928766 eV

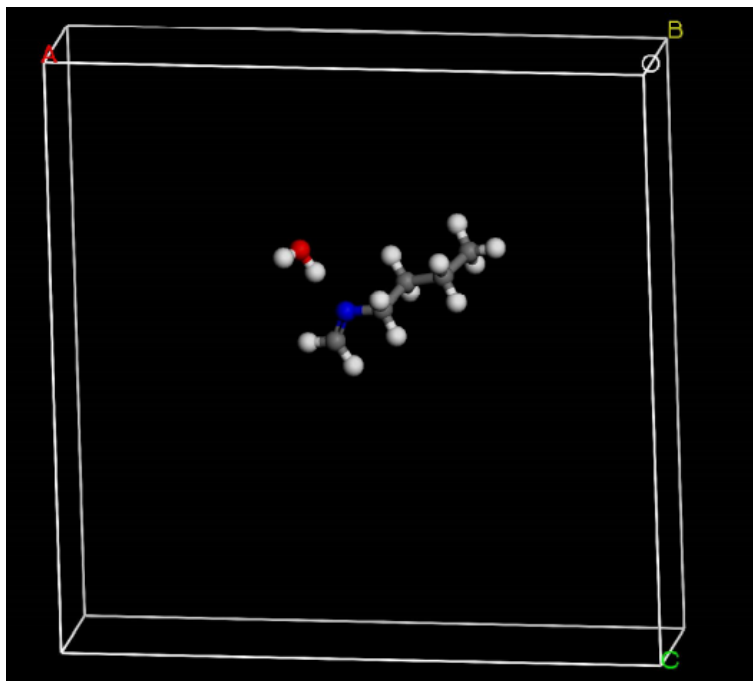
***** Forces *****

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*
*                               Cartesian components (eV/A)                               *
* -----*
*           x           y           z           *
*
* H      1      -0.02456      -0.01188      0.00325      *
* H      2       0.00388       0.01917      -0.00561      *
* H      3       0.01792      -0.01341      0.01669      *
* H      4      -0.05783      -0.01601      -0.01589      *
* H      5      -0.00491       0.00088       0.02208      *
* H      6      -0.01420       0.02116      -0.02415      *
* H      7      -0.00618       0.02345      -0.04505      *
* H      8      -0.00412       0.02799       0.01318      *
* H      9      -0.10210      -0.00634       0.01686      *
* H     10      -0.04684      -0.22231       0.29465      *
* H     11      -0.02636       0.07818      -0.11748      *
* H     12       0.28479      -0.06051      -0.12774      *
* H     13       0.00813      -0.03709      -0.23998      *
* C      1      -0.02182      -0.00366      -0.01932      *
* C      2      -0.01314      -0.00230       0.00412      *
* C      3      -0.07239       0.02687      -0.06049      *
* C      4      -0.18034      -0.02660       0.04172      *
* C      5      -0.21787       0.01282      -0.28384      *
* N      1       0.10381       0.06152       0.29314      *
* O      1       0.37412       0.12807       0.23385      *

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*



BFGS: Final Enthalpy = -1.69149116E+003 eV

***** Forces *****

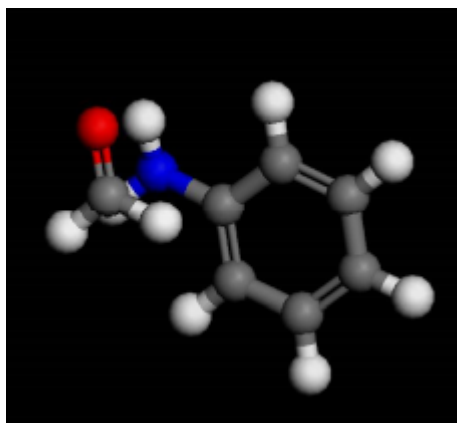
*
 * Cartesian components (eV/A) *
 * ----- *

| | | x | y | z | |
|-----|----|----------|----------|----------|---|
| * H | 1 | 0.00014 | -0.01044 | 0.00221 | * |
| * H | 2 | -0.00542 | 0.00623 | -0.00744 | * |
| * H | 3 | 0.00476 | -0.00406 | 0.00800 | * |
| * H | 4 | -0.00191 | -0.00305 | 0.00160 | * |
| * H | 5 | 0.00365 | 0.00188 | 0.00090 | * |
| * H | 6 | -0.00990 | 0.00446 | -0.01074 | * |
| * H | 7 | 0.00279 | -0.00058 | 0.00943 | * |
| * H | 8 | -0.00743 | 0.00028 | -0.00589 | * |
| * H | 9 | 0.00600 | 0.01468 | -0.00343 | * |
| * H | 10 | 0.00748 | 0.01179 | 0.00018 | * |
| * H | 11 | -0.00132 | -0.00639 | -0.01098 | * |
| * H | 12 | -0.00583 | -0.00122 | 0.00807 | * |
| * H | 13 | 0.01560 | 0.00091 | 0.00141 | * |
| * C | 1 | -0.00048 | -0.00035 | -0.00297 | * |
| * C | 2 | -0.00231 | -0.00483 | -0.00102 | * |
| * C | 3 | -0.00226 | -0.00317 | 0.00682 | * |
| * C | 4 | 0.00204 | -0.00057 | 0.00100 | * |

```

* C      5      -0.00122          0.00710          -0.00021      *
* N      1      -0.00089         -0.01041         -0.00453      *
* O      1      -0.00349         -0.00225          0.00758      *
*

```



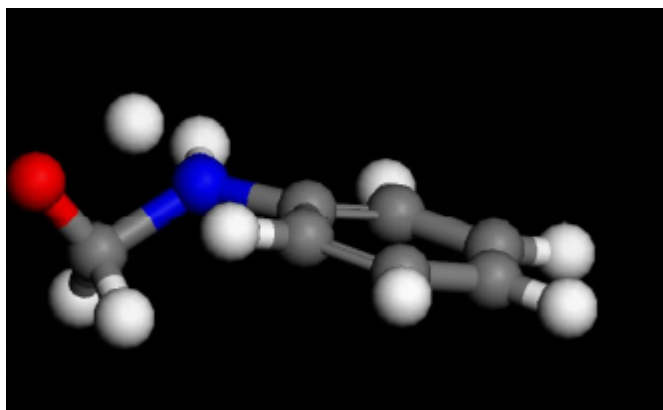
BFGS: Final Enthalpy = -1.93575116E+003 eV
 BFGS: Final <frequency> = 1870.45584 cm-1

***** Forces *****

```

*
*                               Cartesian components (eV/A)                               *
* ----- *
*           x           y           z           *
*
* H      1      -0.00357          0.00166         -0.00056      *
* H      2      -0.00732          0.00403          0.00628      *
* H      3       0.00361          0.00107          0.00479      *
* H      4       0.00042          0.01316          0.00164      *
* H      5       0.00131         -0.00855          0.00114      *
* H      6       0.00072          0.01597          0.00341      *
* H      7       0.00044         -0.00598         -0.00970      *
* H      8       0.00173         -0.01402          0.00007      *
* H      9       0.00632          0.01455          0.00605      *
* C      1       0.00401          0.00076         -0.00917      *
* C      2      -0.00073         -0.00101          0.00268      *
* C      3       0.00339         -0.00210          0.00707      *
* C      4      -0.00523         -0.00379          0.00148      *
* C      5       0.00055         -0.00298         -0.00784      *
* C      6      -0.00416          0.00586         -0.00107      *
* C      7       0.00127         -0.00673          0.00040      *
* N      1      -0.00291         -0.00429         -0.00426      *
* O      1       0.00015         -0.00762         -0.00241      *
*

```

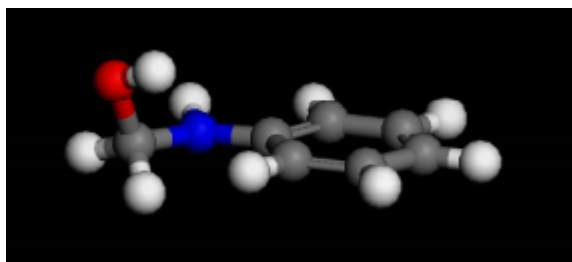


Final energy = -1933.913739552 eV

```

***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 0.12438 -0.21793 0.32846 *
* H 2 0.04241 0.74234 1.16058 *
* H 3 0.51130 0.12861 -0.13722 *
* H 4 0.63870 0.63152 -0.21205 *
* H 5 -0.34858 -0.54480 0.11197 *
* H 6 -0.78335 -0.57469 0.17335 *
* H 7 -0.02417 0.04568 -0.02263 *
* H 8 -0.57479 0.40689 -0.02910 *
* H 9 -0.69084 -1.48871 -2.16449 *
* C 1 -0.24718 -0.11313 0.26479 *
* C 2 0.58140 0.96239 -0.21389 *
* C 3 0.19853 -0.73439 0.06291 *
* C 4 1.16316 1.35504 -0.33171 *
* C 5 -0.23417 -1.39447 -0.38281 *
* C 6 0.07747 0.45908 0.00012 *
* C 7 -0.63542 -0.50874 0.24219 *
* N 1 0.51475 1.26051 0.74301 *
* O 1 -0.31361 -0.41518 0.40650 *
*
*****

```



BFGS: Final Enthalpy = -1.93644423E+003 eV

BFGS: Final <frequency> = 2216.97850 cm-1

***** Forces *****

* * *

* Cartesian components (eV/A) * *

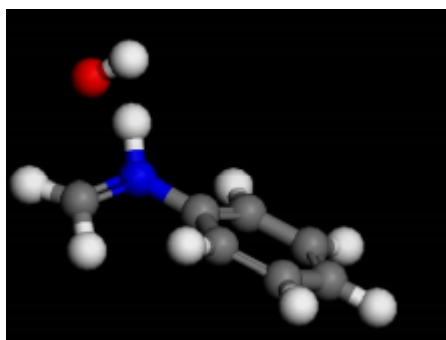
* ----- *

* x y z *

* * *

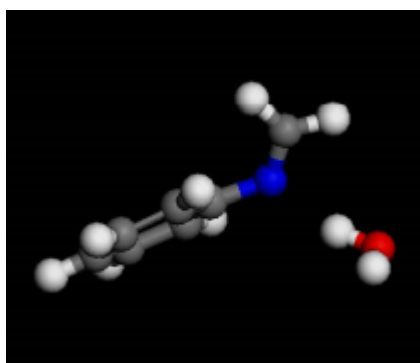
| | | | | | |
|-----|---|----------|----------|----------|---|
| * H | 1 | -0.00031 | 0.00056 | -0.00177 | * |
| * H | 2 | 0.00209 | 0.00185 | -0.00486 | * |
| * H | 3 | 0.00420 | 0.00006 | 0.00077 | * |
| * H | 4 | 0.00073 | 0.00129 | 0.00631 | * |
| * H | 5 | -0.00445 | 0.00457 | -0.00038 | * |
| * H | 6 | -0.00184 | 0.00112 | -0.01358 | * |
| * H | 7 | -0.00144 | 0.00588 | -0.00231 | * |
| * H | 8 | 0.00024 | 0.00507 | 0.00653 | * |
| * H | 9 | 0.00045 | -0.00684 | -0.00329 | * |
| * C | 1 | 0.00080 | 0.00544 | 0.00335 | * |
| * C | 2 | 0.00317 | -0.00810 | 0.00122 | * |
| * C | 3 | 0.00261 | -0.00220 | -0.00081 | * |
| * C | 4 | -0.00549 | 0.00166 | 0.00196 | * |
| * C | 5 | -0.00056 | -0.00409 | 0.00387 | * |
| * C | 6 | 0.00203 | -0.00298 | -0.00308 | * |
| * C | 7 | -0.00514 | -0.00061 | -0.00297 | * |
| * N | 1 | 0.00587 | 0.00098 | 0.00627 | * |
| * O | 1 | -0.00296 | -0.00366 | 0.00278 | * |

* * *



Final energy = -1933.702671346 eV

```
***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 0.20136 0.56461 -0.49574 *
* H 2 0.04435 0.38670 0.81130 *
* H 3 0.09864 0.09121 -0.01487 *
* H 4 -0.04443 -0.00834 0.05908 *
* H 5 -0.00040 -0.13657 0.01496 *
* H 6 0.14760 -0.12864 -0.00929 *
* H 7 0.19946 -0.03044 -0.09497 *
* H 8 -0.00031 0.33857 0.14744 *
* H 9 -0.06275 0.54621 0.20802 *
* C 1 -0.14538 0.08849 -0.99024 *
* C 2 0.06223 -0.03750 -0.03695 *
* C 3 -0.08119 -0.11371 0.04592 *
* C 4 0.09880 -0.13764 0.09941 *
* C 5 -0.03199 -0.03094 0.23460 *
* C 6 0.04829 -0.12111 0.01070 *
* C 7 0.03919 -0.04472 -0.05456 *
* N 1 -0.72574 -0.42502 0.55381 *
* O 1 0.15226 -0.80117 -0.48864 *
*
*****
```



BFGS: Final Enthalpy = -1.93557341E+003 eV

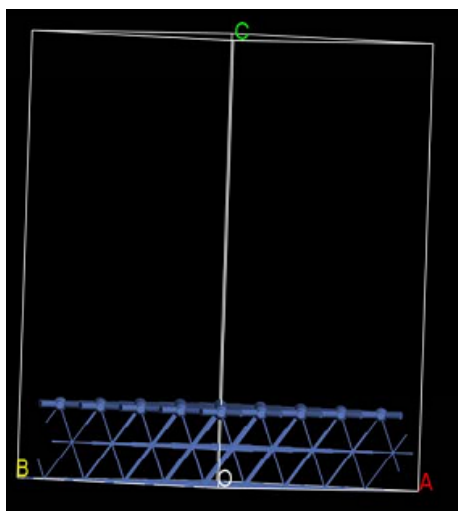
BFGS: Final <frequency> = 2776.48781 cm-1

```
***** Forces *****
```

```

*
*
* Cartesian components (eV/A)
* ----- *
*
* x y z
*
* H 1 -0.01445 0.05079 0.01295
* H 2 -0.05510 0.02688 -0.00395
* H 3 -0.00483 -0.02450 0.02731
* H 4 0.01964 0.00085 0.04385
* H 5 0.03516 -0.02606 0.02815
* H 6 0.00469 -0.03465 0.00955
* H 7 -0.00989 -0.04013 -0.03163
* H 8 -0.00850 0.00165 -0.02063
* H 9 -0.02429 0.03735 0.05383
* C 1 0.00226 -0.00529 -0.04799
* C 2 0.02680 0.00965 -0.03184
* C 3 -0.01630 0.03325 0.02302
* C 4 -0.02996 0.06604 -0.04187
* C 5 -0.00550 -0.01598 -0.01812
* C 6 0.05433 0.02462 0.01289
* C 7 -0.04230 -0.05322 -0.01461
* N 1 0.01419 -0.00819 0.03332
* O 1 0.05406 -0.04307 -0.03425
*
*****

```



BFGS: Final Enthalpy = -1.01539946E+005 eV

***** Forces *****

```

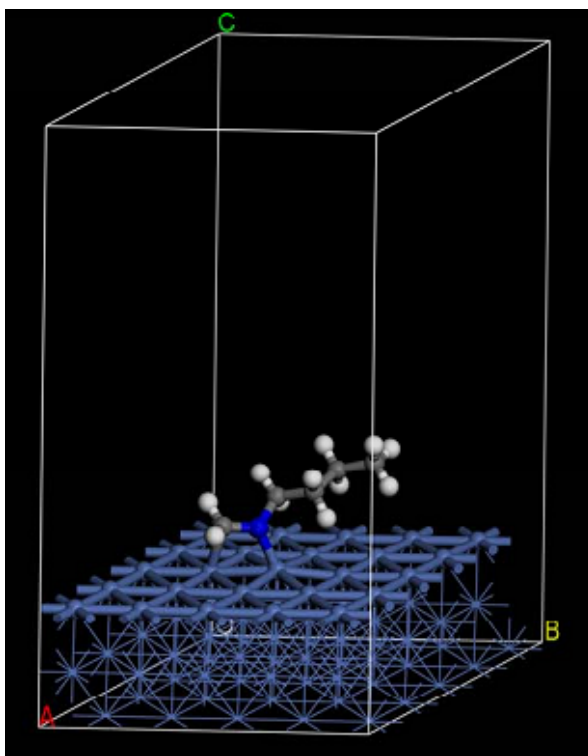
*
*
* Cartesian components (eV/A)
* ----- *
*
* x y z
*

```

| | | | | | |
|------|----|----------|----------|----------|---|
| * | | | | | * |
| * Ni | 1 | -0.02502 | 0.00851 | 0.00430 | * |
| * Ni | 2 | -0.00441 | 0.03026 | 0.01768 | * |
| * Ni | 3 | -0.02275 | -0.05414 | -0.05067 | * |
| * Ni | 4 | -0.02732 | 0.00828 | 0.00172 | * |
| * Ni | 5 | -0.00575 | 0.02737 | 0.01837 | * |
| * Ni | 6 | -0.02621 | -0.05723 | -0.05563 | * |
| * Ni | 7 | -0.02848 | 0.00739 | 0.00269 | * |
| * Ni | 8 | -0.00376 | 0.02827 | 0.02036 | * |
| * Ni | 9 | -0.02664 | -0.05829 | -0.05608 | * |
| * Ni | 10 | -0.02637 | 0.00802 | 0.00554 | * |
| * Ni | 11 | -0.00124 | 0.03090 | 0.02094 | * |
| * Ni | 12 | -0.02298 | -0.05355 | -0.05139 | * |
| * Ni | 13 | -0.02436 | 0.00933 | 0.00573 | * |
| * Ni | 14 | -0.00326 | 0.03233 | 0.01989 | * |
| * Ni | 15 | -0.02303 | -0.05387 | -0.05022 | * |
| * Ni | 16 | 0.02432 | -0.00189 | 0.01912 | * |
| * Ni | 17 | 0.00177 | -0.00858 | 0.00235 | * |
| * Ni | 18 | 0.00955 | -0.00685 | -0.01280 | * |
| * Ni | 19 | 0.02421 | -0.00077 | 0.01787 | * |
| * Ni | 20 | 0.00368 | -0.00633 | 0.00674 | * |
| * Ni | 21 | 0.00924 | -0.00685 | -0.01511 | * |
| * Ni | 22 | 0.02343 | -0.00324 | 0.01477 | * |
| * Ni | 23 | 0.00459 | -0.00587 | 0.00700 | * |
| * Ni | 24 | 0.00760 | -0.00850 | -0.01390 | * |
| * Ni | 25 | 0.02464 | -0.00530 | 0.01879 | * |
| * Ni | 26 | 0.00345 | -0.00545 | 0.00335 | * |
| * Ni | 27 | 0.00831 | -0.00899 | -0.01106 | * |
| * Ni | 28 | 0.02473 | -0.00268 | 0.02018 | * |
| * Ni | 29 | 0.00355 | -0.00771 | -0.00016 | * |
| * Ni | 30 | 0.00806 | -0.00650 | -0.01107 | * |
| * Ni | 31 | -0.01928 | -0.00335 | 0.00053 | * |
| * Ni | 32 | 0.02378 | 0.03510 | 0.01918 | * |
| * Ni | 33 | -0.03331 | -0.00568 | -0.02672 | * |
| * Ni | 34 | -0.02326 | -0.00778 | -0.00009 | * |
| * Ni | 35 | 0.01915 | 0.03192 | 0.01790 | * |
| * Ni | 36 | -0.03340 | -0.00850 | -0.02701 | * |
| * Ni | 37 | -0.02903 | -0.01263 | -0.00628 | * |
| * Ni | 38 | 0.01026 | 0.02390 | 0.01467 | * |
| * Ni | 39 | -0.03569 | -0.00962 | -0.03119 | * |
| * Ni | 40 | -0.02471 | -0.00867 | -0.00597 | * |
| * Ni | 41 | 0.01427 | 0.02502 | 0.01581 | * |
| * Ni | 42 | -0.03176 | -0.00946 | -0.03009 | * |
| * Ni | 43 | -0.01955 | -0.00086 | 0.00000 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 44 | 0.02107 | 0.03176 | 0.01723 | * |
| * Ni | 45 | -0.03172 | -0.00591 | -0.02697 | * |
| * Ni | 46 | -0.00718 | 0.02161 | 0.02542 | * |
| * Ni | 47 | 0.03614 | 0.00220 | 0.01026 | * |
| * Ni | 48 | 0.01668 | -0.01878 | -0.01333 | * |
| * Ni | 49 | -0.00744 | 0.02266 | 0.02406 | * |
| * Ni | 50 | 0.03608 | 0.00095 | 0.01177 | * |
| * Ni | 51 | 0.01753 | -0.01998 | -0.01154 | * |
| * Ni | 52 | -0.00853 | 0.02365 | 0.02410 | * |
| * Ni | 53 | 0.03720 | 0.00177 | 0.01399 | * |
| * Ni | 54 | 0.01594 | -0.01984 | -0.01246 | * |
| * Ni | 55 | -0.00668 | 0.02260 | 0.02517 | * |
| * Ni | 56 | 0.03766 | 0.00311 | 0.01458 | * |
| * Ni | 57 | 0.01425 | -0.01805 | -0.01325 | * |
| * Ni | 58 | -0.00531 | 0.02223 | 0.02747 | * |
| * Ni | 59 | 0.03682 | 0.00345 | 0.01298 | * |
| * Ni | 60 | 0.01541 | -0.01844 | -0.01352 | * |
| * Ni | 61 | 0.00510 | -0.00209 | 0.01923 | * |
| * Ni | 62 | 0.00726 | 0.00728 | 0.00121 | * |
| * Ni | 63 | -0.00115 | 0.01146 | -0.01219 | * |
| * Ni | 64 | 0.00530 | -0.00303 | 0.01899 | * |
| * Ni | 65 | 0.00786 | 0.00637 | 0.00359 | * |
| * Ni | 66 | -0.00081 | 0.00988 | -0.01226 | * |
| * Ni | 67 | 0.00546 | -0.00408 | 0.01960 | * |
| * Ni | 68 | 0.00707 | 0.00536 | 0.00385 | * |
| * Ni | 69 | -0.00122 | 0.00842 | -0.01296 | * |
| * Ni | 70 | 0.00502 | -0.00276 | 0.01864 | * |
| * Ni | 71 | 0.00604 | 0.00549 | 0.00222 | * |
| * Ni | 72 | -0.00090 | 0.01001 | -0.01257 | * |
| * Ni | 73 | 0.00549 | -0.00202 | 0.01884 | * |
| * Ni | 74 | 0.00573 | 0.00654 | 0.00035 | * |
| * Ni | 75 | -0.00120 | 0.01072 | -0.01258 | * |

*



Final energy = -1.02763399E+005 eV

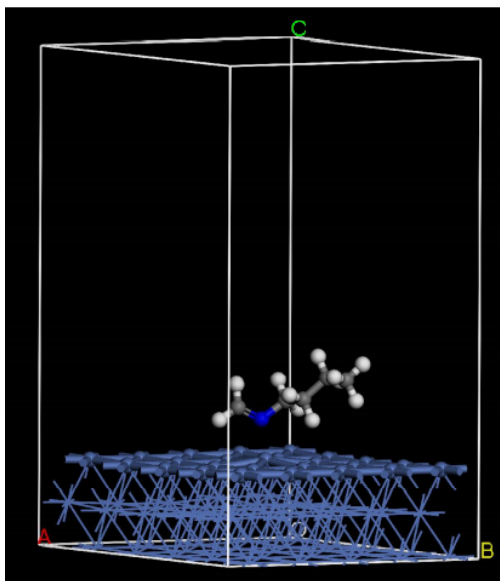
```

***** Forces *****
*
*
* Cartesian components (eV/A)
*
* -----
*
* x y z
*
* H 1 0.01182 0.01246 -0.00772
* H 2 0.00163 -0.01344 0.01506
* H 3 0.02985 0.00395 0.01931
* H 4 0.06036 0.01161 0.06871
* H 5 0.03597 -0.00517 -0.04397
* H 6 0.03623 0.01348 0.01613
* H 7 0.00671 -0.00277 -0.02199
* H 8 0.05952 0.00968 0.03375
* H 9 0.02299 0.03021 0.02183
* H 10 -0.02342 -0.00922 -0.05086
* H 11 -0.10995 0.08945 0.00267
* C 1 0.01514 0.01752 -0.02628
* C 2 -0.12521 0.01316 0.05769
* C 3 -0.04471 0.10232 0.00039
* C 4 -0.07195 -0.02899 -0.05021
* C 5 0.06506 -0.05347 -0.01058
* N 1 0.00155 -0.01104 0.08250
* Ni 1 0.01918 -0.00582 -0.00976

```

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 2 | -0.01307 | -0.01454 | -0.00758 | * |
| * Ni | 3 | -0.00605 | 0.00720 | 0.00233 | * |
| * Ni | 4 | -0.01698 | 0.00237 | -0.00976 | * |
| * Ni | 5 | 0.01220 | -0.00710 | 0.01586 | * |
| * Ni | 6 | -0.00274 | -0.01306 | -0.03177 | * |
| * Ni | 7 | 0.00079 | 0.00898 | 0.00725 | * |
| * Ni | 8 | -0.01159 | -0.01614 | -0.03070 | * |
| * Ni | 9 | -0.00593 | -0.02150 | 0.00227 | * |
| * Ni | 10 | -0.00794 | -0.00695 | -0.01700 | * |
| * Ni | 11 | -0.00342 | -0.01370 | -0.00214 | * |
| * Ni | 12 | -0.00323 | 0.01495 | -0.00163 | * |
| * Ni | 13 | 0.00783 | 0.02081 | 0.00265 | * |
| * Ni | 14 | 0.00249 | -0.00039 | 0.00010 | * |
| * Ni | 15 | 0.01788 | 0.00420 | 0.01691 | * |
| * Ni | 16 | 0.00044 | -0.00334 | 0.00507 | * |
| * Ni | 17 | 0.00539 | 0.00956 | -0.01200 | * |
| * Ni | 18 | 0.01560 | -0.00307 | -0.00505 | * |
| * Ni | 19 | 0.01768 | -0.01760 | -0.00284 | * |
| * Ni | 20 | 0.01517 | 0.01030 | -0.02267 | * |
| * Ni | 21 | -0.01335 | -0.01268 | 0.00370 | * |
| * Ni | 22 | 0.00094 | 0.00226 | -0.00550 | * |
| * Ni | 23 | -0.02514 | -0.00433 | -0.02035 | * |
| * Ni | 24 | 0.00114 | 0.00494 | -0.00797 | * |
| * Ni | 25 | -0.00056 | -0.00435 | -0.01273 | * |
| * Ni | 26 | 0.01375 | -0.00328 | 0.01752 | * |
| * Ni | 27 | 0.01012 | -0.00567 | 0.00475 | * |
| * Ni | 28 | 0.01734 | -0.00216 | 0.01223 | * |
| * Ni | 29 | 0.00014 | -0.00786 | 0.01328 | * |
| * Ni | 30 | 0.00572 | 0.00772 | 0.00061 | * |
| * Ni | 31 | -0.00061 | -0.02019 | -0.00092 | * |
| * Ni | 32 | 0.00032 | 0.00346 | 0.00371 | * |
| * Ni | 33 | 0.00977 | 0.00531 | -0.00090 | * |
| * Ni | 34 | 0.00585 | -0.01484 | -0.00609 | * |
| * Ni | 35 | -0.01931 | -0.00827 | -0.01024 | * |
| * Ni | 36 | 0.00917 | 0.00364 | 0.00151 | * |
| * Ni | 37 | -0.01968 | -0.00151 | -0.03695 | * |
| * Ni | 38 | -0.00238 | -0.00759 | -0.00167 | * |
| * Ni | 39 | -0.00392 | 0.00150 | -0.00374 | * |
| * Ni | 40 | -0.02190 | -0.00597 | -0.00046 | * |
| * Ni | 41 | -0.00687 | -0.01249 | 0.00850 | * |
| * Ni | 42 | -0.01486 | -0.01810 | -0.00133 | * |
| * Ni | 43 | 0.00523 | 0.00053 | 0.00214 | * |
| * Ni | 44 | 0.00027 | -0.01105 | -0.01325 | * |
| * Ni | 45 | 0.01517 | 0.00309 | 0.00096 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 46 | 0.00024 | 0.00836 | -0.00521 | * |
| * Ni | 47 | -0.00377 | -0.01035 | 0.00365 | * |
| * Ni | 48 | 0.00683 | 0.01434 | -0.00197 | * |
| * Ni | 49 | -0.00759 | -0.00720 | 0.00144 | * |
| * Ni | 50 | -0.00353 | -0.02319 | -0.00210 | * |
| * Ni | 51 | 0.00756 | 0.00808 | -0.01125 | * |
| * Ni | 52 | 0.00199 | -0.01486 | -0.00477 | * |
| * Ni | 53 | 0.00108 | -0.00413 | 0.00027 | * |
| * Ni | 54 | -0.00946 | 0.00246 | -0.01231 | * |
| * Ni | 55 | -0.00993 | -0.01111 | -0.01240 | * |
| * Ni | 56 | -0.00948 | -0.01322 | -0.01336 | * |
| * Ni | 57 | -0.00329 | -0.00697 | -0.00689 | * |
| * Ni | 58 | -0.00660 | 0.01813 | -0.00487 | * |
| * Ni | 59 | 0.01630 | 0.01663 | 0.00170 | * |
| * Ni | 60 | 0.01582 | -0.00319 | -0.00201 | * |
| * Ni | 61 | -0.00326 | -0.00675 | 0.02701 | * |
| * Ni | 62 | 0.01486 | 0.00566 | -0.00781 | * |
| * Ni | 63 | -0.01490 | 0.00255 | 0.00889 | * |
| * Ni | 64 | 0.00167 | 0.00489 | -0.00356 | * |
| * Ni | 65 | -0.00694 | 0.00196 | 0.00359 | * |
| * Ni | 66 | 0.00473 | -0.00144 | 0.01723 | * |
| * Ni | 67 | 0.01107 | -0.01637 | 0.01649 | * |
| * Ni | 68 | 0.00543 | -0.01761 | -0.00627 | * |
| * Ni | 69 | 0.00403 | 0.01293 | 0.01135 | * |
| * Ni | 70 | 0.00581 | 0.00144 | -0.00148 | * |
| * Ni | 71 | 0.01478 | 0.00402 | 0.00973 | * |
| * Ni | 72 | -0.00527 | -0.00543 | 0.00239 | * |
| * Ni | 73 | -0.00679 | -0.00995 | 0.01697 | * |
| * Ni | 74 | -0.00990 | 0.02253 | 0.01833 | * |
| * Ni | 75 | 0.00684 | 0.00080 | 0.00446 | * |
| * | | | | | * |



BFGS: Final Enthalpy = -1.02762964E+005 eV

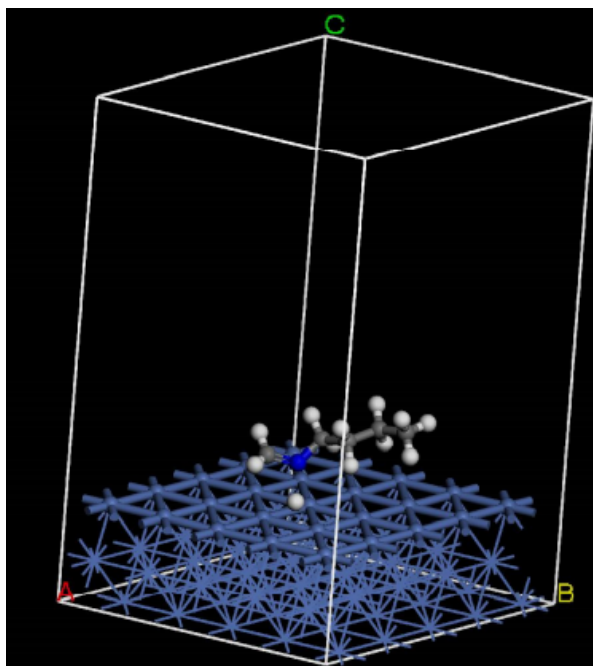
***** Forces *****

| | | Cartesian components (eV/A) | | | | |
|---|----|-----------------------------|----------|----------|----------|---|
| | | x | y | z | | |
| * | | | | | * | |
| * | | | | | * | |
| * | H | 1 | 0.01669 | -0.00592 | -0.05879 | * |
| * | H | 2 | 0.00343 | 0.01303 | 0.02817 | * |
| * | H | 3 | -0.04952 | 0.03358 | 0.03412 | * |
| * | H | 4 | 0.07792 | -0.06514 | -0.05443 | * |
| * | H | 5 | -0.02951 | -0.01582 | -0.03620 | * |
| * | H | 6 | 0.04552 | 0.02217 | 0.02019 | * |
| * | H | 7 | -0.02965 | 0.02395 | -0.04773 | * |
| * | H | 8 | -0.07625 | -0.00348 | 0.03275 | * |
| * | H | 9 | 0.02102 | -0.00024 | 0.04039 | * |
| * | H | 10 | -0.00519 | 0.00194 | -0.00169 | * |
| * | H | 11 | 0.01384 | -0.03660 | 0.04079 | * |
| * | C | 1 | 0.05379 | 0.01212 | 0.05812 | * |
| * | C | 2 | -0.13884 | -0.00940 | -0.00570 | * |
| * | C | 3 | 0.01891 | -0.06465 | -0.05612 | * |
| * | C | 4 | -0.00649 | 0.01373 | 0.00960 | * |
| * | C | 5 | 0.00274 | -0.01808 | 0.00655 | * |
| * | N | 1 | 0.04245 | 0.05900 | -0.02968 | * |
| * | Ni | 1 | -0.00577 | -0.00567 | -0.00763 | * |
| * | Ni | 2 | -0.01467 | -0.01490 | 0.00410 | * |
| * | Ni | 3 | -0.01037 | -0.00518 | -0.00309 | * |
| * | Ni | 4 | 0.00046 | -0.00227 | -0.01146 | * |
| * | Ni | 5 | 0.00310 | -0.01412 | -0.00993 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 6 | -0.00004 | 0.00085 | 0.01078 | * |
| * Ni | 7 | 0.01379 | -0.00527 | 0.00409 | * |
| * Ni | 8 | 0.00413 | 0.00323 | -0.00348 | * |
| * Ni | 9 | -0.00743 | -0.00028 | 0.00460 | * |
| * Ni | 10 | 0.00309 | 0.00452 | -0.00273 | * |
| * Ni | 11 | 0.00734 | -0.00836 | -0.00019 | * |
| * Ni | 12 | 0.00324 | 0.00762 | 0.00236 | * |
| * Ni | 13 | -0.00471 | 0.00289 | -0.00792 | * |
| * Ni | 14 | -0.00748 | 0.00269 | -0.00651 | * |
| * Ni | 15 | -0.00013 | -0.00868 | 0.00492 | * |
| * Ni | 16 | 0.01124 | 0.02230 | -0.00390 | * |
| * Ni | 17 | 0.00454 | 0.00503 | -0.00149 | * |
| * Ni | 18 | -0.00859 | 0.00677 | -0.00272 | * |
| * Ni | 19 | 0.00043 | 0.00457 | -0.01635 | * |
| * Ni | 20 | 0.01486 | 0.01441 | -0.01480 | * |
| * Ni | 21 | 0.00111 | 0.00532 | 0.00800 | * |
| * Ni | 22 | 0.00193 | -0.00606 | -0.01146 | * |
| * Ni | 23 | 0.00020 | 0.00522 | 0.00512 | * |
| * Ni | 24 | 0.01854 | -0.00775 | 0.00080 | * |
| * Ni | 25 | -0.00361 | 0.00686 | 0.00944 | * |
| * Ni | 26 | -0.00963 | -0.01304 | -0.00048 | * |
| * Ni | 27 | -0.00085 | -0.00656 | 0.00124 | * |
| * Ni | 28 | -0.00904 | -0.00937 | 0.00774 | * |
| * Ni | 29 | 0.00315 | -0.00298 | 0.01502 | * |
| * Ni | 30 | -0.00956 | 0.02096 | 0.01694 | * |
| * Ni | 31 | 0.00024 | 0.01349 | 0.00399 | * |
| * Ni | 32 | 0.00954 | 0.00592 | -0.01652 | * |
| * Ni | 33 | 0.00071 | -0.00172 | -0.00443 | * |
| * Ni | 34 | 0.00743 | -0.00349 | -0.00921 | * |
| * Ni | 35 | 0.01308 | 0.00267 | 0.01371 | * |
| * Ni | 36 | -0.00229 | 0.00414 | 0.00697 | * |
| * Ni | 37 | -0.00781 | -0.01148 | -0.01287 | * |
| * Ni | 38 | 0.00918 | 0.00417 | -0.00880 | * |
| * Ni | 39 | 0.00942 | 0.01072 | 0.00020 | * |
| * Ni | 40 | -0.00528 | -0.00874 | -0.01365 | * |
| * Ni | 41 | 0.00316 | -0.00327 | -0.00181 | * |
| * Ni | 42 | -0.02106 | 0.00281 | -0.00154 | * |
| * Ni | 43 | -0.00050 | -0.00158 | -0.01703 | * |
| * Ni | 44 | -0.00042 | 0.01146 | -0.00308 | * |
| * Ni | 45 | -0.00191 | -0.01235 | -0.00171 | * |
| * Ni | 46 | 0.01124 | 0.00765 | -0.00188 | * |
| * Ni | 47 | -0.00205 | 0.01084 | 0.01500 | * |
| * Ni | 48 | -0.00055 | 0.01635 | 0.01123 | * |
| * Ni | 49 | 0.00474 | -0.02033 | -0.00212 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 50 | 0.00857 | -0.00492 | 0.01101 | * |
| * Ni | 51 | -0.00607 | 0.00162 | -0.01242 | * |
| * Ni | 52 | -0.01290 | -0.00737 | -0.00976 | * |
| * Ni | 53 | 0.00805 | 0.00151 | 0.01927 | * |
| * Ni | 54 | 0.00691 | 0.00429 | 0.00534 | * |
| * Ni | 55 | -0.01090 | 0.00084 | 0.00269 | * |
| * Ni | 56 | 0.00664 | 0.00028 | 0.02194 | * |
| * Ni | 57 | -0.00736 | 0.00449 | 0.00691 | * |
| * Ni | 58 | 0.00360 | 0.01348 | 0.00103 | * |
| * Ni | 59 | -0.00536 | 0.00407 | 0.00503 | * |
| * Ni | 60 | 0.01487 | 0.00288 | 0.01296 | * |
| * Ni | 61 | 0.00375 | 0.00370 | -0.01639 | * |
| * Ni | 62 | -0.00294 | 0.01327 | 0.00242 | * |
| * Ni | 63 | 0.00120 | 0.00223 | -0.02005 | * |
| * Ni | 64 | 0.00598 | 0.01306 | -0.00912 | * |
| * Ni | 65 | -0.00106 | -0.01955 | 0.00171 | * |
| * Ni | 66 | 0.00417 | -0.00323 | -0.01098 | * |
| * Ni | 67 | -0.00303 | -0.00281 | 0.00251 | * |
| * Ni | 68 | 0.00225 | 0.00258 | 0.01313 | * |
| * Ni | 69 | -0.00747 | -0.01900 | 0.01179 | * |
| * Ni | 70 | 0.00161 | -0.00699 | 0.00928 | * |
| * Ni | 71 | -0.01340 | 0.01248 | 0.00763 | * |
| * Ni | 72 | -0.01634 | -0.00663 | 0.01783 | * |
| * Ni | 73 | 0.01617 | 0.00268 | 0.00225 | * |
| * Ni | 74 | 0.00877 | -0.01103 | 0.00333 | * |
| * Ni | 75 | 0.00733 | 0.00787 | -0.00712 | * |

*



Final energy = -102778.3878944 eV

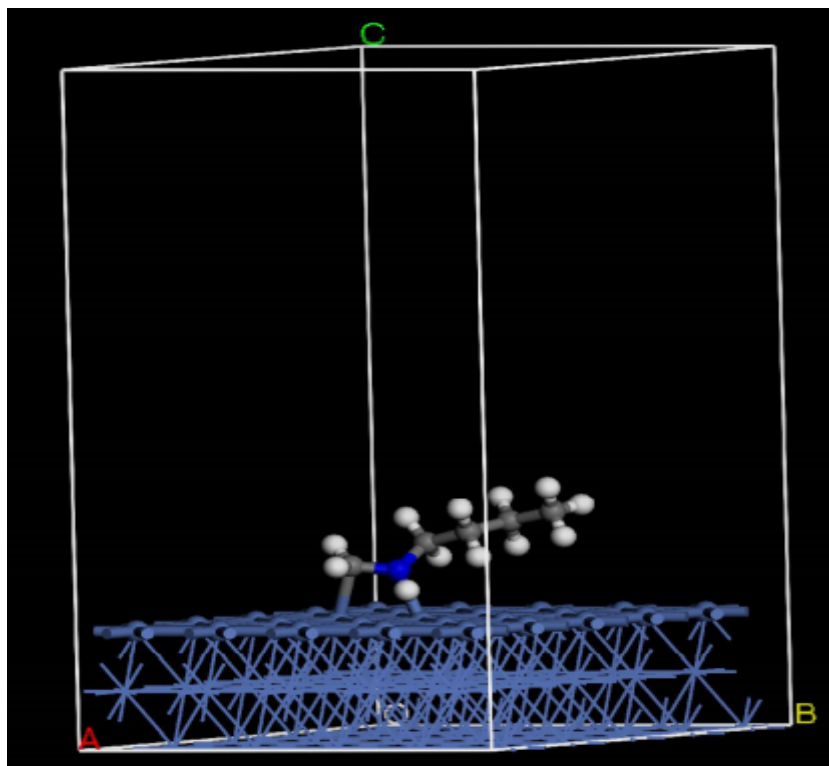
***** Forces *****

| ***** Forces ***** | | | | |
|---------------------------------|----|----------|----------|------------|
| * Cartesian components (eV/A) * | | | | |
| * ----- * | | | | |
| | | x | y | z |
| * ----- * | | | | |
| * H | 1 | 0.02115 | 0.01890 | 0.00227 * |
| * H | 2 | 0.09196 | 0.06026 | 0.04570 * |
| * H | 3 | 0.00912 | -0.01584 | 0.00773 * |
| * H | 4 | 0.04322 | 0.10058 | 0.08307 * |
| * H | 5 | -0.01993 | 0.02259 | 0.03374 * |
| * H | 6 | -0.04975 | -0.00122 | 0.06676 * |
| * H | 7 | 0.00479 | 0.04522 | 0.07832 * |
| * H | 8 | -0.04667 | 0.05991 | 0.09960 * |
| * H | 9 | -0.06964 | -0.01155 | -0.02028 * |
| * H | 10 | 0.01440 | 0.11803 | 0.15332 * |
| * H | 11 | 0.01811 | 0.03018 | -0.10980 * |
| * H | 12 | 0.03968 | -0.02701 | 0.01846 * |
| * C | 1 | -0.20456 | -0.24341 | 0.09818 * |
| * C | 2 | 0.27903 | -0.04095 | -0.14664 * |
| * C | 3 | -0.36670 | -0.10292 | 0.21913 * |
| * C | 4 | 0.38395 | 0.11716 | -0.20324 * |
| * C | 5 | -0.22592 | -0.02070 | -0.07019 * |
| * N | 1 | -0.19994 | 0.31869 | -0.02079 * |
| * Ni | 1 | -0.02001 | -0.05719 | -0.02972 * |
| * Ni | 2 | -0.08392 | -0.10466 | 0.00609 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 3 | 0.00779 | 0.03591 | 0.12708 * |
| * Ni | 4 | -0.02797 | -0.03544 | 0.02986 * |
| * Ni | 5 | -0.04887 | -0.05722 | -0.11051 * |
| * Ni | 6 | 0.14034 | 0.05092 | 0.14019 * |
| * Ni | 7 | -0.04563 | -0.07950 | -0.04201 * |
| * Ni | 8 | -0.03330 | -0.03022 | -0.09170 * |
| * Ni | 9 | 0.06120 | 0.03014 | 0.11457 * |
| * Ni | 10 | -0.03919 | -0.05061 | 0.01657 * |
| * Ni | 11 | -0.04914 | -0.00542 | -0.07603 * |
| * Ni | 12 | 0.01682 | 0.06027 | 0.10653 * |
| * Ni | 13 | 0.05568 | 0.00873 | -0.03757 * |
| * Ni | 14 | -0.07513 | -0.05221 | -0.09874 * |
| * Ni | 15 | 0.00339 | 0.03205 | 0.06771 * |
| * Ni | 16 | -0.07762 | -0.10899 | -0.07664 * |
| * Ni | 17 | 0.34879 | 0.26960 | 0.06715 * |
| * Ni | 18 | 0.01367 | 0.09804 | 0.08265 * |
| * Ni | 19 | 0.01564 | -0.00072 | -0.05839 * |
| * Ni | 20 | -0.29718 | -0.37570 | -0.20943 * |
| * Ni | 21 | 0.05134 | 0.00887 | 0.00308 * |
| * Ni | 22 | 0.39471 | 0.18641 | 0.41894 * |
| * Ni | 23 | -0.13373 | -0.11738 | 0.10774 * |
| * Ni | 24 | 0.13890 | 0.09098 | 0.09405 * |
| * Ni | 25 | -0.08480 | -0.22135 | -0.07846 * |
| * Ni | 26 | -0.14833 | -0.10741 | 0.01898 * |
| * Ni | 27 | 0.03229 | 0.02598 | 0.06043 * |
| * Ni | 28 | -0.01762 | -0.05580 | -0.02501 * |
| * Ni | 29 | -0.24674 | -0.15957 | -0.05184 * |
| * Ni | 30 | 0.04825 | 0.09034 | 0.11075 * |
| * Ni | 31 | -0.17293 | 0.00583 | -0.08355 * |
| * Ni | 32 | 0.17546 | 0.09872 | 0.07503 * |
| * Ni | 33 | 0.02337 | 0.05687 | -0.03348 * |
| * Ni | 34 | -0.39748 | -0.04806 | -0.24437 * |
| * Ni | 35 | 0.16429 | 0.09492 | 0.06110 * |
| * Ni | 36 | 0.00391 | 0.02071 | -0.02764 * |
| * Ni | 37 | 0.34420 | 0.30669 | 0.61831 * |
| * Ni | 38 | 0.07309 | 0.08305 | -0.24752 * |
| * Ni | 39 | 0.04336 | 0.04513 | -0.03722 * |
| * Ni | 40 | -0.01049 | -0.30701 | -0.12394 * |
| * Ni | 41 | 0.07399 | -0.03257 | -0.12193 * |
| * Ni | 42 | 0.09969 | 0.04043 | -0.00602 * |
| * Ni | 43 | -0.12314 | -0.06188 | -0.03927 * |
| * Ni | 44 | 0.12484 | 0.16206 | -0.06162 * |
| * Ni | 45 | 0.06594 | 0.07639 | -0.03993 * |
| * Ni | 46 | -0.07477 | -0.12048 | -0.12723 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 47 | 0.20523 | 0.15812 | 0.39272 * |
| * Ni | 48 | -0.00367 | 0.04797 | -0.03481 * |
| * Ni | 49 | -0.10845 | -0.04622 | -0.13353 * |
| * Ni | 50 | 0.07863 | 0.15967 | 0.32826 * |
| * Ni | 51 | 0.03218 | 0.05133 | -0.01169 * |
| * Ni | 52 | -0.10067 | 0.02129 | -0.10154 * |
| * Ni | 53 | 0.15316 | 0.02568 | 0.29652 * |
| * Ni | 54 | 0.01616 | -0.00960 | -0.02227 * |
| * Ni | 55 | -0.02823 | 0.01649 | -0.20600 * |
| * Ni | 56 | 0.08531 | 0.05861 | 0.30489 * |
| * Ni | 57 | 0.03571 | 0.03190 | -0.03825 * |
| * Ni | 58 | 0.03071 | -0.05776 | -0.09677 * |
| * Ni | 59 | 0.14307 | 0.09301 | 0.39042 * |
| * Ni | 60 | 0.09576 | 0.04203 | -0.01689 * |
| * Ni | 61 | -0.04857 | -0.08729 | 0.01657 * |
| * Ni | 62 | -0.13393 | -0.16253 | -0.37812 * |
| * Ni | 63 | 0.08301 | 0.06540 | 0.06151 * |
| * Ni | 64 | -0.03910 | -0.07232 | 0.01827 * |
| * Ni | 65 | -0.13484 | -0.11551 | -0.40029 * |
| * Ni | 66 | -0.00309 | 0.06954 | 0.04938 * |
| * Ni | 67 | -0.01713 | -0.05619 | 0.00861 * |
| * Ni | 68 | -0.08876 | -0.16864 | -0.40276 * |
| * Ni | 69 | 0.09945 | 0.07400 | 0.07230 * |
| * Ni | 70 | -0.13322 | -0.07543 | -0.02810 * |
| * Ni | 71 | -0.11702 | -0.11220 | -0.27306 * |
| * Ni | 72 | 0.06758 | 0.06049 | 0.08530 * |
| * Ni | 73 | -0.08125 | -0.08782 | -0.02726 * |
| * Ni | 74 | -0.19036 | -0.16447 | -0.43653 * |
| * Ni | 75 | 0.06705 | 0.02286 | 0.10077 * |

* *



Final energy = -102777.69835 eV

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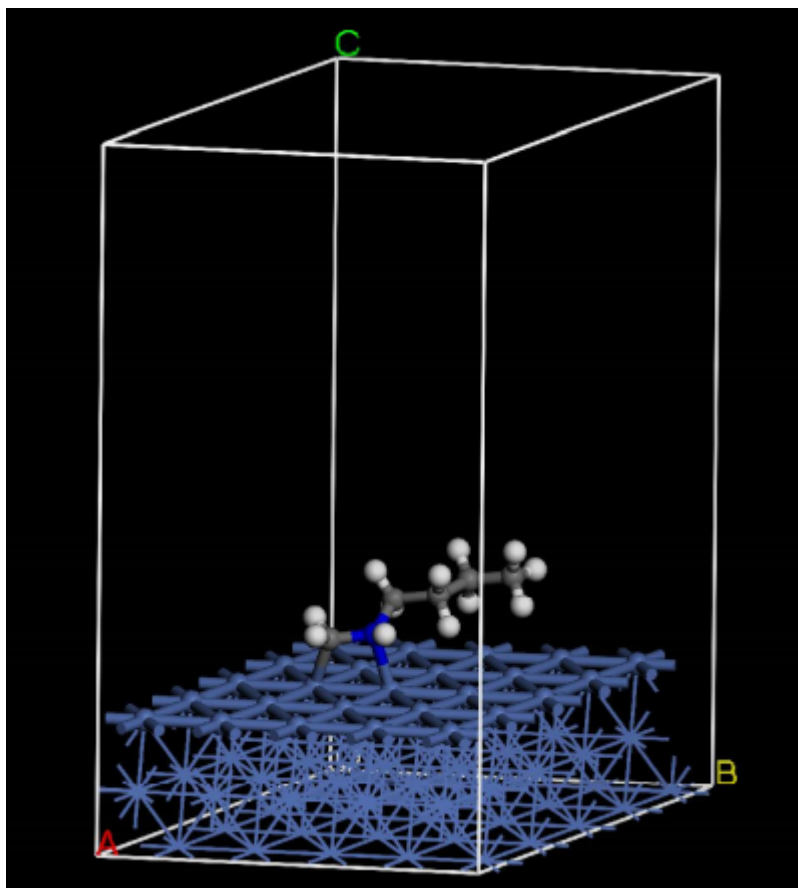
Transition State Found!

***** Forces *****

| | | Cartesian components (eV/A) | | | | |
|---|---|-----------------------------|----------|----------|----------|---|
| | | x | y | z | | |
| * | | | | | * | |
| * | | | | | * | |
| * | H | 1 | 0.06530 | -0.13079 | 0.00187 | * |
| * | H | 2 | -0.00621 | -0.03927 | -0.03944 | * |
| * | H | 3 | 0.16475 | 0.00878 | 0.06717 | * |
| * | H | 4 | -0.19884 | -0.04350 | 0.01947 | * |
| * | H | 5 | 0.03530 | 0.03693 | 0.17896 | * |
| * | H | 6 | 0.33178 | 0.09139 | 0.07084 | * |
| * | H | 7 | 0.03716 | 0.03996 | -0.18616 | * |
| * | H | 8 | 0.25621 | -0.29590 | -0.14434 | * |
| * | H | 9 | 0.07140 | -0.19672 | -0.26215 | * |
| * | H | 10 | -0.03211 | 0.16245 | -0.23866 | * |
| * | H | 11 | 0.17631 | -0.22947 | 0.09493 | * |
| * | H | 12 | -0.92627 | -0.27943 | -0.23857 | * |
| * | C | 1 | -0.34763 | 0.01415 | 0.10972 | * |
| * | C | 2 | 0.34687 | 0.07703 | -0.32131 | * |
| * | C | 3 | -0.52723 | -0.03119 | 0.05504 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * C | 4 | 0.11542 | 0.26291 | -0.08418 | * |
| * C | 5 | 0.05615 | 0.34875 | -0.23286 | * |
| * N | 1 | 0.18785 | -0.00235 | 0.87477 | * |
| * Ni | 1 | -0.00582 | -0.09677 | 0.16243 | * |
| * Ni | 2 | -0.03477 | -0.07793 | 0.05218 | * |
| * Ni | 3 | -0.04460 | -0.06054 | 0.03107 | * |
| * Ni | 4 | 0.01789 | -0.06970 | 0.06003 | * |
| * Ni | 5 | -0.00725 | -0.01404 | 0.04147 | * |
| * Ni | 6 | -0.02724 | -0.05113 | 0.01382 | * |
| * Ni | 7 | 0.05635 | -0.11858 | 0.11860 | * |
| * Ni | 8 | -0.06355 | -0.10806 | 0.09526 | * |
| * Ni | 9 | -0.00776 | -0.03449 | 0.04617 | * |
| * Ni | 10 | 0.01164 | -0.08002 | 0.13571 | * |
| * Ni | 11 | -0.06925 | -0.01609 | 0.03622 | * |
| * Ni | 12 | -0.02762 | -0.06079 | 0.05734 | * |
| * Ni | 13 | 0.01871 | -0.06513 | 0.16467 | * |
| * Ni | 14 | 0.00352 | -0.04482 | -0.01584 | * |
| * Ni | 15 | -0.03947 | -0.04701 | 0.00690 | * |
| * Ni | 16 | 0.04262 | 0.16296 | -0.14091 | * |
| * Ni | 17 | 0.01509 | 0.04130 | -0.07907 | * |
| * Ni | 18 | 0.00612 | 0.09480 | -0.10029 | * |
| * Ni | 19 | 0.05692 | 0.11213 | -0.09593 | * |
| * Ni | 20 | 0.13651 | 0.06773 | -0.01994 | * |
| * Ni | 21 | 0.02083 | 0.06423 | -0.05197 | * |
| * Ni | 22 | -0.10026 | -0.02733 | -0.03818 | * |
| * Ni | 23 | 0.01725 | 0.12420 | -0.06301 | * |
| * Ni | 24 | 0.01855 | 0.06383 | -0.04657 | * |
| * Ni | 25 | 0.06735 | 0.12357 | -0.05637 | * |
| * Ni | 26 | 0.07438 | 0.12038 | -0.09202 | * |
| * Ni | 27 | -0.01379 | 0.12773 | -0.09299 | * |
| * Ni | 28 | 0.08850 | 0.12080 | -0.11063 | * |
| * Ni | 29 | 0.06765 | 0.11036 | -0.05160 | * |
| * Ni | 30 | -0.00874 | 0.06818 | -0.09227 | * |
| * Ni | 31 | 0.00291 | -0.05411 | 0.12197 | * |
| * Ni | 32 | -0.10137 | -0.14234 | 0.00803 | * |
| * Ni | 33 | -0.00253 | -0.12428 | 0.11936 | * |
| * Ni | 34 | -0.00350 | -0.09657 | 0.12045 | * |
| * Ni | 35 | 0.03119 | -0.13745 | 0.11910 | * |
| * Ni | 36 | -0.03594 | -0.11280 | 0.13318 | * |
| * Ni | 37 | -0.10289 | 0.13374 | -0.12438 | * |
| * Ni | 38 | -0.04190 | -0.04260 | 0.08527 | * |
| * Ni | 39 | -0.02948 | -0.10135 | 0.07986 | * |
| * Ni | 40 | 0.04331 | -0.36085 | 0.13023 | * |
| * Ni | 41 | -0.05451 | -0.05309 | 0.08441 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 42 | -0.04845 | -0.08498 | 0.06457 | * |
| * Ni | 43 | -0.06978 | -0.00408 | 0.05907 | * |
| * Ni | 44 | -0.06324 | -0.07361 | 0.02445 | * |
| * Ni | 45 | -0.00329 | -0.13017 | 0.06768 | * |
| * Ni | 46 | 0.02294 | 0.08074 | 0.01860 | * |
| * Ni | 47 | -0.04796 | -0.06281 | -0.00446 | * |
| * Ni | 48 | -0.03444 | 0.07053 | -0.09533 | * |
| * Ni | 49 | 0.03745 | 0.07805 | 0.01894 | * |
| * Ni | 50 | -0.00837 | -0.10824 | 0.01790 | * |
| * Ni | 51 | -0.04044 | 0.09352 | -0.09941 | * |
| * Ni | 52 | 0.05196 | -0.02215 | 0.02001 | * |
| * Ni | 53 | 0.03195 | 0.04690 | 0.03089 | * |
| * Ni | 54 | 0.03488 | 0.02189 | -0.05909 | * |
| * Ni | 55 | -0.04247 | 0.30899 | -0.18155 | * |
| * Ni | 56 | 0.05055 | 0.13227 | 0.00778 | * |
| * Ni | 57 | -0.01023 | 0.02082 | -0.08394 | * |
| * Ni | 58 | 0.07168 | 0.00791 | 0.00718 | * |
| * Ni | 59 | 0.01822 | 0.03338 | -0.03915 | * |
| * Ni | 60 | 0.02103 | 0.01166 | -0.06216 | * |
| * Ni | 61 | -0.00690 | 0.15092 | -0.09973 | * |
| * Ni | 62 | -0.05312 | 0.09135 | -0.13307 | * |
| * Ni | 63 | 0.02597 | -0.12022 | 0.04795 | * |
| * Ni | 64 | 0.10045 | 0.17137 | -0.06155 | * |
| * Ni | 65 | -0.03597 | 0.08297 | -0.16722 | * |
| * Ni | 66 | 0.05670 | -0.03846 | 0.09632 | * |
| * Ni | 67 | 0.09843 | 0.14467 | -0.00193 | * |
| * Ni | 68 | 0.01668 | 0.00186 | -0.09031 | * |
| * Ni | 69 | 0.02191 | 0.00060 | 0.05069 | * |
| * Ni | 70 | 0.02845 | 0.01103 | 0.01859 | * |
| * Ni | 71 | 0.05762 | 0.00312 | 0.06076 | * |
| * Ni | 72 | -0.04359 | -0.02615 | 0.03721 | * |
| * Ni | 73 | -0.09667 | 0.06033 | -0.03811 | * |
| * Ni | 74 | 0.08447 | -0.00090 | 0.11000 | * |
| * Ni | 75 | -0.00765 | -0.08494 | -0.01843 | * |
| * | | | | | * |
| ***** | | | | | |



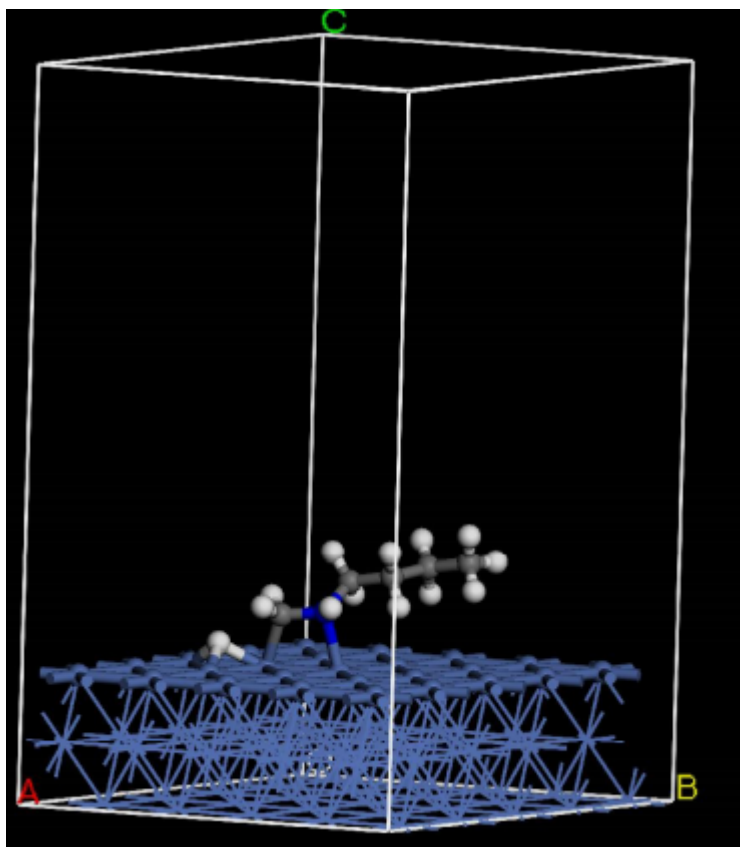
Final energy = -102778.4687424 eV

***** Forces *****

| ***** Forces ***** | | | | |
|---------------------------------|----|----------|----------|----------|
| * Cartesian components (eV/A) * | | | | |
| *-----* | | | | |
| | | x | y | z |
| * H | 1 | -0.01017 | 0.03794 | 0.03026 |
| * H | 2 | 0.03564 | 0.02212 | 0.01786 |
| * H | 3 | -0.07667 | 0.01154 | -0.00269 |
| * H | 4 | -0.02253 | 0.04609 | 0.02054 |
| * H | 5 | 0.01613 | 0.03308 | 0.05295 |
| * H | 6 | 0.03734 | 0.02615 | 0.03435 |
| * H | 7 | -0.00318 | 0.05625 | 0.02602 |
| * H | 8 | -0.07473 | 0.02688 | -0.01925 |
| * H | 9 | -0.00142 | 0.03572 | 0.07737 |
| * H | 10 | 0.01340 | 0.03415 | -0.00416 |
| * H | 11 | 0.01156 | -0.01264 | 0.01662 |
| * H | 12 | 0.02077 | -0.00851 | -0.02942 |
| * C | 1 | -0.03018 | -0.02055 | -0.01051 |

| | | | | | |
|------|----|----------|----------|----------|---|
| * C | 2 | 0.03308 | 0.02914 | -0.00087 | * |
| * C | 3 | -0.01073 | 0.01731 | -0.03357 | * |
| * C | 4 | 0.04757 | -0.06754 | -0.04218 | * |
| * C | 5 | 0.01384 | 0.00260 | 0.01627 | * |
| * N | 1 | 0.01561 | -0.06090 | -0.05104 | * |
| * Ni | 1 | -0.01282 | -0.01104 | -0.01132 | * |
| * Ni | 2 | 0.00102 | -0.00446 | -0.00227 | * |
| * Ni | 3 | -0.00246 | -0.00050 | -0.00308 | * |
| * Ni | 4 | 0.00363 | -0.00142 | 0.00086 | * |
| * Ni | 5 | -0.00277 | 0.00387 | -0.00714 | * |
| * Ni | 6 | 0.01247 | 0.00810 | 0.00915 | * |
| * Ni | 7 | 0.00117 | -0.00032 | 0.00491 | * |
| * Ni | 8 | 0.00139 | -0.00683 | 0.00148 | * |
| * Ni | 9 | 0.00224 | 0.00621 | -0.00225 | * |
| * Ni | 10 | -0.00193 | 0.00416 | -0.00203 | * |
| * Ni | 11 | 0.00162 | 0.00423 | 0.00248 | * |
| * Ni | 12 | 0.00394 | 0.00076 | -0.00089 | * |
| * Ni | 13 | -0.00157 | 0.00157 | -0.00268 | * |
| * Ni | 14 | -0.00152 | -0.00098 | -0.00119 | * |
| * Ni | 15 | -0.00372 | -0.00591 | -0.00439 | * |
| * Ni | 16 | -0.01036 | -0.01671 | -0.01329 | * |
| * Ni | 17 | -0.00317 | 0.00136 | -0.00553 | * |
| * Ni | 18 | -0.00034 | -0.00342 | -0.00062 | * |
| * Ni | 19 | -0.02914 | -0.04103 | -0.02490 | * |
| * Ni | 20 | 0.00583 | -0.00664 | 0.00235 | * |
| * Ni | 21 | -0.00365 | -0.00280 | -0.00933 | * |
| * Ni | 22 | -0.00604 | -0.01337 | -0.01409 | * |
| * Ni | 23 | -0.01480 | -0.00703 | -0.01443 | * |
| * Ni | 24 | 0.00360 | -0.00073 | 0.00153 | * |
| * Ni | 25 | 0.01274 | 0.00751 | 0.01167 | * |
| * Ni | 26 | 0.00403 | -0.00655 | -0.00283 | * |
| * Ni | 27 | -0.00426 | -0.00617 | -0.00877 | * |
| * Ni | 28 | -0.00344 | -0.00098 | -0.00921 | * |
| * Ni | 29 | -0.00609 | -0.00737 | -0.00583 | * |
| * Ni | 30 | -0.00342 | -0.00749 | -0.00721 | * |
| * Ni | 31 | -0.00376 | -0.00737 | -0.00655 | * |
| * Ni | 32 | 0.00463 | -0.00631 | 0.00443 | * |
| * Ni | 33 | 0.00191 | -0.00012 | -0.00188 | * |
| * Ni | 34 | 0.00421 | -0.00838 | -0.00413 | * |
| * Ni | 35 | 0.00750 | 0.00811 | 0.00532 | * |
| * Ni | 36 | -0.00062 | -0.00199 | -0.00053 | * |
| * Ni | 37 | -0.01788 | -0.02654 | -0.02679 | * |
| * Ni | 38 | 0.01152 | 0.00103 | 0.01350 | * |
| * Ni | 39 | -0.00137 | -0.00017 | -0.00544 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 40 | -0.00196 | -0.00547 | -0.00438 | * |
| * Ni | 41 | 0.00107 | 0.00183 | 0.00016 | * |
| * Ni | 42 | 0.00175 | -0.00327 | -0.00252 | * |
| * Ni | 43 | -0.00541 | -0.00841 | -0.00023 | * |
| * Ni | 44 | 0.00242 | -0.00257 | -0.00059 | * |
| * Ni | 45 | 0.00690 | 0.00193 | 0.00088 | * |
| * Ni | 46 | 0.00255 | -0.01098 | -0.00677 | * |
| * Ni | 47 | 0.00473 | 0.00020 | 0.00511 | * |
| * Ni | 48 | 0.00334 | 0.00266 | 0.00155 | * |
| * Ni | 49 | 0.00385 | -0.01623 | -0.00063 | * |
| * Ni | 50 | -0.00388 | -0.00569 | 0.00145 | * |
| * Ni | 51 | 0.00276 | 0.00296 | 0.00278 | * |
| * Ni | 52 | 0.01075 | -0.00489 | 0.01038 | * |
| * Ni | 53 | 0.00145 | 0.00190 | 0.00185 | * |
| * Ni | 54 | 0.00216 | 0.00493 | 0.00326 | * |
| * Ni | 55 | 0.01339 | 0.00300 | 0.01512 | * |
| * Ni | 56 | 0.00025 | -0.00639 | 0.00363 | * |
| * Ni | 57 | -0.00038 | -0.00009 | 0.00187 | * |
| * Ni | 58 | -0.00126 | 0.00333 | 0.00493 | * |
| * Ni | 59 | -0.00218 | -0.00181 | -0.00082 | * |
| * Ni | 60 | -0.00539 | -0.00746 | -0.00807 | * |
| * Ni | 61 | -0.01380 | -0.01424 | -0.00892 | * |
| * Ni | 62 | -0.00220 | 0.00264 | 0.00140 | * |
| * Ni | 63 | -0.00349 | -0.00546 | -0.00919 | * |
| * Ni | 64 | 0.01042 | 0.00463 | 0.01222 | * |
| * Ni | 65 | 0.00395 | 0.00112 | 0.00758 | * |
| * Ni | 66 | 0.00154 | 0.00548 | -0.00128 | * |
| * Ni | 67 | -0.00247 | -0.00392 | 0.00203 | * |
| * Ni | 68 | 0.00202 | 0.00456 | 0.00465 | * |
| * Ni | 69 | 0.00631 | 0.00426 | 0.00417 | * |
| * Ni | 70 | 0.00095 | 0.00180 | 0.00080 | * |
| * Ni | 71 | 0.00223 | 0.00356 | 0.00604 | * |
| * Ni | 72 | -0.00055 | 0.00205 | 0.00039 | * |
| * Ni | 73 | 0.00218 | 0.00116 | 0.00202 | * |
| * Ni | 74 | -0.00353 | -0.00411 | -0.00522 | * |
| * Ni | 75 | -0.00410 | -0.00612 | -0.00329 | * |
| * | | | | | * |
| ***** | | | | | |



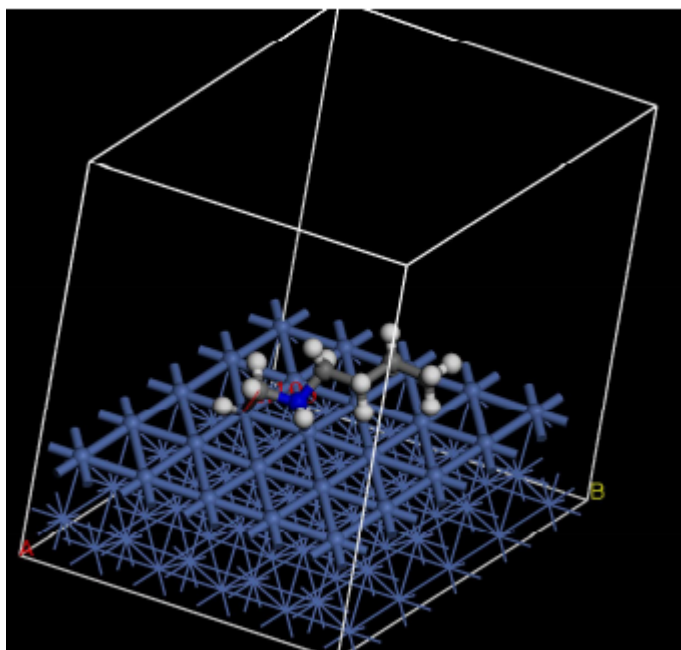
Final energy = -102795.0284123 eV

***** Forces *****

| ***** Forces ***** | | | | |
|---------------------------------|----|----------|----------|----------|
| * Cartesian components (eV/A) * | | | | |
| *-----* | | | | |
| | | x | y | z |
| * H | 1 | 0.00335 | -0.00259 | -0.00908 |
| * H | 2 | -0.00392 | 0.01785 | 0.00401 |
| * H | 3 | -0.03056 | 0.03671 | -0.00919 |
| * H | 4 | 0.00014 | 0.02534 | 0.01840 |
| * H | 5 | 0.01594 | 0.02883 | 0.00552 |
| * H | 6 | -0.02805 | 0.00274 | -0.01394 |
| * H | 7 | -0.00463 | 0.04190 | -0.00684 |
| * H | 8 | -0.05529 | -0.00320 | -0.03984 |
| * H | 9 | 0.00335 | -0.02043 | -0.00591 |
| * H | 10 | -0.01530 | -0.00486 | -0.00206 |
| * H | 11 | 0.00288 | -0.00176 | -0.02977 |
| * H | 12 | 0.02668 | 0.01649 | -0.05543 |
| * H | 13 | 0.06897 | 0.02102 | 0.00442 |
| * C | 1 | -0.01564 | 0.01373 | 0.01086 |
| * C | 2 | -0.00028 | 0.02234 | -0.00083 |
| * C | 3 | 0.00734 | 0.04885 | -0.05411 |

| | | | | | |
|------|----|----------|----------|----------|---|
| * C | 4 | -0.00592 | 0.03030 | -0.07362 | * |
| * C | 5 | 0.03891 | 0.01035 | -0.07866 | * |
| * N | 1 | -0.02407 | 0.03542 | -0.00145 | * |
| * Ni | 1 | -0.00985 | -0.01222 | -0.01383 | * |
| * Ni | 2 | 0.01889 | -0.00207 | 0.00838 | * |
| * Ni | 3 | 0.00611 | 0.00352 | 0.01337 | * |
| * Ni | 4 | -0.01142 | -0.00869 | 0.00615 | * |
| * Ni | 5 | -0.00746 | -0.00995 | 0.00404 | * |
| * Ni | 6 | 0.00445 | 0.00309 | 0.01467 | * |
| * Ni | 7 | 0.03264 | 0.04248 | -0.02216 | * |
| * Ni | 8 | 0.01203 | 0.00019 | 0.01366 | * |
| * Ni | 9 | 0.00225 | 0.00075 | -0.00575 | * |
| * Ni | 10 | 0.00967 | -0.00646 | 0.03220 | * |
| * Ni | 11 | -0.01236 | -0.01529 | -0.02639 | * |
| * Ni | 12 | 0.00808 | 0.01308 | 0.02612 | * |
| * Ni | 13 | -0.00646 | -0.00670 | -0.01833 | * |
| * Ni | 14 | 0.00608 | -0.00863 | -0.01200 | * |
| * Ni | 15 | 0.01872 | 0.01131 | 0.01823 | * |
| * Ni | 16 | -0.00275 | -0.00127 | 0.00520 | * |
| * Ni | 17 | 0.00463 | 0.00459 | 0.01031 | * |
| * Ni | 18 | -0.00502 | -0.00529 | 0.00275 | * |
| * Ni | 19 | -0.04000 | -0.03160 | -0.02576 | * |
| * Ni | 20 | 0.00496 | 0.00956 | 0.01196 | * |
| * Ni | 21 | 0.01366 | 0.00606 | 0.02118 | * |
| * Ni | 22 | -0.03296 | -0.05509 | 0.02884 | * |
| * Ni | 23 | -0.02543 | -0.03456 | -0.01941 | * |
| * Ni | 24 | 0.00312 | -0.00882 | -0.01191 | * |
| * Ni | 25 | -0.03915 | -0.01300 | -0.00049 | * |
| * Ni | 26 | -0.00804 | -0.00038 | -0.00971 | * |
| * Ni | 27 | 0.00493 | 0.00571 | 0.02446 | * |
| * Ni | 28 | -0.00590 | -0.00935 | -0.01568 | * |
| * Ni | 29 | -0.00580 | -0.01408 | -0.01242 | * |
| * Ni | 30 | 0.00630 | 0.00271 | 0.00924 | * |
| * Ni | 31 | 0.00455 | -0.01874 | -0.00399 | * |
| * Ni | 32 | 0.00670 | 0.00859 | 0.01413 | * |
| * Ni | 33 | -0.00818 | -0.00114 | 0.00156 | * |
| * Ni | 34 | 0.00903 | -0.00397 | 0.00014 | * |
| * Ni | 35 | -0.00446 | -0.01466 | -0.00562 | * |
| * Ni | 36 | 0.01155 | 0.00132 | 0.02238 | * |
| * Ni | 37 | -0.00026 | -0.02524 | 0.01060 | * |
| * Ni | 38 | 0.00367 | -0.00673 | 0.00313 | * |
| * Ni | 39 | 0.00611 | 0.00796 | -0.00966 | * |
| * Ni | 40 | -0.00176 | -0.04717 | 0.00590 | * |
| * Ni | 41 | 0.00081 | 0.01074 | 0.00792 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 42 | 0.02380 | 0.00268 | 0.03122 | * |
| * Ni | 43 | -0.01637 | -0.00576 | -0.03154 | * |
| * Ni | 44 | 0.00454 | 0.00326 | -0.00301 | * |
| * Ni | 45 | 0.01128 | 0.00840 | 0.01396 | * |
| * Ni | 46 | -0.00134 | -0.01218 | 0.00775 | * |
| * Ni | 47 | -0.00824 | -0.00132 | 0.01259 | * |
| * Ni | 48 | 0.00120 | 0.00368 | 0.01150 | * |
| * Ni | 49 | 0.00482 | -0.01224 | 0.00937 | * |
| * Ni | 50 | 0.01056 | 0.00206 | 0.01391 | * |
| * Ni | 51 | -0.01079 | -0.00984 | 0.01246 | * |
| * Ni | 52 | -0.01293 | -0.02786 | 0.01398 | * |
| * Ni | 53 | -0.00736 | 0.01527 | 0.00056 | * |
| * Ni | 54 | 0.01712 | 0.00788 | 0.00808 | * |
| * Ni | 55 | 0.00116 | -0.01404 | -0.00361 | * |
| * Ni | 56 | 0.00926 | 0.00017 | 0.01612 | * |
| * Ni | 57 | 0.01450 | 0.00462 | 0.03098 | * |
| * Ni | 58 | 0.00104 | 0.00308 | -0.01107 | * |
| * Ni | 59 | -0.01159 | -0.00237 | -0.01285 | * |
| * Ni | 60 | 0.00770 | 0.00932 | 0.01202 | * |
| * Ni | 61 | -0.00197 | 0.00037 | -0.00642 | * |
| * Ni | 62 | 0.00554 | -0.00803 | 0.00476 | * |
| * Ni | 63 | 0.00637 | 0.00178 | 0.01614 | * |
| * Ni | 64 | -0.00334 | -0.00506 | 0.01931 | * |
| * Ni | 65 | -0.00270 | -0.01821 | 0.00663 | * |
| * Ni | 66 | 0.00442 | 0.00633 | 0.02629 | * |
| * Ni | 67 | -0.03119 | -0.03564 | 0.01579 | * |
| * Ni | 68 | 0.00387 | 0.01320 | 0.00459 | * |
| * Ni | 69 | 0.00600 | 0.00302 | -0.00079 | * |
| * Ni | 70 | 0.00946 | -0.01175 | 0.02331 | * |
| * Ni | 71 | 0.00099 | -0.00817 | -0.00037 | * |
| * Ni | 72 | 0.00036 | -0.00147 | 0.01539 | * |
| * Ni | 73 | -0.00296 | -0.00648 | -0.02606 | * |
| * Ni | 74 | -0.00149 | 0.00083 | -0.00675 | * |
| * Ni | 75 | 0.01267 | 0.00486 | 0.00989 | * |
| * | | | | | * |
| ***** | | | | | |



Final energy = -102794.3430549 eV

+++++

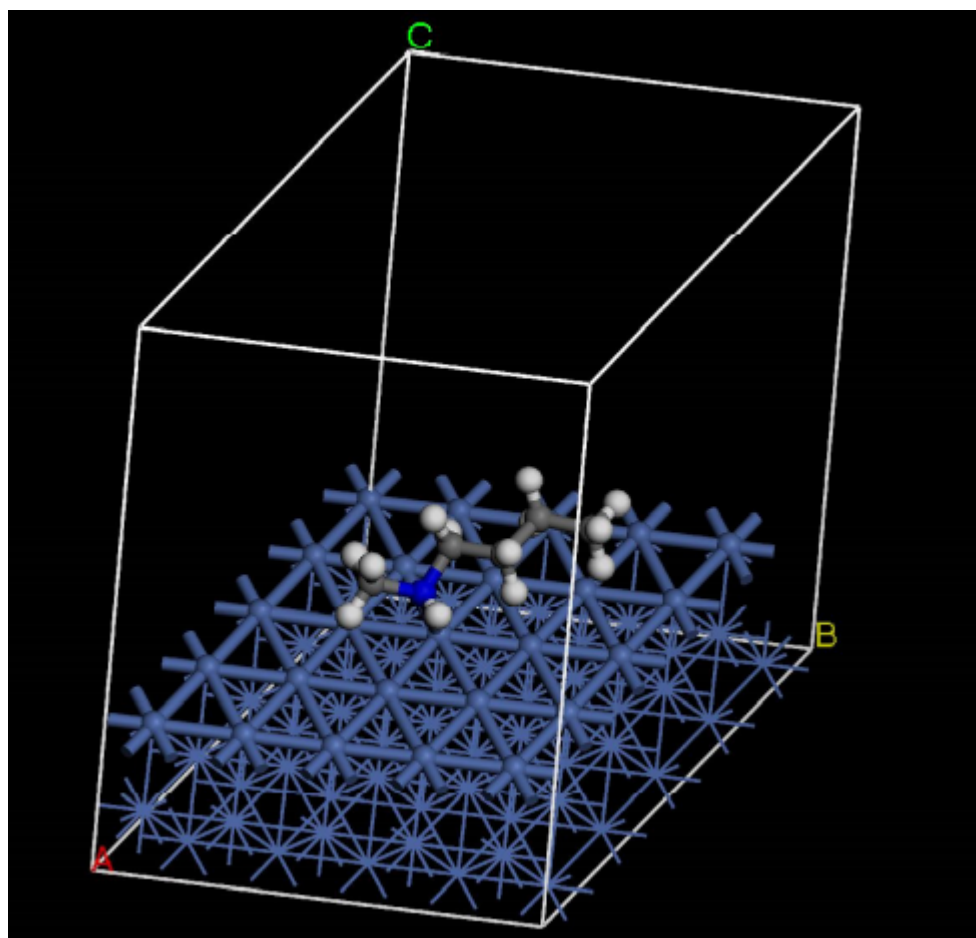
Transition State Found!

***** Forces *****

| ***** Forces ***** | | | | |
|---------------------------------|----|----------|----------|----------|
| * Cartesian components (eV/A) * | | | | |
| *-----* | | | | |
| | | x | y | z |
| * H | 1 | 0.00159 | 0.05740 | -0.02263 |
| * H | 2 | 0.01573 | 0.03935 | -0.01111 |
| * H | 3 | 0.06201 | 0.06636 | -0.01816 |
| * H | 4 | -0.04762 | 0.02115 | 0.00404 |
| * H | 5 | 0.02311 | 0.05349 | 0.05065 |
| * H | 6 | 0.05269 | 0.04187 | -0.01215 |
| * H | 7 | -0.01121 | 0.01324 | -0.00998 |
| * H | 8 | 0.01952 | -0.01469 | 0.03035 |
| * H | 9 | 0.05137 | -0.02188 | 0.05042 |
| * H | 10 | -0.19577 | 0.03045 | 0.10286 |
| * H | 11 | -0.22653 | -0.19360 | -0.18124 |
| * H | 12 | 0.23163 | 0.08958 | -0.11262 |
| * H | 13 | 0.57407 | -0.22078 | -0.02073 |
| * C | 1 | -0.07860 | 0.04159 | 0.03990 |

| | | | | | |
|------|----|----------|----------|----------|---|
| * C | 2 | 0.13848 | -0.06241 | -0.00341 | * |
| * C | 3 | -0.10450 | 0.02943 | 0.17061 | * |
| * C | 4 | 0.16624 | -0.04137 | -0.26046 | * |
| * C | 5 | 0.11330 | 0.40716 | -0.00317 | * |
| * N | 1 | -0.25995 | 0.06397 | 0.35491 | * |
| * Ni | 1 | 0.12053 | 0.08989 | 0.01516 | * |
| * Ni | 2 | 0.08474 | 0.04475 | 0.02040 | * |
| * Ni | 3 | 0.06105 | 0.01082 | 0.06512 | * |
| * Ni | 4 | 0.10050 | 0.09234 | 0.06267 | * |
| * Ni | 5 | 0.07276 | -0.04730 | -0.01064 | * |
| * Ni | 6 | 0.00603 | 0.02445 | 0.03087 | * |
| * Ni | 7 | -0.03551 | -0.05259 | 0.04881 | * |
| * Ni | 8 | -0.01708 | 0.04887 | 0.03437 | * |
| * Ni | 9 | -0.03193 | 0.00024 | -0.01070 | * |
| * Ni | 10 | 0.02900 | -0.01859 | 0.00867 | * |
| * Ni | 11 | -0.07341 | -0.00830 | 0.04490 | * |
| * Ni | 12 | -0.06985 | 0.01925 | -0.04749 | * |
| * Ni | 13 | 0.03367 | -0.05760 | -0.07222 | * |
| * Ni | 14 | -0.31398 | -0.18747 | 0.07727 | * |
| * Ni | 15 | -0.08699 | -0.02645 | 0.01508 | * |
| * Ni | 16 | 0.12034 | 0.11163 | -0.00246 | * |
| * Ni | 17 | 0.02936 | 0.05980 | -0.06039 | * |
| * Ni | 18 | 0.05750 | -0.02448 | -0.01775 | * |
| * Ni | 19 | 0.05685 | 0.06735 | 0.05826 | * |
| * Ni | 20 | 0.02558 | -0.06053 | 0.00591 | * |
| * Ni | 21 | -0.00362 | -0.01069 | -0.00153 | * |
| * Ni | 22 | -0.58666 | -0.02674 | -0.11879 | * |
| * Ni | 23 | 0.00368 | 0.04263 | 0.03162 | * |
| * Ni | 24 | -0.00226 | 0.02431 | 0.00175 | * |
| * Ni | 25 | 0.04639 | 0.02277 | 0.01404 | * |
| * Ni | 26 | -0.01130 | -0.01830 | -0.00881 | * |
| * Ni | 27 | -0.03221 | -0.03408 | 0.01338 | * |
| * Ni | 28 | 0.06559 | -0.07178 | 0.00294 | * |
| * Ni | 29 | -0.03602 | -0.04028 | 0.03519 | * |
| * Ni | 30 | -0.07468 | 0.00578 | 0.01743 | * |
| * Ni | 31 | 0.04137 | 0.01470 | -0.00927 | * |
| * Ni | 32 | 0.00580 | -0.00299 | -0.02545 | * |
| * Ni | 33 | 0.02699 | -0.02943 | -0.05982 | * |
| * Ni | 34 | 0.02989 | 0.05124 | 0.03263 | * |
| * Ni | 35 | -0.05618 | -0.01945 | -0.05405 | * |
| * Ni | 36 | 0.00704 | -0.05623 | 0.00408 | * |
| * Ni | 37 | 0.00314 | 0.04785 | -0.02854 | * |
| * Ni | 38 | -0.06120 | -0.07404 | -0.01574 | * |
| * Ni | 39 | 0.01749 | 0.02005 | 0.01821 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 40 | 0.02432 | 0.00536 | 0.03190 | * |
| * Ni | 41 | 0.02383 | 0.07045 | 0.04269 | * |
| * Ni | 42 | -0.02132 | 0.01987 | 0.00403 | * |
| * Ni | 43 | 0.03188 | 0.02121 | -0.01469 | * |
| * Ni | 44 | -0.02517 | -0.04548 | 0.00174 | * |
| * Ni | 45 | -0.05758 | 0.01189 | 0.01529 | * |
| * Ni | 46 | -0.04796 | 0.00556 | -0.05264 | * |
| * Ni | 47 | -0.01724 | 0.01487 | -0.02263 | * |
| * Ni | 48 | 0.01881 | -0.07905 | -0.07718 | * |
| * Ni | 49 | 0.02664 | 0.01367 | 0.02059 | * |
| * Ni | 50 | 0.03644 | -0.04335 | -0.00659 | * |
| * Ni | 51 | -0.00676 | -0.05029 | -0.03234 | * |
| * Ni | 52 | 0.01685 | 0.05081 | 0.01916 | * |
| * Ni | 53 | -0.03201 | 0.00153 | -0.07106 | * |
| * Ni | 54 | 0.02722 | -0.02190 | -0.00085 | * |
| * Ni | 55 | 0.01744 | 0.02108 | 0.04240 | * |
| * Ni | 56 | -0.04619 | -0.06092 | -0.00798 | * |
| * Ni | 57 | -0.01754 | -0.01492 | -0.02201 | * |
| * Ni | 58 | 0.02193 | -0.01137 | 0.04932 | * |
| * Ni | 59 | 0.04536 | 0.11059 | 0.08271 | * |
| * Ni | 60 | -0.03109 | -0.00047 | 0.01790 | * |
| * Ni | 61 | -0.09841 | -0.07843 | -0.08626 | * |
| * Ni | 62 | -0.04223 | -0.04616 | -0.06298 | * |
| * Ni | 63 | -0.09758 | -0.28518 | -0.21544 | * |
| * Ni | 64 | -0.00462 | -0.00359 | 0.02179 | * |
| * Ni | 65 | 0.00259 | 0.04581 | -0.04542 | * |
| * Ni | 66 | 0.04847 | -0.04235 | -0.05503 | * |
| * Ni | 67 | -0.00045 | -0.01147 | 0.02595 | * |
| * Ni | 68 | 0.02864 | -0.01185 | -0.00530 | * |
| * Ni | 69 | 0.01198 | -0.05921 | -0.01326 | * |
| * Ni | 70 | -0.01995 | 0.03533 | 0.03562 | * |
| * Ni | 71 | 0.02231 | 0.00498 | -0.04949 | * |
| * Ni | 72 | 0.00117 | -0.03647 | 0.01201 | * |
| * Ni | 73 | -0.00049 | 0.06494 | 0.05047 | * |
| * Ni | 74 | 0.01216 | 0.03176 | 0.07602 | * |
| * Ni | 75 | 0.07060 | 0.04104 | 0.02835 | * |
| * | | | | | * |
| ***** | | | | | |



Final energy = -102795.3248242 eV

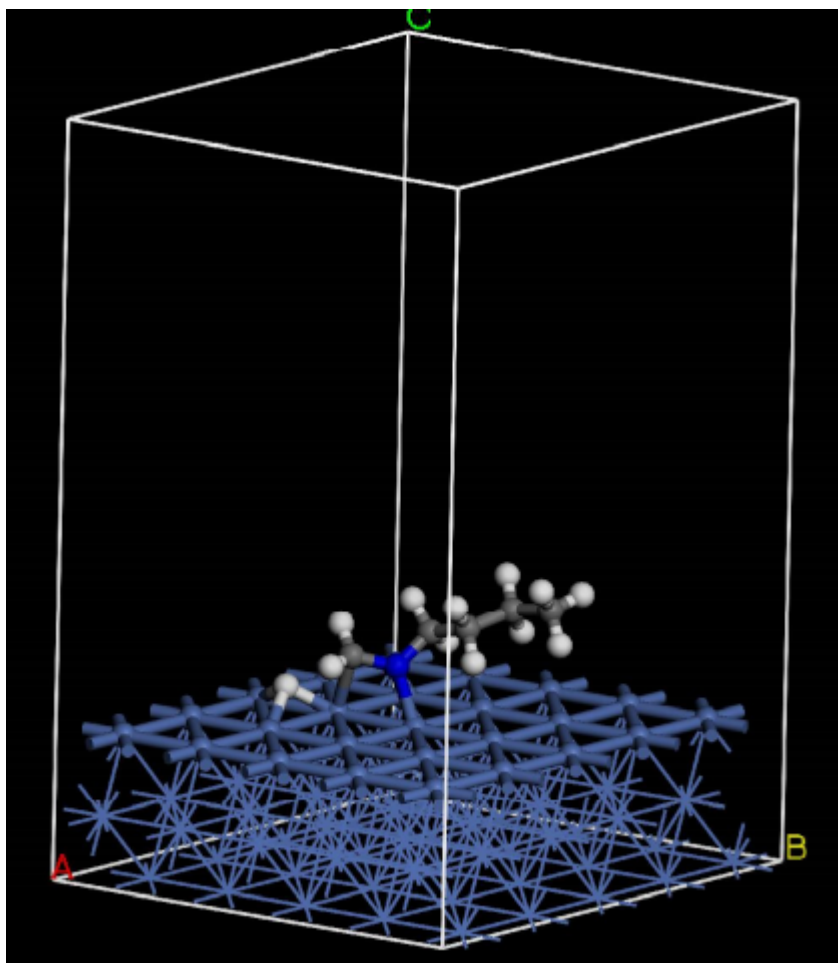
```

***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 0.11955 0.01073 0.05320 *
* H 2 0.06815 0.13291 0.09595 *
* H 3 0.01486 0.10860 0.04592 *
* H 4 0.13645 0.11004 0.08418 *
* H 5 0.02571 0.06488 0.02332 *
* H 6 0.04403 0.02757 0.01117 *
* H 7 0.03123 0.05912 -0.04126 *
* H 8 0.05820 0.09938 0.03269 *
* H 9 0.10690 0.16118 0.17164 *
* H 10 -0.00901 0.00349 -0.05988 *
* H 11 -0.06003 -0.00892 0.08744 *
* H 12 0.08605 0.05270 -0.03373 *
* H 13 -0.00887 0.02683 -0.04765 *

```

| | | | | |
|------|----|----------|----------|------------|
| * C | 1 | -0.21461 | -0.27959 | 0.04223 * |
| * C | 2 | 0.28336 | 0.01346 | -0.20380 * |
| * C | 3 | -0.46120 | 0.10923 | 0.03137 * |
| * C | 4 | 0.08982 | -0.11864 | -0.21374 * |
| * C | 5 | 0.18558 | 0.29299 | -0.08185 * |
| * N | 1 | -0.07957 | 0.27977 | 0.26323 * |
| * Ni | 1 | -0.09994 | -0.06049 | -0.04084 * |
| * Ni | 2 | 0.01223 | 0.14809 | 0.09484 * |
| * Ni | 3 | -0.00081 | 0.01455 | 0.04801 * |
| * Ni | 4 | -0.09944 | -0.07113 | -0.05037 * |
| * Ni | 5 | -0.12742 | -0.30523 | -0.14755 * |
| * Ni | 6 | 0.04340 | -0.03141 | 0.06851 * |
| * Ni | 7 | 0.02740 | -0.04797 | -0.18670 * |
| * Ni | 8 | -0.10464 | -0.08646 | -0.08715 * |
| * Ni | 9 | 0.14679 | 0.06069 | 0.06818 * |
| * Ni | 10 | -0.01801 | -0.01132 | 0.01389 * |
| * Ni | 11 | -0.38205 | -0.16061 | -0.13873 * |
| * Ni | 12 | 0.09847 | 0.10898 | 0.08933 * |
| * Ni | 13 | -0.01515 | -0.06417 | -0.05226 * |
| * Ni | 14 | 0.38776 | 0.10278 | 0.16540 * |
| * Ni | 15 | -0.02765 | 0.03329 | 0.03335 * |
| * Ni | 16 | -0.11494 | -0.11489 | -0.12914 * |
| * Ni | 17 | 0.00470 | 0.06120 | 0.09896 * |
| * Ni | 18 | -0.01942 | 0.02812 | 0.01509 * |
| * Ni | 19 | -0.26558 | -0.13199 | -0.16823 * |
| * Ni | 20 | 0.06220 | 0.19034 | 0.03646 * |
| * Ni | 21 | 0.03453 | -0.00450 | 0.04767 * |
| * Ni | 22 | -0.08068 | -0.18366 | -0.18199 * |
| * Ni | 23 | -0.00818 | -0.05851 | -0.04642 * |
| * Ni | 24 | 0.10073 | 0.05237 | 0.00187 * |
| * Ni | 25 | -0.06915 | -0.19371 | -0.05070 * |
| * Ni | 26 | -0.41370 | -0.17597 | -0.14613 * |
| * Ni | 27 | 0.07364 | 0.05529 | 0.04886 * |
| * Ni | 28 | 0.02816 | -0.06333 | -0.06619 * |
| * Ni | 29 | 0.38839 | 0.16885 | 0.16859 * |
| * Ni | 30 | 0.00365 | 0.03765 | 0.03578 * |
| * Ni | 31 | -0.19715 | -0.07112 | -0.04724 * |
| * Ni | 32 | 0.10733 | 0.08097 | 0.24055 * |
| * Ni | 33 | -0.08001 | 0.06035 | -0.00202 * |
| * Ni | 34 | -0.23819 | -0.05532 | -0.21676 * |
| * Ni | 35 | 0.22260 | 0.20026 | 0.36065 * |
| * Ni | 36 | -0.00182 | 0.03492 | -0.01302 * |
| * Ni | 37 | 0.45787 | 0.15548 | 0.48929 * |
| * Ni | 38 | 0.00001 | -0.07250 | -0.05254 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 39 | 0.10146 | 0.00888 | 0.07045 * |
| * Ni | 40 | -0.16492 | -0.32521 | -0.21442 * |
| * Ni | 41 | -0.41989 | -0.20364 | -0.18641 * |
| * Ni | 42 | 0.12566 | 0.02928 | 0.03633 * |
| * Ni | 43 | -0.02825 | -0.07311 | -0.03746 * |
| * Ni | 44 | 0.43337 | 0.13562 | 0.16735 * |
| * Ni | 45 | -0.07729 | 0.07410 | 0.07775 * |
| * Ni | 46 | -0.14588 | -0.10999 | -0.07168 * |
| * Ni | 47 | -0.00502 | 0.21390 | 0.20745 * |
| * Ni | 48 | -0.04248 | 0.04147 | 0.01426 * |
| * Ni | 49 | -0.11524 | 0.00414 | -0.14839 * |
| * Ni | 50 | -0.02604 | -0.17295 | -0.27031 * |
| * Ni | 51 | 0.08943 | 0.06475 | 0.01627 * |
| * Ni | 52 | -0.00028 | -0.05161 | -0.05962 * |
| * Ni | 53 | -0.00195 | -0.10545 | -0.07890 * |
| * Ni | 54 | 0.12604 | 0.03957 | 0.03438 * |
| * Ni | 55 | -0.11123 | -0.11091 | -0.11228 * |
| * Ni | 56 | -0.41863 | -0.17415 | -0.16074 * |
| * Ni | 57 | 0.06988 | 0.04341 | 0.05215 * |
| * Ni | 58 | 0.06229 | -0.06050 | -0.03693 * |
| * Ni | 59 | 0.45620 | 0.12838 | 0.15882 * |
| * Ni | 60 | -0.05647 | 0.05406 | 0.06563 * |
| * Ni | 61 | -0.11063 | -0.05299 | -0.06971 * |
| * Ni | 62 | -0.05078 | 0.10158 | 0.15422 * |
| * Ni | 63 | 0.00118 | 0.02316 | 0.06497 * |
| * Ni | 64 | -0.15503 | -0.05026 | -0.07501 * |
| * Ni | 65 | 0.02292 | -0.19197 | -0.15434 * |
| * Ni | 66 | 0.10917 | 0.03494 | 0.06427 * |
| * Ni | 67 | -0.00554 | -0.09266 | -0.11326 * |
| * Ni | 68 | -0.08656 | -0.05919 | -0.05794 * |
| * Ni | 69 | 0.08399 | 0.02765 | 0.02258 * |
| * Ni | 70 | -0.03514 | -0.06489 | -0.03233 * |
| * Ni | 71 | -0.39416 | -0.10088 | -0.12614 * |
| * Ni | 72 | 0.10979 | 0.09428 | 0.08434 * |
| * Ni | 73 | 0.02256 | -0.08060 | -0.05115 * |
| * Ni | 74 | 0.39864 | 0.14232 | 0.18013 * |
| * Ni | 75 | -0.01373 | 0.04383 | 0.02394 * |
| * | | | | * |



Final energy = -102778.4793301 eV

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***** Forces *****
```

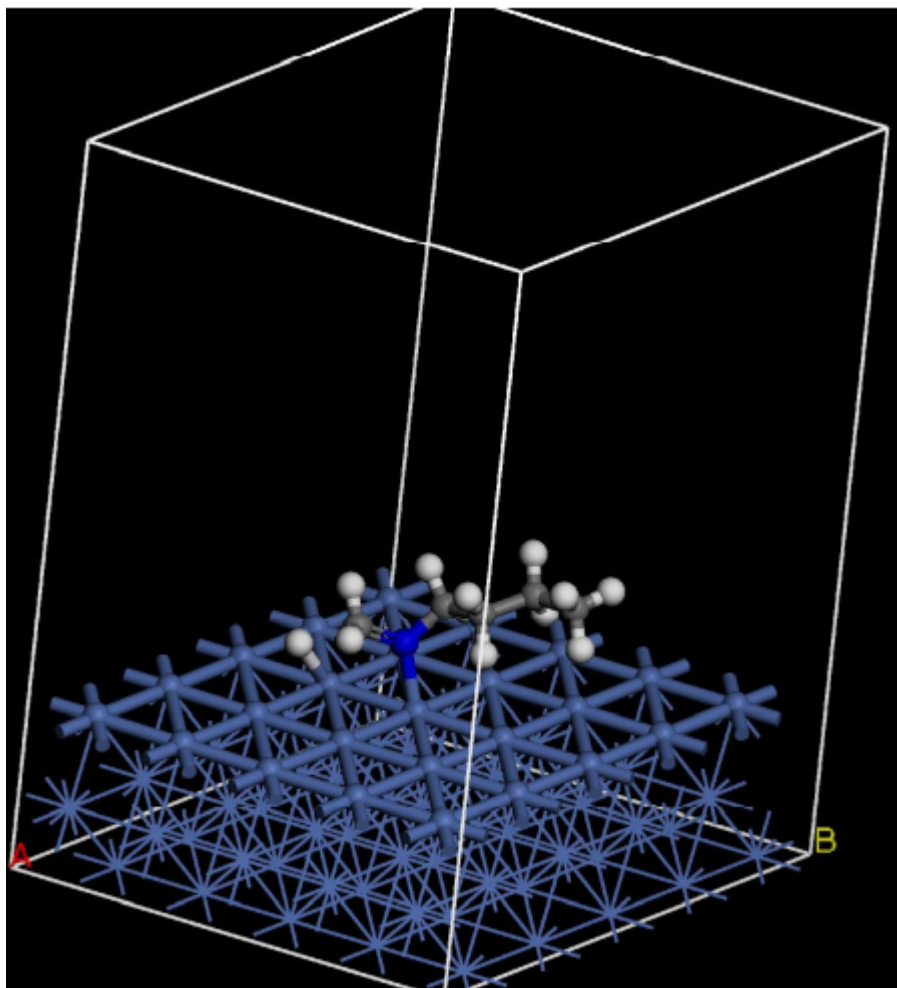
| | | Cartesian components (eV/A) | | | |
|-------|----|-----------------------------|----------|----------|---|
| ----- | | | | | |
| | | x | y | z | |
| * H | 1 | 0.01294 | 0.04540 | 0.00783 | * |
| * H | 2 | 0.10461 | 0.04036 | 0.06213 | * |
| * H | 3 | -0.03886 | 0.00973 | -0.01099 | * |
| * H | 4 | 0.02843 | 0.07711 | 0.06467 | * |
| * H | 5 | -0.02750 | -0.00160 | 0.00254 | * |
| * H | 6 | -0.03622 | -0.00312 | 0.02416 | * |
| * H | 7 | 0.04005 | 0.06327 | 0.04372 | * |
| * H | 8 | -0.02797 | 0.01295 | -0.02208 | * |
| * H | 9 | -0.05354 | 0.06894 | 0.01962 | * |
| * H | 10 | 0.12718 | 0.09870 | 0.08441 | * |
| * H | 11 | 0.06515 | 0.03393 | -0.06175 | * |
| * H | 12 | -0.02581 | -0.12928 | -0.03949 | * |

| | | | | |
|------|----|----------|----------|------------|
| * C | 1 | -0.15644 | -0.18441 | 0.08298 * |
| * C | 2 | 0.33310 | 0.00853 | -0.12855 * |
| * C | 3 | -0.40778 | -0.07084 | 0.18250 * |
| * C | 4 | 0.38633 | 0.23523 | -0.04093 * |
| * C | 5 | -0.08755 | 0.05439 | -0.11673 * |
| * N | 1 | -0.06339 | 0.41229 | 0.00279 * |
| * Ni | 1 | 0.01962 | -0.07872 | -0.00521 * |
| * Ni | 2 | -0.14662 | -0.22832 | -0.11408 * |
| * Ni | 3 | -0.00651 | 0.02998 | 0.12089 * |
| * Ni | 4 | -0.09962 | -0.01179 | 0.00137 * |
| * Ni | 5 | -0.04968 | -0.09419 | -0.11769 * |
| * Ni | 6 | 0.04001 | 0.03730 | 0.16870 * |
| * Ni | 7 | -0.04365 | -0.08775 | 0.02725 * |
| * Ni | 8 | -0.15894 | -0.11556 | -0.21289 * |
| * Ni | 9 | 0.08759 | 0.09460 | 0.10937 * |
| * Ni | 10 | -0.00144 | -0.15675 | 0.03565 * |
| * Ni | 11 | -0.13875 | -0.08816 | -0.36577 * |
| * Ni | 12 | 0.11066 | 0.09388 | 0.14365 * |
| * Ni | 13 | -0.02318 | -0.08898 | -0.03116 * |
| * Ni | 14 | -0.07075 | -0.04901 | -0.14394 * |
| * Ni | 15 | 0.12570 | 0.11369 | 0.14638 * |
| * Ni | 16 | -0.10261 | -0.05048 | -0.02600 * |
| * Ni | 17 | 0.17014 | 0.15799 | -0.01591 * |
| * Ni | 18 | 0.00670 | -0.00664 | 0.06514 * |
| * Ni | 19 | -0.19860 | -0.09644 | -0.08394 * |
| * Ni | 20 | -0.14995 | -0.21106 | -0.03432 * |
| * Ni | 21 | 0.00762 | -0.01584 | 0.01914 * |
| * Ni | 22 | 0.44586 | 0.36697 | 0.45422 * |
| * Ni | 23 | -0.16290 | -0.21901 | -0.07853 * |
| * Ni | 24 | 0.04189 | 0.06494 | 0.07422 * |
| * Ni | 25 | 0.01160 | -0.22357 | 0.06990 * |
| * Ni | 26 | -0.23429 | -0.15990 | -0.07874 * |
| * Ni | 27 | 0.11771 | 0.13076 | 0.11412 * |
| * Ni | 28 | -0.02489 | -0.08138 | -0.01414 * |
| * Ni | 29 | -0.27537 | -0.19255 | -0.04044 * |
| * Ni | 30 | 0.03671 | 0.06174 | 0.06084 * |
| * Ni | 31 | -0.12232 | -0.04570 | -0.06384 * |
| * Ni | 32 | 0.28218 | 0.23044 | 0.10964 * |
| * Ni | 33 | -0.04419 | 0.02542 | -0.12629 * |
| * Ni | 34 | -0.32946 | -0.06053 | -0.23089 * |
| * Ni | 35 | 0.22812 | 0.16142 | 0.06049 * |
| * Ni | 36 | -0.02634 | -0.00942 | -0.05593 * |
| * Ni | 37 | 0.18077 | 0.08043 | 0.38418 * |
| * Ni | 38 | 0.15519 | 0.13987 | -0.11130 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 39 | 0.06707 | 0.04054 | -0.02107 * |
| * Ni | 40 | -0.17756 | -0.23402 | -0.27741 * |
| * Ni | 41 | -0.19221 | -0.24258 | -0.05912 * |
| * Ni | 42 | -0.00054 | -0.05300 | -0.03039 * |
| * Ni | 43 | -0.09490 | -0.05427 | -0.03172 * |
| * Ni | 44 | 0.27668 | 0.18662 | 0.04383 * |
| * Ni | 45 | 0.07239 | 0.08944 | 0.04286 * |
| * Ni | 46 | -0.12309 | -0.15162 | -0.09939 * |
| * Ni | 47 | 0.15155 | 0.11717 | 0.44332 * |
| * Ni | 48 | 0.02346 | 0.06313 | -0.06262 * |
| * Ni | 49 | -0.13141 | -0.05937 | -0.17154 * |
| * Ni | 50 | 0.04112 | 0.05713 | 0.14786 * |
| * Ni | 51 | 0.06120 | 0.05637 | -0.01896 * |
| * Ni | 52 | -0.00382 | -0.00734 | -0.08202 * |
| * Ni | 53 | 0.03317 | -0.01698 | 0.06093 * |
| * Ni | 54 | 0.06589 | -0.01205 | -0.00271 * |
| * Ni | 55 | -0.03068 | -0.04587 | -0.10917 * |
| * Ni | 56 | 0.11254 | 0.16666 | 0.14340 * |
| * Ni | 57 | -0.00259 | 0.06785 | 0.02126 * |
| * Ni | 58 | -0.01134 | -0.02352 | -0.11745 * |
| * Ni | 59 | 0.09586 | 0.08160 | 0.23574 * |
| * Ni | 60 | 0.12079 | 0.09184 | 0.00606 * |
| * Ni | 61 | -0.02549 | -0.04578 | 0.02394 * |
| * Ni | 62 | -0.11556 | -0.13787 | -0.35428 * |
| * Ni | 63 | 0.12685 | 0.07748 | 0.04116 * |
| * Ni | 64 | -0.02311 | -0.03953 | -0.03205 * |
| * Ni | 65 | -0.20580 | -0.12964 | -0.34879 * |
| * Ni | 66 | 0.01143 | 0.05952 | 0.00536 * |
| * Ni | 67 | -0.02174 | -0.10283 | -0.02980 * |
| * Ni | 68 | 0.18279 | 0.10769 | 0.34679 * |
| * Ni | 69 | 0.03317 | 0.11638 | 0.04833 * |
| * Ni | 70 | -0.13051 | -0.12301 | -0.07369 * |
| * Ni | 71 | 0.08561 | 0.14054 | 0.36836 * |
| * Ni | 72 | -0.04152 | -0.01519 | -0.03504 * |
| * Ni | 73 | -0.05691 | -0.03149 | -0.04993 * |
| * Ni | 74 | -0.08860 | -0.20295 | -0.35250 * |
| * Ni | 75 | 0.08509 | 0.01971 | 0.00951 * |

*

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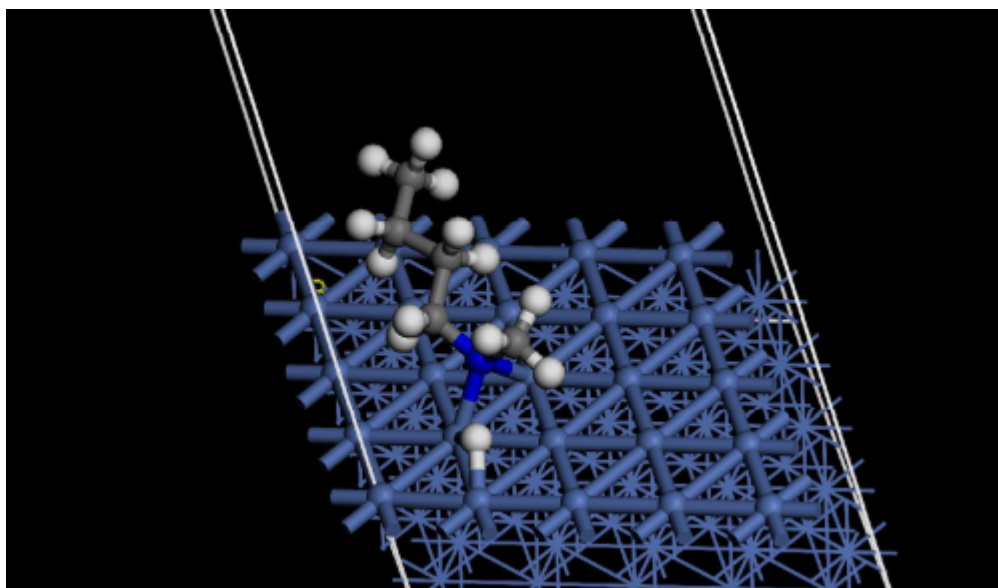
Final energy = -102778.0913945 eV

***** Forces *****

| ***** Forces ***** | | | | | |
|---------------------------------|----|----------|----------|----------|---|
| * Cartesian components (eV/A) * | | | | | |
| *-----* | | | | | |
| | x | y | z | | |
| * H | 1 | 0.02058 | 0.00920 | -0.01910 | * |
| * H | 2 | 0.05592 | 0.00706 | 0.01907 | * |
| * H | 3 | 0.11754 | 0.04833 | 0.04385 | * |
| * H | 4 | -0.11790 | 0.04436 | -0.02535 | * |
| * H | 5 | -0.00656 | 0.02090 | 0.01477 | * |
| * H | 6 | 0.10682 | 0.02791 | 0.08018 | * |
| * H | 7 | -0.03991 | 0.02339 | 0.02053 | * |
| * H | 8 | -0.02596 | 0.10364 | 0.04883 | * |
| * H | 9 | -0.02046 | -0.00031 | 0.09555 | * |
| * H | 10 | 0.00696 | -0.29110 | 0.00296 | * |
| * H | 11 | -0.44912 | 0.02356 | 0.13636 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * H | 12 | -0.03699 | -0.17920 | 0.13247 | * |
| * C | 1 | -0.16238 | 0.02752 | 0.00205 | * |
| * C | 2 | 0.20019 | 0.01314 | 0.12335 | * |
| * C | 3 | -0.27729 | -0.06165 | -0.08677 | * |
| * C | 4 | 0.00200 | -0.07738 | -0.03143 | * |
| * C | 5 | 0.32633 | -0.33122 | -0.49840 | * |
| * N | 1 | -0.36914 | 0.17881 | 0.21951 | * |
| * Ni | 1 | 0.05175 | 0.02998 | -0.00379 | * |
| * Ni | 2 | 0.10698 | 0.01104 | -0.01967 | * |
| * Ni | 3 | 0.01647 | 0.05312 | 0.04226 | * |
| * Ni | 4 | 0.04961 | -0.01323 | -0.07526 | * |
| * Ni | 5 | 0.10232 | 0.19541 | 0.05896 | * |
| * Ni | 6 | -0.02493 | 0.03710 | 0.05291 | * |
| * Ni | 7 | -0.01720 | -0.07417 | -0.00863 | * |
| * Ni | 8 | 0.05541 | 0.05510 | 0.06987 | * |
| * Ni | 9 | -0.05264 | 0.02460 | -0.01544 | * |
| * Ni | 10 | -0.04923 | -0.05397 | -0.02413 | * |
| * Ni | 11 | 0.04749 | -0.04932 | 0.02230 | * |
| * Ni | 12 | -0.06113 | -0.07209 | -0.06029 | * |
| * Ni | 13 | -0.05198 | 0.00225 | -0.03684 | * |
| * Ni | 14 | -0.02587 | 0.01688 | 0.03401 | * |
| * Ni | 15 | 0.04426 | 0.02423 | 0.03717 | * |
| * Ni | 16 | 0.09796 | 0.02530 | 0.02234 | * |
| * Ni | 17 | 0.02253 | -0.10131 | 0.03435 | * |
| * Ni | 18 | 0.00810 | 0.00126 | 0.04298 | * |
| * Ni | 19 | 0.28165 | 0.00960 | -0.02039 | * |
| * Ni | 20 | 0.04338 | 0.10700 | 0.10470 | * |
| * Ni | 21 | -0.02182 | 0.03729 | 0.04457 | * |
| * Ni | 22 | -0.01201 | 0.50727 | -0.01798 | * |
| * Ni | 23 | 0.01693 | 0.08005 | 0.12005 | * |
| * Ni | 24 | -0.03393 | -0.02672 | -0.00739 | * |
| * Ni | 25 | 0.05572 | -0.14005 | -0.03704 | * |
| * Ni | 26 | -0.01245 | 0.02598 | 0.01285 | * |
| * Ni | 27 | 0.01258 | 0.01774 | -0.04167 | * |
| * Ni | 28 | -0.01346 | -0.03099 | -0.00322 | * |
| * Ni | 29 | -0.05507 | -0.00085 | -0.00975 | * |
| * Ni | 30 | 0.00998 | -0.02065 | 0.05342 | * |
| * Ni | 31 | 0.01692 | 0.03093 | 0.01680 | * |
| * Ni | 32 | 0.00318 | -0.02649 | 0.01295 | * |
| * Ni | 33 | 0.00912 | -0.01832 | 0.03319 | * |
| * Ni | 34 | 0.05536 | -0.00078 | -0.10726 | * |
| * Ni | 35 | 0.03649 | 0.02933 | 0.02872 | * |
| * Ni | 36 | -0.04456 | 0.00362 | 0.03478 | * |
| * Ni | 37 | 0.06667 | -0.00689 | -0.24853 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 38 | 0.05091 | -0.01100 | 0.02391 | * |
| * Ni | 39 | -0.05956 | -0.04163 | -0.02775 | * |
| * Ni | 40 | -0.08428 | -0.03694 | -0.06111 | * |
| * Ni | 41 | 0.01132 | 0.01645 | -0.04103 | * |
| * Ni | 42 | 0.06226 | -0.03249 | -0.01090 | * |
| * Ni | 43 | 0.00054 | -0.04674 | 0.05697 | * |
| * Ni | 44 | -0.07261 | -0.04982 | -0.02409 | * |
| * Ni | 45 | -0.00315 | 0.02620 | 0.03828 | * |
| * Ni | 46 | 0.06763 | 0.02732 | 0.01602 | * |
| * Ni | 47 | 0.03734 | -0.04661 | -0.01632 | * |
| * Ni | 48 | 0.00037 | -0.02172 | 0.00871 | * |
| * Ni | 49 | 0.06962 | -0.02610 | -0.08198 | * |
| * Ni | 50 | -0.05248 | 0.01231 | -0.04002 | * |
| * Ni | 51 | -0.05312 | 0.01629 | 0.02371 | * |
| * Ni | 52 | 0.01823 | -0.02900 | -0.02952 | * |
| * Ni | 53 | 0.05006 | -0.01351 | 0.00580 | * |
| * Ni | 54 | -0.03659 | -0.03501 | -0.03243 | * |
| * Ni | 55 | -0.05875 | -0.03648 | -0.02458 | * |
| * Ni | 56 | 0.00015 | 0.02632 | -0.03155 | * |
| * Ni | 57 | 0.01936 | -0.05760 | 0.03820 | * |
| * Ni | 58 | 0.06937 | 0.01884 | 0.04929 | * |
| * Ni | 59 | -0.04106 | -0.06073 | -0.05381 | * |
| * Ni | 60 | -0.01551 | 0.06468 | 0.03601 | * |
| * Ni | 61 | 0.04619 | -0.01394 | -0.01254 | * |
| * Ni | 62 | 0.06049 | 0.02331 | -0.01062 | * |
| * Ni | 63 | 0.00278 | 0.00467 | 0.01662 | * |
| * Ni | 64 | 0.03985 | -0.02097 | -0.10724 | * |
| * Ni | 65 | 0.01675 | 0.09065 | -0.01098 | * |
| * Ni | 66 | -0.07284 | 0.01705 | 0.03413 | * |
| * Ni | 67 | -0.01926 | -0.00375 | -0.05371 | * |
| * Ni | 68 | 0.06292 | 0.04618 | 0.03309 | * |
| * Ni | 69 | -0.05447 | -0.02324 | -0.01579 | * |
| * Ni | 70 | -0.00901 | -0.05224 | -0.01488 | * |
| * Ni | 71 | 0.02080 | -0.05531 | -0.02140 | * |
| * Ni | 72 | -0.07568 | -0.03950 | -0.01851 | * |
| * Ni | 73 | 0.02238 | 0.04195 | -0.03771 | * |
| * Ni | 74 | -0.12274 | 0.03076 | -0.04461 | * |
| * Ni | 75 | 0.03654 | 0.01517 | 0.02201 | * |
| * | | | | | * |
| ***** | | | | | |



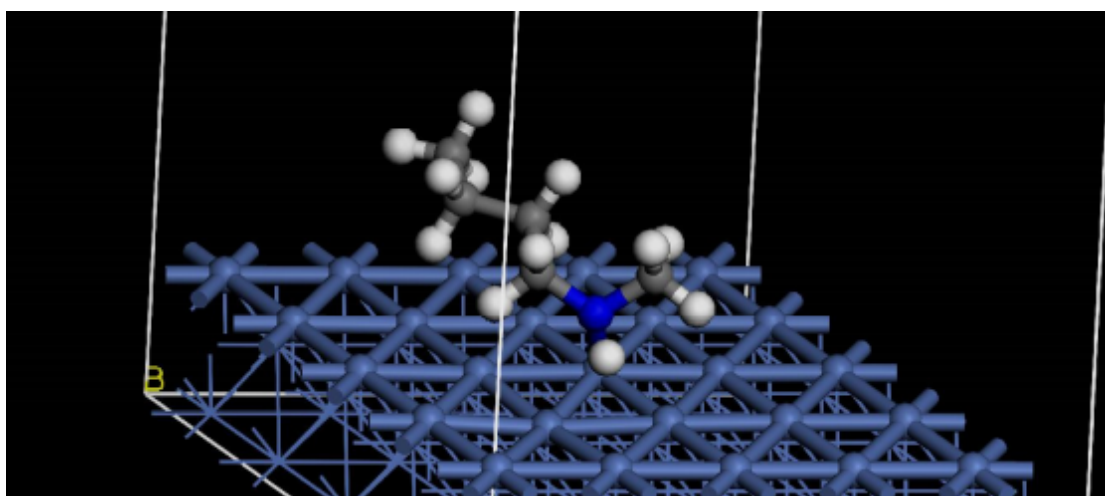
Final energy = -102795.1968992 eV

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***** Forces *****
```

| ***** Forces ***** | | | | | |
|---------------------------------|----|----------|----------|----------|---|
| * Cartesian components (eV/A) * | | | | | |
| *-----* | | | | | |
| | | x | y | z | |
| * H | 1 | 0.02157 | 0.05368 | -0.00289 | * |
| * H | 2 | -0.03420 | -0.00984 | -0.02832 | * |
| * H | 3 | 0.02862 | -0.03944 | -0.01230 | * |
| * H | 4 | 0.01007 | 0.04265 | 0.02784 | * |
| * H | 5 | 0.02048 | -0.00235 | -0.05038 | * |
| * H | 6 | 0.00325 | -0.01223 | -0.04233 | * |
| * H | 7 | -0.02726 | 0.04452 | -0.02196 | * |
| * H | 8 | -0.00172 | -0.02526 | -0.00947 | * |
| * H | 9 | 0.03314 | -0.00394 | -0.02179 | * |
| * H | 10 | -0.01880 | 0.03864 | 0.02810 | * |
| * H | 11 | -0.05451 | -0.01732 | 0.07817 | * |
| * H | 12 | 0.02464 | 0.04443 | -0.00098 | * |
| * H | 13 | 0.05263 | -0.03309 | 0.00046 | * |
| * C | 1 | 0.08439 | 0.01109 | -0.04920 | * |
| * C | 2 | -0.01243 | 0.00769 | -0.04814 | * |
| * C | 3 | 0.01866 | 0.01151 | -0.07165 | * |
| * C | 4 | -0.00120 | 0.02212 | 0.01924 | * |
| * C | 5 | 0.02416 | 0.00359 | -0.03851 | * |
| * N | 1 | -0.01693 | 0.00288 | -0.02786 | * |
| * Ni | 1 | 0.01317 | -0.01195 | 0.00987 | * |
| * Ni | 2 | 0.00499 | 0.01139 | 0.00845 | * |
| * Ni | 3 | -0.02424 | 0.00188 | 0.01129 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 4 | 0.00879 | 0.01638 | -0.00931 | * |
| * Ni | 5 | 0.00905 | 0.00205 | -0.01052 | * |
| * Ni | 6 | -0.02598 | -0.00399 | 0.00992 | * |
| * Ni | 7 | 0.02623 | -0.01272 | 0.00109 | * |
| * Ni | 8 | 0.00744 | 0.00739 | -0.01397 | * |
| * Ni | 9 | -0.02741 | 0.00191 | 0.03009 | * |
| * Ni | 10 | 0.02969 | 0.00311 | -0.02291 | * |
| * Ni | 11 | 0.00936 | 0.00401 | -0.00162 | * |
| * Ni | 12 | -0.02746 | -0.00563 | 0.02583 | * |
| * Ni | 13 | 0.01042 | -0.00330 | -0.02025 | * |
| * Ni | 14 | 0.00911 | -0.00313 | -0.00367 | * |
| * Ni | 15 | -0.02220 | 0.00255 | 0.01988 | * |
| * Ni | 16 | -0.00659 | 0.00210 | -0.00712 | * |
| * Ni | 17 | 0.01354 | 0.00024 | 0.00058 | * |
| * Ni | 18 | -0.02395 | -0.00284 | 0.01204 | * |
| * Ni | 19 | 0.02303 | -0.02703 | 0.01210 | * |
| * Ni | 20 | -0.00368 | -0.01584 | -0.00835 | * |
| * Ni | 21 | -0.02681 | -0.00876 | 0.01558 | * |
| * Ni | 22 | -0.00203 | -0.00636 | -0.01853 | * |
| * Ni | 23 | 0.00819 | 0.00209 | -0.01637 | * |
| * Ni | 24 | -0.02162 | -0.00373 | 0.02851 | * |
| * Ni | 25 | 0.01148 | 0.00767 | -0.01146 | * |
| * Ni | 26 | 0.01302 | -0.00222 | -0.01328 | * |
| * Ni | 27 | -0.03008 | -0.01177 | 0.02461 | * |
| * Ni | 28 | 0.00007 | 0.01211 | -0.01377 | * |
| * Ni | 29 | 0.01099 | 0.00544 | -0.00447 | * |
| * Ni | 30 | -0.01964 | -0.00201 | 0.01883 | * |
| * Ni | 31 | 0.02809 | -0.00546 | -0.01819 | * |
| * Ni | 32 | -0.00074 | 0.00809 | -0.00230 | * |
| * Ni | 33 | -0.01897 | 0.00523 | 0.02174 | * |
| * Ni | 34 | 0.00697 | -0.00264 | -0.00736 | * |
| * Ni | 35 | 0.01045 | -0.00270 | -0.00266 | * |
| * Ni | 36 | -0.02994 | -0.00796 | 0.01557 | * |
| * Ni | 37 | 0.01144 | -0.01214 | -0.01869 | * |
| * Ni | 38 | 0.00438 | 0.00502 | -0.00600 | * |
| * Ni | 39 | -0.02790 | -0.00431 | 0.03888 | * |
| * Ni | 40 | 0.00369 | 0.00601 | -0.01007 | * |
| * Ni | 41 | -0.00018 | 0.00351 | -0.00564 | * |
| * Ni | 42 | -0.02883 | -0.01111 | 0.02553 | * |
| * Ni | 43 | 0.01538 | 0.00459 | -0.00946 | * |
| * Ni | 44 | 0.00576 | -0.00154 | 0.00157 | * |
| * Ni | 45 | -0.02091 | 0.00221 | 0.02737 | * |
| * Ni | 46 | 0.03299 | -0.00280 | -0.00231 | * |
| * Ni | 47 | 0.00169 | 0.00194 | 0.01121 | * |

| | | | | | |
|-------|----|----------|----------|----------|---|
| * Ni | 48 | -0.02318 | 0.00469 | 0.02127 | * |
| * Ni | 49 | 0.01072 | -0.02146 | 0.01261 | * |
| * Ni | 50 | 0.00550 | -0.00179 | 0.00678 | * |
| * Ni | 51 | -0.03381 | -0.01156 | 0.01134 | * |
| * Ni | 52 | 0.01470 | -0.00792 | -0.01759 | * |
| * Ni | 53 | 0.01367 | -0.00017 | -0.00538 | * |
| * Ni | 54 | -0.02933 | -0.01191 | 0.02885 | * |
| * Ni | 55 | 0.00627 | 0.01351 | -0.02084 | * |
| * Ni | 56 | 0.00970 | 0.00215 | -0.00892 | * |
| * Ni | 57 | -0.03098 | -0.00476 | 0.03449 | * |
| * Ni | 58 | 0.00712 | 0.00428 | -0.00924 | * |
| * Ni | 59 | 0.00546 | 0.00884 | -0.00235 | * |
| * Ni | 60 | -0.02576 | -0.00014 | 0.02291 | * |
| * Ni | 61 | 0.03156 | -0.02486 | -0.00646 | * |
| * Ni | 62 | 0.01466 | 0.00102 | 0.00868 | * |
| * Ni | 63 | -0.02558 | -0.00028 | 0.01504 | * |
| * Ni | 64 | -0.00240 | -0.03218 | 0.01629 | * |
| * Ni | 65 | 0.00187 | 0.00115 | 0.00384 | * |
| * Ni | 66 | -0.02597 | 0.00294 | 0.01919 | * |
| * Ni | 67 | 0.01945 | -0.02119 | 0.00654 | * |
| * Ni | 68 | 0.01471 | -0.00161 | -0.00896 | * |
| * Ni | 69 | -0.02730 | -0.00636 | 0.03094 | * |
| * Ni | 70 | 0.01420 | 0.01920 | -0.02632 | * |
| * Ni | 71 | 0.01322 | 0.00234 | -0.00425 | * |
| * Ni | 72 | -0.03195 | -0.00936 | 0.02827 | * |
| * Ni | 73 | 0.00076 | 0.00478 | -0.01149 | * |
| * Ni | 74 | 0.00683 | 0.00609 | -0.00687 | * |
| * Ni | 75 | -0.02895 | 0.00027 | 0.02131 | * |
| * | | | | | * |
| ***** | | | | | |



Final energy = -102793.7335605 eV

***** Forces *****

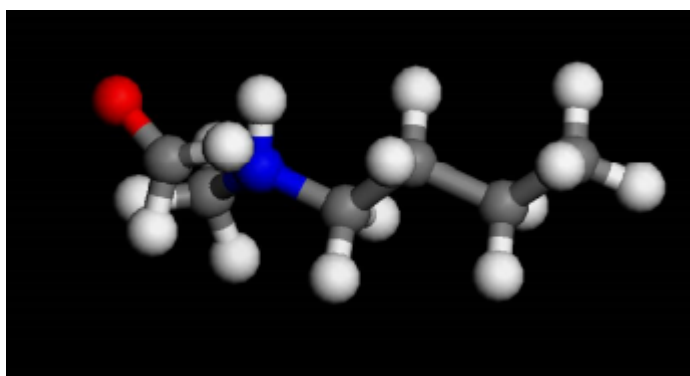
| * Cartesian components (eV/A) * | | | | |
|---------------------------------|----|----------|----------|----------|
| * ----- * | | | | |
| | x | y | z | |
| * H | 1 | -0.16158 | -0.11887 | -0.18946 |
| * H | 2 | -0.18648 | -0.17703 | -0.21507 |
| * H | 3 | -0.08603 | -0.08072 | -0.18145 |
| * H | 4 | -0.08471 | -0.03345 | -0.10205 |
| * H | 5 | -0.12735 | -0.13964 | -0.17140 |
| * H | 6 | -0.11965 | -0.10441 | -0.17348 |
| * H | 7 | -0.14435 | -0.06312 | -0.23460 |
| * H | 8 | -0.12041 | -0.16343 | -0.11417 |
| * H | 9 | -0.10454 | -0.04167 | -0.12380 |
| * H | 10 | -0.12728 | -0.08593 | -0.21759 |
| * H | 11 | -0.07481 | -0.00663 | -0.08530 |
| * H | 12 | -0.25073 | 0.04638 | -0.16455 |
| * H | 13 | -0.91847 | -0.08499 | -1.61494 |
| * C | 1 | -0.05141 | 0.04416 | -0.22642 |
| * C | 2 | -0.15224 | -0.15077 | -0.04564 |
| * C | 3 | 0.02165 | -0.10088 | -0.18508 |
| * C | 4 | -0.76206 | -0.62987 | 0.05372 |
| * C | 5 | 0.13892 | -0.20077 | -0.15274 |
| * N | 1 | -0.24735 | -0.90496 | 0.29380 |
| * Ni | 1 | 0.49028 | 0.39868 | 0.40898 |
| * Ni | 2 | 0.19075 | 0.18325 | 0.03339 |
| * Ni | 3 | 0.16633 | 0.11824 | 0.18835 |
| * Ni | 4 | 0.49066 | 0.64932 | -0.05814 |
| * Ni | 5 | 0.02220 | -0.01629 | 0.00594 |
| * Ni | 6 | 0.16638 | 0.08646 | 0.17177 |
| * Ni | 7 | 0.42196 | 0.60389 | 0.34560 |
| * Ni | 8 | 0.10686 | 0.11894 | 0.05829 |
| * Ni | 9 | 0.19945 | 0.14393 | 0.23481 |
| * Ni | 10 | 0.20857 | 0.28523 | 0.17336 |
| * Ni | 11 | 0.02167 | 0.03055 | -0.02753 |
| * Ni | 12 | 0.15382 | 0.16116 | 0.18924 |
| * Ni | 13 | -0.02558 | 0.08857 | 0.03598 |
| * Ni | 14 | -0.06408 | -0.04803 | -0.06944 |
| * Ni | 15 | 0.02432 | 0.05330 | 0.06358 |
| * Ni | 16 | 0.45773 | 0.27583 | 0.30714 |
| * Ni | 17 | 0.14246 | -0.01896 | 0.12088 |
| * Ni | 18 | 0.14066 | 0.06312 | 0.14598 |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 19 | 0.50109 | -0.09454 | 0.65540 | * |
| * Ni | 20 | -0.08245 | -0.08131 | -0.00441 | * |
| * Ni | 21 | 0.06942 | 0.00368 | 0.05056 | * |
| * Ni | 22 | -0.11324 | 0.40864 | 0.10877 | * |
| * Ni | 23 | 0.01633 | 0.00847 | -0.00738 | * |
| * Ni | 24 | 0.05543 | -0.05194 | 0.02061 | * |
| * Ni | 25 | 0.32726 | 0.43651 | 0.28942 | * |
| * Ni | 26 | 0.02473 | 0.02077 | 0.02549 | * |
| * Ni | 27 | 0.15313 | 0.13309 | 0.19688 | * |
| * Ni | 28 | 0.07605 | 0.18153 | 0.13923 | * |
| * Ni | 29 | -0.02873 | -0.00457 | -0.03577 | * |
| * Ni | 30 | 0.07974 | 0.07136 | 0.11498 | * |
| * Ni | 31 | 0.10727 | 0.11302 | 0.05846 | * |
| * Ni | 32 | -0.11342 | -0.09528 | -0.08201 | * |
| * Ni | 33 | 0.04365 | -0.02305 | 0.05359 | * |
| * Ni | 34 | -0.06913 | -0.02923 | -0.08458 | * |
| * Ni | 35 | -0.08945 | -0.04599 | -0.04130 | * |
| * Ni | 36 | -0.00192 | -0.02384 | 0.03366 | * |
| * Ni | 37 | -0.00217 | 0.04145 | 0.21303 | * |
| * Ni | 38 | -0.08390 | -0.07866 | -0.14475 | * |
| * Ni | 39 | -0.05001 | -0.08406 | -0.02819 | * |
| * Ni | 40 | 0.27758 | 0.35962 | 0.34666 | * |
| * Ni | 41 | -0.04259 | -0.06481 | -0.05534 | * |
| * Ni | 42 | 0.05655 | 0.01781 | 0.10381 | * |
| * Ni | 43 | 0.11423 | 0.19864 | 0.15114 | * |
| * Ni | 44 | -0.03581 | -0.02650 | -0.03879 | * |
| * Ni | 45 | 0.07251 | 0.03793 | 0.11704 | * |
| * Ni | 46 | 0.13070 | 0.11249 | 0.09620 | * |
| * Ni | 47 | -0.05855 | -0.09684 | -0.06736 | * |
| * Ni | 48 | 0.02484 | -0.05418 | 0.04640 | * |
| * Ni | 49 | 0.01841 | 0.00269 | -0.01566 | * |
| * Ni | 50 | -0.11550 | -0.13583 | -0.03891 | * |
| * Ni | 51 | -0.01152 | -0.04480 | 0.02123 | * |
| * Ni | 52 | -0.07070 | -0.05285 | -0.10762 | * |
| * Ni | 53 | -0.05764 | -0.08134 | -0.08921 | * |
| * Ni | 54 | -0.06266 | -0.08706 | -0.01551 | * |
| * Ni | 55 | 0.01966 | 0.04159 | -0.03483 | * |
| * Ni | 56 | -0.06693 | -0.06843 | -0.05652 | * |
| * Ni | 57 | -0.06803 | -0.08813 | -0.02218 | * |
| * Ni | 58 | 0.06119 | 0.06541 | 0.03732 | * |
| * Ni | 59 | -0.09265 | -0.11003 | -0.09854 | * |
| * Ni | 60 | -0.01942 | -0.06186 | 0.03006 | * |
| * Ni | 61 | 0.05524 | 0.01294 | 0.03284 | * |
| * Ni | 62 | 0.01674 | 0.01350 | 0.00534 | * |

```

* Ni      63      -0.03378          -0.08775          0.01331          *
* Ni      64       0.07105           0.07210           0.06958          *
* Ni      65      -0.06495          -0.09927          -0.02665         *
* Ni      66      -0.02138          -0.06807           0.02531          *
* Ni      67      -0.10257          -0.10343          -0.04453         *
* Ni      68      -0.06536          -0.07681          -0.07469         *
* Ni      69      -0.05736          -0.08758           0.00774          *
* Ni      70      -0.04942           0.02132          -0.04376         *
* Ni      71      -0.07644          -0.10126          -0.10123         *
* Ni      72      -0.07690          -0.10541          -0.01256         *
* Ni      73      -0.07158          -0.04399          -0.05915         *
* Ni      74      -0.06573          -0.07328          -0.06612         *
* Ni      75      -0.10648          -0.12315          -0.04447         *
*
*****

```



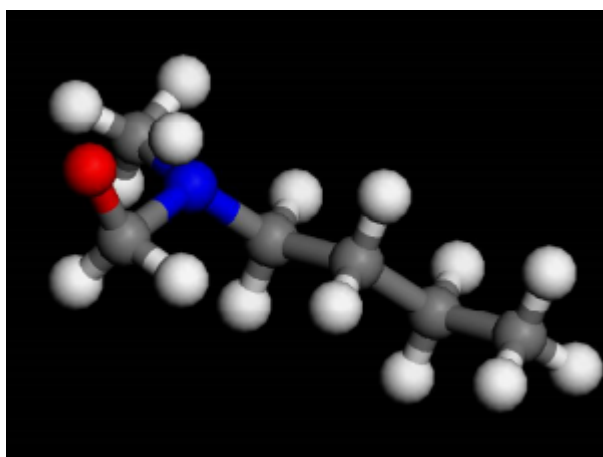
BFGS: Final Enthalpy = -1.87816874E+003 eV

```

***** Forces *****
*
* Cartesian components (eV/A)
* -----*
* x y z
*
* H 1 0.00282 -0.00421 0.00317
* H 2 0.00269 0.00084 -0.00275
* H 3 0.00235 0.00109 -0.00075
* H 4 0.00074 0.00318 -0.00014
* H 5 -0.00453 -0.00641 0.00463
* H 6 0.00443 0.00489 -0.00288
* H 7 -0.00962 -0.00189 -0.00670
* H 8 -0.00496 -0.00442 0.00118
* H 9 -0.00185 0.00418 -0.00024

```


| | | | | | |
|-----|----|----------|----------|----------|---|
| * H | 10 | 0.00082 | -0.00610 | 0.00047 | * |
| * H | 11 | 0.00071 | 0.00508 | -0.00244 | * |
| * H | 12 | -0.00408 | 0.00516 | 0.00040 | * |
| * H | 13 | 0.00125 | -0.00052 | 0.00143 | * |
| * H | 14 | 0.00143 | -0.00607 | 0.00125 | * |
| * H | 15 | -0.00005 | 0.00020 | 0.00015 | * |
| * C | 1 | -0.00248 | 0.00080 | 0.00140 | * |
| * C | 2 | -0.00195 | -0.00340 | -0.00101 | * |
| * C | 3 | 0.00616 | -0.00246 | -0.00488 | * |
| * C | 4 | 0.00003 | -0.00128 | -0.00007 | * |
| * C | 5 | 0.00290 | 0.00067 | 0.00575 | * |
| * C | 6 | 0.00201 | -0.00020 | -0.00058 | * |
| * N | 1 | 0.00157 | 0.00398 | 0.00151 | * |
| * O | 1 | -0.00036 | 0.00690 | 0.00110 | * |
| * | | | | | * |

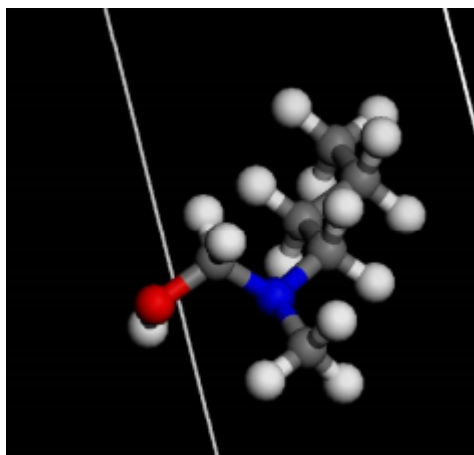


Final energy = -1876.719719048 eV

***** Forces *****

| ***** Forces ***** | | | | | |
|---------------------------------|---|----------|----------|----------|---|
| * Cartesian components (eV/A) * | | | | | |
| * ----- * | | | | | |
| | | x | y | z | |
| * | | | | | * |
| * | | | | | * |
| * H | 1 | -0.07030 | -0.08348 | -0.01878 | * |
| * H | 2 | -0.03835 | -0.01751 | 0.03738 | * |
| * H | 3 | 0.02231 | -0.05977 | -0.02973 | * |
| * H | 4 | 0.05577 | -0.00333 | 0.00041 | * |
| * H | 5 | 0.08682 | 0.06697 | -0.03990 | * |
| * H | 6 | -0.05592 | 0.16062 | 0.02703 | * |
| * H | 7 | -0.08667 | 0.02736 | 0.12098 | * |
| * H | 8 | 0.32246 | 0.35577 | 0.09967 | * |

| | | | | | |
|-----|----|----------|----------|----------|---|
| * H | 9 | 0.26484 | 0.27430 | -0.00104 | * |
| * H | 10 | -0.52299 | -0.57007 | 0.23756 | * |
| * H | 11 | 0.56997 | -0.43481 | -0.34833 | * |
| * H | 12 | 0.39794 | -0.61996 | -0.16297 | * |
| * H | 13 | 0.59619 | 0.22963 | 0.31401 | * |
| * H | 14 | 0.05757 | 0.41083 | -0.27371 | * |
| * H | 15 | 0.37125 | 0.05010 | -0.15215 | * |
| * C | 1 | 0.18077 | 0.15894 | 0.05402 | * |
| * C | 2 | -0.05954 | -0.00170 | 0.17512 | * |
| * C | 3 | 0.22215 | 0.21372 | -0.37226 | * |
| * C | 4 | 0.13027 | 0.14174 | 0.25563 | * |
| * C | 5 | -0.65612 | -0.08907 | -0.03196 | * |
| * C | 6 | -1.08033 | -0.12308 | -0.99665 | * |
| * N | 1 | 0.19069 | 0.12716 | 0.11248 | * |
| * O | 1 | -0.89878 | -0.21437 | 0.99321 | * |
| * | | | | | * |



BFGS: Final Enthalpy = -1.87875245E+003 eV

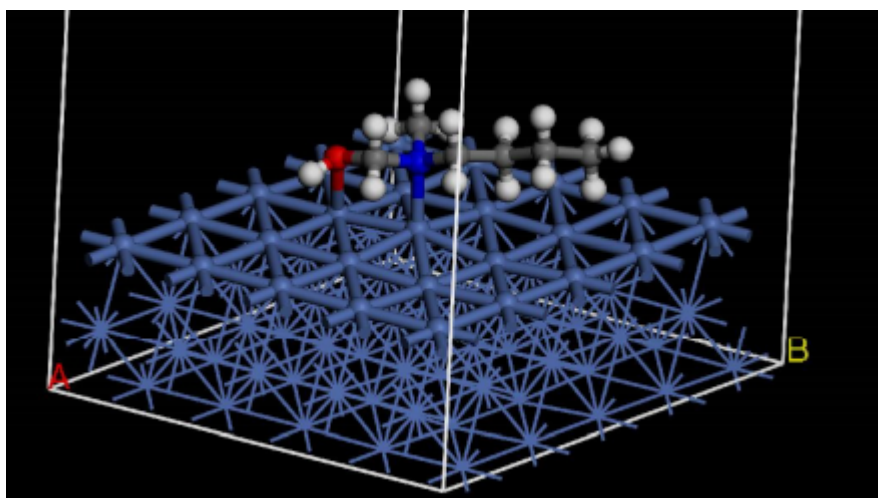
***** Forces *****

| | | | | | |
|-----|---|-----------------------------|----------|----------|---|
| * | | | | * | |
| * | | Cartesian components (eV/A) | | * | |
| * | | ----- | | * | |
| * | | x | y | z | * |
| * | | | | | * |
| * H | 1 | -0.00104 | -0.00112 | -0.00339 | * |
| * H | 2 | -0.00011 | -0.00018 | -0.00806 | * |
| * H | 3 | 0.00314 | 0.00063 | -0.00237 | * |
| * H | 4 | 0.00275 | -0.00173 | -0.00108 | * |
| * H | 5 | -0.00045 | -0.00126 | -0.00039 | * |

```

* H      6    -0.00064      0.00284      -0.00151      *
* H      7    -0.00054      0.00104      0.00189      *
* H      8     0.00102      0.00324      -0.00201      *
* H      9     0.00259      0.00202      0.00268      *
* H     10    -0.00016      0.00047      0.00031      *
* H     11     0.00126      0.00092      0.00733      *
* H     12    -0.00019     -0.00503      0.00244      *
* H     13     0.00446     -0.00004      0.00269      *
* H     14    -0.00156     -0.00531     -0.00219      *
* H     15    -0.00090     -0.00268      0.00495      *
* C      1    -0.00241      0.00043      0.00331      *
* C      2    -0.00240     -0.00039      0.00365      *
* C      3    -0.00178      0.00413      0.00028      *
* C      4     0.00057      0.00298     -0.00091      *
* C      5    -0.00036      0.00088     -0.00365      *
* C      6    -0.00315     -0.00148      0.00212      *
* N      1    -0.00173      0.00571      0.00102      *
* O      1     0.00163     -0.00607     -0.00709      *
*
*****

```



Final energy = -103421.8322497 eV

```

***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 0.06260 0.03824 0.02604 *
* H 2 0.04824 0.03749 0.04468 *
* H 3 0.01892 -0.01085 0.03607 *

```

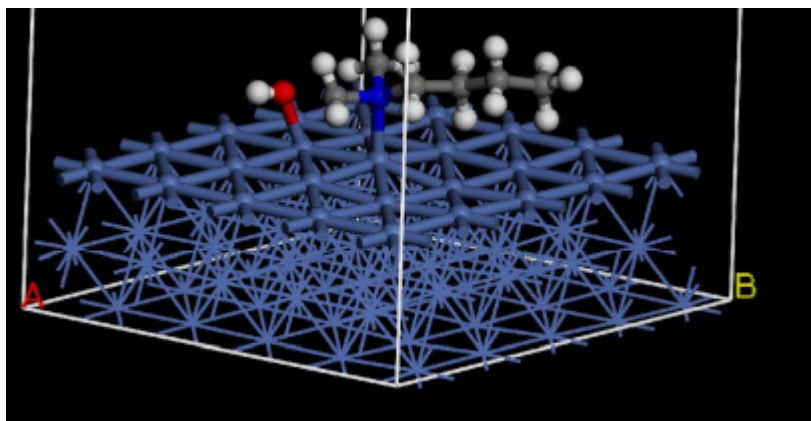
| | | | | |
|------|----|----------|----------|------------|
| * H | 4 | 0.03489 | 0.03392 | 0.00807 * |
| * H | 5 | -0.02155 | 0.02450 | 0.03497 * |
| * H | 6 | 0.05314 | 0.03595 | 0.07369 * |
| * H | 7 | 0.06064 | -0.00505 | -0.00394 * |
| * H | 8 | 0.05472 | 0.02920 | 0.01380 * |
| * H | 9 | -0.03326 | -0.02413 | 0.03921 * |
| * H | 10 | -0.00656 | 0.00483 | 0.00914 * |
| * H | 11 | -0.02661 | 0.01904 | 0.09658 * |
| * H | 12 | 0.13357 | -0.20260 | -0.01720 * |
| * H | 13 | 0.05736 | 0.04797 | 0.01781 * |
| * H | 14 | 0.07438 | 0.00896 | 0.04163 * |
| * H | 15 | 0.07495 | 0.05351 | 0.02405 * |
| * C | 1 | 0.26181 | 0.04565 | 0.12654 * |
| * C | 2 | -0.08525 | -0.03815 | 0.01443 * |
| * C | 3 | 0.17377 | 0.20566 | 0.07916 * |
| * C | 4 | -0.19307 | 0.04652 | -0.07080 * |
| * C | 5 | 0.05338 | -0.11138 | 0.31552 * |
| * C | 6 | 0.01962 | -0.06610 | -0.08486 * |
| * N | 1 | 0.06830 | 0.03661 | 0.04874 * |
| * O | 1 | 0.10180 | 0.50842 | -0.15938 * |
| * Ni | 1 | -0.07279 | -0.11498 | -0.37748 * |
| * Ni | 2 | 0.38892 | 0.34256 | 0.28370 * |
| * Ni | 3 | -0.08955 | 0.09438 | -0.14015 * |
| * Ni | 4 | -0.02329 | 0.16018 | -0.06873 * |
| * Ni | 5 | 0.01403 | -0.00262 | -0.10121 * |
| * Ni | 6 | 0.06033 | -0.07536 | -0.03243 * |
| * Ni | 7 | -0.06279 | -0.10638 | -0.36895 * |
| * Ni | 8 | -0.17915 | -0.06236 | -0.08949 * |
| * Ni | 9 | 0.09313 | 0.05781 | 0.08300 * |
| * Ni | 10 | 0.07655 | 0.01856 | -0.24088 * |
| * Ni | 11 | -0.08049 | -0.08912 | -0.08912 * |
| * Ni | 12 | 0.08177 | 0.09410 | 0.09706 * |
| * Ni | 13 | 0.08486 | 0.11953 | -0.29310 * |
| * Ni | 14 | -0.11361 | -0.18699 | -0.07990 * |
| * Ni | 15 | 0.05967 | 0.09708 | 0.14204 * |
| * Ni | 16 | -0.06484 | 0.00235 | 0.02051 * |
| * Ni | 17 | -0.22362 | -0.11748 | -0.20647 * |
| * Ni | 18 | -0.14756 | -0.11192 | 0.23985 * |
| * Ni | 19 | -0.11856 | 0.02959 | 0.29853 * |
| * Ni | 20 | -0.14057 | -0.18311 | 0.09440 * |
| * Ni | 21 | -0.08262 | -0.07217 | 0.32842 * |
| * Ni | 22 | -0.06893 | -0.20284 | 0.13378 * |
| * Ni | 23 | -0.23596 | -0.21507 | -0.00530 * |
| * Ni | 24 | 0.03452 | -0.03524 | 0.25283 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 25 | 0.03003 | -0.22914 | -0.02219 * |
| * Ni | 26 | -0.08167 | -0.05629 | -0.10895 * |
| * Ni | 27 | 0.03157 | -0.09213 | 0.27509 * |
| * Ni | 28 | -0.09470 | -0.04376 | 0.06202 * |
| * Ni | 29 | -0.01829 | -0.06112 | -0.12394 * |
| * Ni | 30 | -0.07705 | -0.07711 | 0.33394 * |
| * Ni | 31 | -0.20115 | -0.17827 | 0.02220 * |
| * Ni | 32 | 0.08369 | 0.04687 | -0.16418 * |
| * Ni | 33 | 0.03685 | 0.01863 | -0.12991 * |
| * Ni | 34 | -0.24420 | -0.05093 | -0.08075 * |
| * Ni | 35 | -0.02556 | -0.16442 | -0.21280 * |
| * Ni | 36 | -0.01254 | -0.05187 | -0.10313 * |
| * Ni | 37 | -0.11726 | 0.05372 | -0.08609 * |
| * Ni | 38 | -0.00197 | 0.16136 | -0.14265 * |
| * Ni | 39 | 0.01569 | -0.01558 | 0.01144 * |
| * Ni | 40 | 0.07608 | -0.10287 | -0.34742 * |
| * Ni | 41 | 0.06319 | 0.04349 | -0.31332 * |
| * Ni | 42 | 0.04605 | 0.00882 | -0.02268 * |
| * Ni | 43 | 0.02943 | -0.14412 | -0.10805 * |
| * Ni | 44 | 0.13278 | 0.18437 | -0.04883 * |
| * Ni | 45 | 0.04209 | 0.14705 | -0.06677 * |
| * Ni | 46 | -0.18561 | -0.08778 | -0.25217 * |
| * Ni | 47 | 0.01810 | 0.09605 | -0.05729 * |
| * Ni | 48 | -0.12464 | -0.11324 | 0.15062 * |
| * Ni | 49 | 0.05232 | -0.00915 | -0.19605 * |
| * Ni | 50 | 0.29799 | 0.20112 | 0.19441 * |
| * Ni | 51 | -0.14895 | -0.08413 | 0.02223 * |
| * Ni | 52 | 0.13762 | 0.10325 | -0.21533 * |
| * Ni | 53 | 0.23724 | 0.20842 | -0.02959 * |
| * Ni | 54 | 0.13087 | 0.14147 | 0.28148 * |
| * Ni | 55 | 0.06326 | 0.12947 | -0.14240 * |
| * Ni | 56 | 0.26301 | 0.40710 | 0.31897 * |
| * Ni | 57 | 0.09475 | 0.16318 | 0.28289 * |
| * Ni | 58 | -0.14440 | -0.12300 | -0.35809 * |
| * Ni | 59 | -0.01221 | 0.09291 | 0.03132 * |
| * Ni | 60 | -0.06168 | -0.16126 | 0.10666 * |
| * Ni | 61 | -0.22553 | -0.21906 | -0.04676 * |
| * Ni | 62 | 0.32467 | 0.34918 | 0.56394 * |
| * Ni | 63 | -0.02460 | 0.05634 | -0.27725 * |
| * Ni | 64 | -0.31405 | -0.13289 | -0.13122 * |
| * Ni | 65 | 0.17293 | 0.20097 | 0.39873 * |
| * Ni | 66 | 0.01419 | -0.04530 | -0.33014 * |
| * Ni | 67 | -0.21566 | -0.19512 | -0.09540 * |
| * Ni | 68 | -0.23115 | -0.18016 | 0.22077 * |

```

* Ni      69      0.09724      0.03114      -0.16231 *
* Ni      70     -0.19862     -0.23379      0.10600 *
* Ni      71     -0.12328     -0.25933      0.25629 *
* Ni      72      0.16022      0.20598     -0.09764 *
* Ni      73     -0.18159     -0.31492     -0.04968 *
* Ni      74      0.14241      0.06257      0.41407 *
* Ni      75      0.09685      0.15457     -0.12495 *
*
*****

```



Final energy = -103420.2451462 eV

***** Forces *****

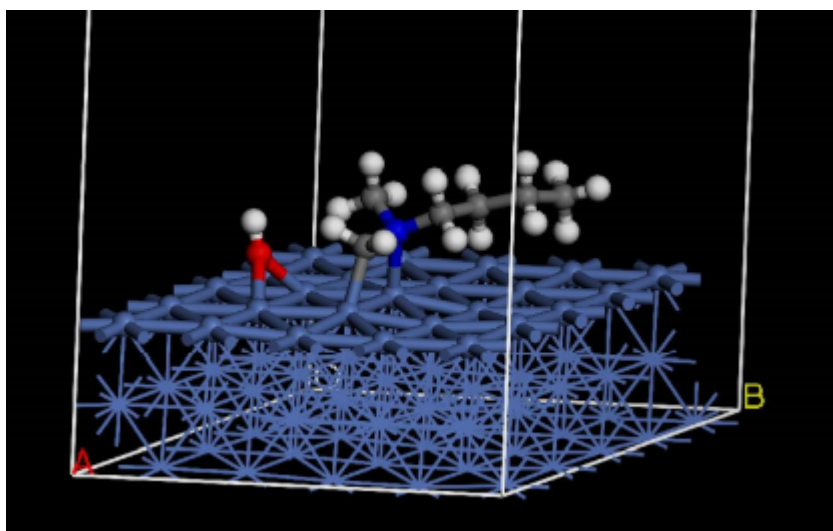
```

*
*
* Cartesian components (eV/A)
* -----
*
*      x      y      z
*
* H      1      0.06989      0.02240      0.03410
* H      2      0.01137      0.02362      0.00436
* H      3      0.06320      0.03125     -0.00159
* H      4      0.00891      0.02478      0.03174
* H      5      0.06676      0.00531     -0.02127
* H      6     -0.12475     -0.00074     -0.07698
* H      7      0.01573      0.02000      0.00299
* H      8     -0.04098      0.05291     -0.09493
* H      9     -0.06741      0.03321      0.02627
* H     10      0.25107     -0.14158      0.65330
* H     11      0.17246      0.11350     -0.28695
* H     12     -0.11333     -0.11128     -0.16814
* H     13     -0.05608     -0.17615      0.19810
* H     14      0.33526     -0.24075      0.03579
* H     15      0.09877      0.07950      0.15344
* C      1      0.01740      0.08741      0.00588
* C      2      0.01734     -0.05771      0.01369

```

| | | | | | |
|------|----|----------|----------|----------|---|
| * C | 3 | 0.11565 | -0.01260 | 0.11314 | * |
| * C | 4 | -0.05315 | -0.01414 | 0.00400 | * |
| * C | 5 | 0.31711 | -0.69794 | -0.01504 | * |
| * C | 6 | 0.00021 | 0.12961 | -0.19721 | * |
| * N | 1 | -0.35531 | 1.45261 | -0.48835 | * |
| * O | 1 | -0.19757 | 0.02586 | 0.26180 | * |
| * Ni | 1 | -0.09221 | -0.07500 | 0.02027 | * |
| * Ni | 2 | -0.05456 | -0.03774 | -0.04652 | * |
| * Ni | 3 | 0.05116 | 0.07783 | 0.08708 | * |
| * Ni | 4 | 0.02307 | -0.00286 | 0.00166 | * |
| * Ni | 5 | -0.00952 | 0.03370 | 0.04983 | * |
| * Ni | 6 | 0.04637 | 0.10344 | 0.05461 | * |
| * Ni | 7 | -0.07980 | -0.08534 | 0.13816 | * |
| * Ni | 8 | -0.04811 | -0.06684 | 0.03650 | * |
| * Ni | 9 | 0.08747 | 0.01582 | 0.05438 | * |
| * Ni | 10 | 0.04218 | 0.02077 | 0.08897 | * |
| * Ni | 11 | 0.00170 | 0.05018 | 0.07278 | * |
| * Ni | 12 | 0.00818 | 0.00753 | 0.01098 | * |
| * Ni | 13 | 0.01714 | 0.07707 | 0.07137 | * |
| * Ni | 14 | -0.07679 | -0.06550 | -0.01007 | * |
| * Ni | 15 | 0.03724 | 0.05415 | 0.05803 | * |
| * Ni | 16 | 0.08854 | 0.07133 | 0.09596 | * |
| * Ni | 17 | -0.00193 | 0.01595 | 0.08097 | * |
| * Ni | 18 | -0.01816 | 0.01816 | 0.10802 | * |
| * Ni | 19 | 0.07442 | -0.04697 | -0.00141 | * |
| * Ni | 20 | 0.12446 | 0.01301 | 0.20444 | * |
| * Ni | 21 | 0.06403 | 0.10638 | 0.13498 | * |
| * Ni | 22 | -0.32703 | -0.20465 | -0.28627 | * |
| * Ni | 23 | 0.04458 | 0.07049 | 0.09261 | * |
| * Ni | 24 | 0.02464 | 0.04710 | 0.00902 | * |
| * Ni | 25 | 0.13176 | -0.00970 | 0.00602 | * |
| * Ni | 26 | 0.03534 | 0.02617 | -0.04924 | * |
| * Ni | 27 | 0.04015 | -0.00556 | -0.00241 | * |
| * Ni | 28 | 0.07223 | 0.06291 | 0.05384 | * |
| * Ni | 29 | -0.00528 | 0.01584 | -0.03893 | * |
| * Ni | 30 | 0.01436 | -0.00138 | 0.08318 | * |
| * Ni | 31 | -0.04507 | -0.06541 | -0.11128 | * |
| * Ni | 32 | 0.04174 | 0.07498 | -0.01345 | * |
| * Ni | 33 | -0.17725 | -0.17691 | -0.19191 | * |
| * Ni | 34 | -0.08094 | -0.01299 | -0.14565 | * |
| * Ni | 35 | 0.13839 | 0.09846 | 0.00449 | * |
| * Ni | 36 | 0.02095 | -0.06451 | -0.11260 | * |
| * Ni | 37 | 0.01121 | -0.06037 | 0.07504 | * |
| * Ni | 38 | 0.01852 | -0.01723 | 0.05249 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 39 | 0.08350 | 0.08232 | 0.04774 | * |
| * Ni | 40 | -0.04001 | -0.08283 | -0.07461 | * |
| * Ni | 41 | -0.06425 | -0.02548 | 0.01930 | * |
| * Ni | 42 | 0.15806 | 0.15044 | 0.11802 | * |
| * Ni | 43 | 0.12314 | 0.06929 | 0.07323 | * |
| * Ni | 44 | -0.01592 | -0.00165 | 0.04308 | * |
| * Ni | 45 | -0.10691 | 0.08931 | 0.05058 | * |
| * Ni | 46 | -0.11366 | -0.13021 | -0.10717 | * |
| * Ni | 47 | -0.00332 | -0.07397 | -0.08198 | * |
| * Ni | 48 | -0.11316 | -0.09315 | -0.15147 | * |
| * Ni | 49 | -0.11089 | -0.02441 | -0.03594 | * |
| * Ni | 50 | -0.01924 | -0.00387 | -0.00758 | * |
| * Ni | 51 | 0.04342 | -0.06154 | 0.00159 | * |
| * Ni | 52 | -0.02285 | -0.05715 | 0.04183 | * |
| * Ni | 53 | -0.07910 | 0.01325 | 0.00183 | * |
| * Ni | 54 | 0.01022 | 0.08399 | 0.08444 | * |
| * Ni | 55 | 0.03646 | 0.04014 | 0.13460 | * |
| * Ni | 56 | -0.08072 | -0.16478 | -0.16041 | * |
| * Ni | 57 | 0.05737 | 0.02794 | 0.05563 | * |
| * Ni | 58 | -0.03227 | -0.04145 | -0.02503 | * |
| * Ni | 59 | -0.09192 | -0.08021 | -0.09921 | * |
| * Ni | 60 | -0.17582 | -0.07221 | -0.04643 | * |
| * Ni | 61 | -0.12301 | -0.10249 | -0.09019 | * |
| * Ni | 62 | -0.04142 | -0.02964 | -0.07462 | * |
| * Ni | 63 | 0.05465 | -0.01709 | -0.01847 | * |
| * Ni | 64 | -0.08151 | -0.14537 | -0.11406 | * |
| * Ni | 65 | -0.11012 | -0.15541 | -0.09239 | * |
| * Ni | 66 | -0.08052 | -0.00964 | -0.06356 | * |
| * Ni | 67 | -0.03631 | 0.03018 | -0.09615 | * |
| * Ni | 68 | 0.05757 | 0.07383 | -0.02595 | * |
| * Ni | 69 | 0.07865 | 0.02084 | 0.03790 | * |
| * Ni | 70 | 0.08708 | 0.11163 | 0.04747 | * |
| * Ni | 71 | 0.04197 | 0.02594 | -0.04971 | * |
| * Ni | 72 | 0.00754 | 0.00296 | 0.00639 | * |
| * Ni | 73 | 0.02783 | -0.06695 | -0.09744 | * |
| * Ni | 74 | -0.12016 | -0.15769 | -0.16563 | * |
| * Ni | 75 | -0.00011 | 0.06379 | -0.00971 | * |
| * | | | | | * |



Final energy = -103422.4146730 eV

```

***** Forces *****
*
*           Cartesian components (eV/A)           *
* -----*
*           x           y           z           *
*
* H      1      0.07873      -0.00361      0.00767 *
* H      2      0.00307       0.01632      0.04712 *
* H      3      0.01216      -0.01885      0.04260 *
* H      4     -0.00527      -0.01407     -0.00035 *
* H      5     -0.00593       0.01087      0.02265 *
* H      6      0.03704       0.03087      0.03342 *
* H      7      0.03510       0.01738      0.00725 *
* H      8     -0.04892      -0.03292     -0.03167 *
* H      9     -0.00725      -0.01292      0.00146 *
* H     10      0.02482       0.02066     -0.00441 *
* H     11      0.03978       0.05462      0.05980 *
* H     12      0.03503       0.01620      0.03227 *
* H     13      0.01869       0.00040      0.00140 *
* H     14      0.00167       0.01960      0.01243 *
* H     15      0.02210      -0.00977      0.02265 *
* C      1      0.13713       0.10388      0.16171 *
* C      2      0.06487       0.07898      0.00812 *
* C      3     -0.01556       0.00868      0.03471 *
* C      4     -0.00914       0.00353      0.06201 *
* C      5      0.01971       0.01030     -0.04973 *
* C      6      0.05132       0.09806      0.08969 *
* N      1      0.01735      -0.01386      0.00157 *
* O      1     -0.01185       0.07368     -0.06532 *

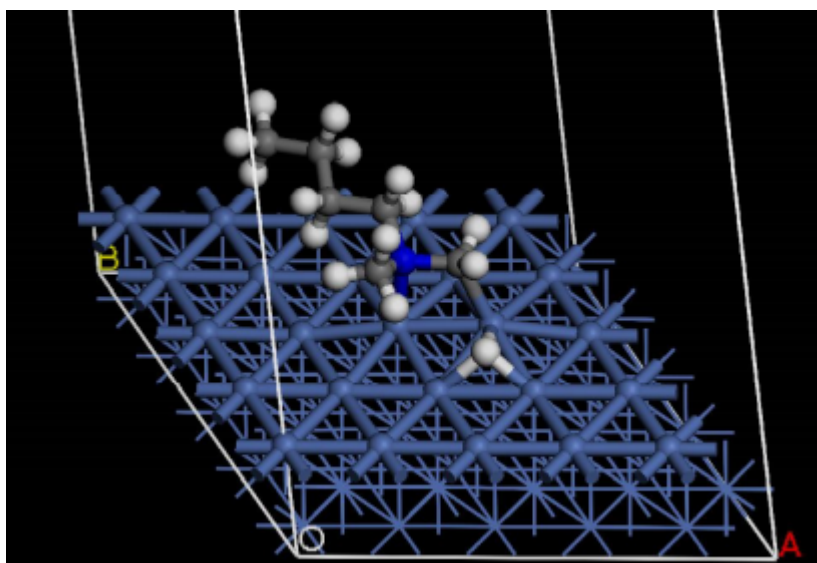
```

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 1 | 0.06786 | 0.04545 | 0.08346 * |
| * Ni | 2 | 0.33411 | 0.57551 | 0.02430 * |
| * Ni | 3 | 0.03102 | 0.07644 | -0.04250 * |
| * Ni | 4 | -0.13974 | -0.10978 | -0.10833 * |
| * Ni | 5 | -0.03513 | -0.08968 | -0.05271 * |
| * Ni | 6 | 0.14029 | 0.02034 | 0.07357 * |
| * Ni | 7 | -0.10348 | -0.10518 | -0.12746 * |
| * Ni | 8 | 0.09926 | 0.04511 | -0.00599 * |
| * Ni | 9 | 0.04020 | 0.01337 | -0.00960 * |
| * Ni | 10 | -0.09777 | -0.05455 | -0.11515 * |
| * Ni | 11 | 0.01528 | -0.07187 | -0.04423 * |
| * Ni | 12 | -0.02422 | -0.07747 | -0.04643 * |
| * Ni | 13 | -0.06873 | -0.07559 | -0.05950 * |
| * Ni | 14 | -0.16688 | -0.20525 | -0.16342 * |
| * Ni | 15 | -0.06414 | -0.03723 | -0.04838 * |
| * Ni | 16 | 0.17579 | 0.12358 | 0.06498 * |
| * Ni | 17 | 0.07843 | -0.04410 | 0.28285 * |
| * Ni | 18 | 0.04981 | 0.04735 | 0.04753 * |
| * Ni | 19 | -0.00232 | 0.00354 | -0.02225 * |
| * Ni | 20 | -0.02910 | 0.05468 | 0.11892 * |
| * Ni | 21 | 0.04603 | 0.05303 | 0.04680 * |
| * Ni | 22 | -0.06441 | -0.05933 | -0.08806 * |
| * Ni | 23 | -0.18191 | -0.04997 | 0.11790 * |
| * Ni | 24 | 0.00352 | 0.04519 | -0.03847 * |
| * Ni | 25 | 0.06388 | 0.06464 | 0.08641 * |
| * Ni | 26 | 0.01768 | 0.02895 | 0.14357 * |
| * Ni | 27 | -0.01141 | -0.01770 | -0.05987 * |
| * Ni | 28 | -0.04898 | -0.09018 | -0.01287 * |
| * Ni | 29 | -0.06318 | -0.14085 | -0.05653 * |
| * Ni | 30 | -0.09634 | -0.07747 | -0.08014 * |
| * Ni | 31 | 0.08096 | 0.07176 | 0.13079 * |
| * Ni | 32 | -0.10939 | -0.09148 | -0.13291 * |
| * Ni | 33 | -0.00512 | -0.01008 | 0.03935 * |
| * Ni | 34 | -0.07447 | -0.04367 | -0.04107 * |
| * Ni | 35 | -0.08644 | -0.05959 | -0.14166 * |
| * Ni | 36 | 0.00338 | 0.01751 | -0.02191 * |
| * Ni | 37 | 0.11123 | 0.02676 | 0.04653 * |
| * Ni | 38 | -0.31954 | -0.19561 | -0.26854 * |
| * Ni | 39 | 0.09872 | 0.07304 | 0.06892 * |
| * Ni | 40 | 0.17260 | 0.07439 | 0.11531 * |
| * Ni | 41 | -0.32025 | -0.30392 | -0.53206 * |
| * Ni | 42 | 0.09381 | 0.03443 | 0.09470 * |
| * Ni | 43 | 0.12619 | 0.07555 | 0.21739 * |
| * Ni | 44 | -0.12368 | 0.02699 | -0.09589 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 45 | 0.10179 | 0.12311 | 0.09463 * |
| * Ni | 46 | -0.00799 | 0.01595 | 0.03176 * |
| * Ni | 47 | -0.02067 | -0.06298 | -0.04072 * |
| * Ni | 48 | -0.06583 | -0.00754 | -0.04774 * |
| * Ni | 49 | -0.07584 | -0.06368 | -0.08589 * |
| * Ni | 50 | 0.17356 | 0.10340 | 0.18184 * |
| * Ni | 51 | -0.10775 | -0.10169 | -0.07437 * |
| * Ni | 52 | 0.14299 | 0.08292 | 0.12941 * |
| * Ni | 53 | 0.02438 | 0.08762 | -0.02712 * |
| * Ni | 54 | -0.01771 | -0.01084 | 0.02001 * |
| * Ni | 55 | -0.06810 | 0.00163 | -0.05050 * |
| * Ni | 56 | 0.07277 | 0.07639 | 0.22124 * |
| * Ni | 57 | 0.01020 | -0.00545 | 0.03148 * |
| * Ni | 58 | 0.07483 | 0.08454 | -0.03507 * |
| * Ni | 59 | -0.03966 | -0.11056 | -0.02002 * |
| * Ni | 60 | -0.07508 | -0.03546 | -0.05462 * |
| * Ni | 61 | -0.01179 | 0.03990 | 0.04056 * |
| * Ni | 62 | -0.01259 | -0.07313 | 0.03756 * |
| * Ni | 63 | -0.08862 | -0.07998 | 0.03212 * |
| * Ni | 64 | -0.02006 | 0.02236 | -0.00424 * |
| * Ni | 65 | 0.10742 | 0.10995 | 0.03814 * |
| * Ni | 66 | 0.01955 | 0.02393 | -0.00833 * |
| * Ni | 67 | 0.03608 | -0.01471 | 0.00313 * |
| * Ni | 68 | -0.05062 | -0.11751 | -0.09980 * |
| * Ni | 69 | -0.08693 | -0.09534 | -0.09058 * |
| * Ni | 70 | 0.05456 | 0.03961 | 0.06891 * |
| * Ni | 71 | -0.07671 | -0.02162 | -0.10187 * |
| * Ni | 72 | -0.05453 | -0.01788 | -0.10207 * |
| * Ni | 73 | 0.08406 | 0.11399 | 0.07217 * |
| * Ni | 74 | -0.10763 | -0.07495 | 0.01123 * |
| * Ni | 75 | -0.02215 | -0.07703 | -0.05561 * |

*

*



Final energy = -102982.1606534 eV

```

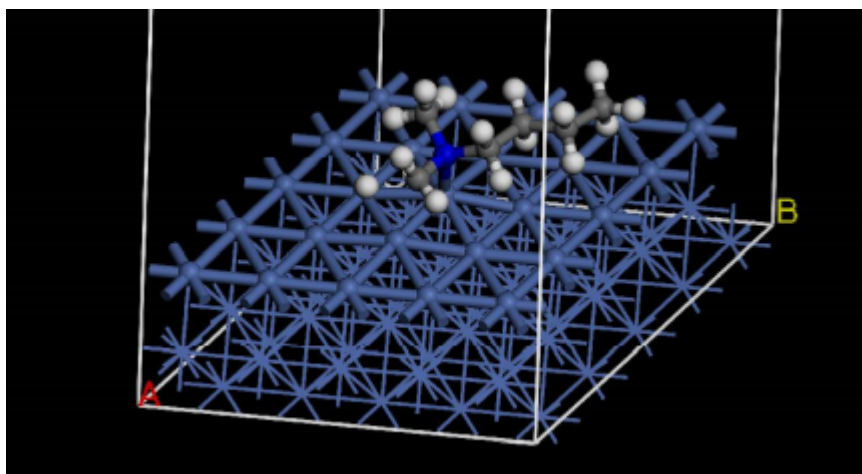
***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 -0.00393 0.00287 0.03140 *
* H 2 -0.00460 0.01571 0.04332 *
* H 3 -0.01122 0.02422 0.02669 *
* H 4 0.01310 0.03981 0.04137 *
* H 5 -0.02201 0.00002 0.04161 *
* H 6 0.04949 0.01148 0.04538 *
* H 7 0.05209 0.01371 0.03743 *
* H 8 -0.01183 -0.02726 -0.02154 *
* H 9 0.01086 -0.00763 -0.00925 *
* H 10 -0.01491 -0.01569 -0.01182 *
* H 11 -0.00582 -0.00156 -0.01485 *
* H 12 -0.01324 -0.01893 -0.00016 *
* H 13 0.01904 -0.00087 0.01289 *
* H 14 0.02511 0.02343 0.02890 *
* H 15 0.01061 0.06559 0.01608 *
* C 1 0.06720 -0.00850 -0.02343 *
* C 2 -0.08291 0.10558 -0.00308 *
* C 3 0.14789 -0.07721 -0.11385 *
* C 4 -0.17239 0.01080 0.00213 *
* C 5 0.01692 0.06845 0.19608 *
* C 6 0.03975 -0.14486 -0.09952 *

```

| | | | | |
|------|----|----------|----------|------------|
| * N | 1 | 0.03532 | 0.01907 | 0.07605 * |
| * Ni | 1 | 0.04648 | 0.00676 | 0.02114 * |
| * Ni | 2 | -0.23854 | -0.19706 | -0.19286 * |
| * Ni | 3 | 0.05239 | 0.07932 | 0.13854 * |
| * Ni | 4 | -0.03194 | -0.01418 | 0.03955 * |
| * Ni | 5 | -0.32083 | -0.34532 | -0.01815 * |
| * Ni | 6 | 0.08489 | 0.05592 | 0.14269 * |
| * Ni | 7 | -0.06859 | -0.14749 | 0.06724 * |
| * Ni | 8 | -0.03841 | 0.04103 | 0.03600 * |
| * Ni | 9 | 0.03209 | 0.07863 | 0.10138 * |
| * Ni | 10 | -0.05646 | -0.08775 | -0.01203 * |
| * Ni | 11 | -0.05430 | -0.10187 | 0.10879 * |
| * Ni | 12 | -0.01726 | -0.07366 | 0.02703 * |
| * Ni | 13 | -0.02131 | 0.04192 | 0.05963 * |
| * Ni | 14 | -0.16219 | -0.22009 | -0.14227 * |
| * Ni | 15 | -0.02745 | -0.01855 | 0.05110 * |
| * Ni | 16 | -0.03334 | 0.02818 | -0.04219 * |
| * Ni | 17 | -0.20921 | -0.10419 | -0.16994 * |
| * Ni | 18 | -0.01695 | -0.04776 | 0.03499 * |
| * Ni | 19 | 0.01629 | 0.00144 | -0.02490 * |
| * Ni | 20 | 0.20041 | 0.29601 | -0.13600 * |
| * Ni | 21 | 0.06261 | 0.07422 | 0.06191 * |
| * Ni | 22 | 0.05498 | 0.05282 | 0.15841 * |
| * Ni | 23 | 0.19373 | -0.02337 | -0.29278 * |
| * Ni | 24 | 0.06748 | 0.13213 | 0.12358 * |
| * Ni | 25 | -0.01531 | -0.26495 | 0.04780 * |
| * Ni | 26 | 0.14298 | 0.17500 | 0.01123 * |
| * Ni | 27 | 0.12997 | 0.17417 | 0.03783 * |
| * Ni | 28 | -0.09607 | -0.15216 | -0.12734 * |
| * Ni | 29 | 0.28685 | 0.33992 | 0.05819 * |
| * Ni | 30 | -0.08516 | -0.11855 | -0.04983 * |
| * Ni | 31 | -0.04816 | -0.10111 | -0.09395 * |
| * Ni | 32 | 0.20838 | 0.18366 | 0.13228 * |
| * Ni | 33 | -0.02868 | -0.05132 | -0.09333 * |
| * Ni | 34 | -0.04980 | 0.01501 | -0.07400 * |
| * Ni | 35 | 0.24491 | -0.02767 | 0.18589 * |
| * Ni | 36 | -0.06457 | -0.10570 | -0.12897 * |
| * Ni | 37 | 0.04641 | 0.19279 | -0.11666 * |
| * Ni | 38 | 0.03364 | -0.06722 | 0.11734 * |
| * Ni | 39 | 0.04223 | 0.07063 | 0.04539 * |
| * Ni | 40 | -0.17415 | 0.14819 | -0.22890 * |
| * Ni | 41 | -0.29108 | -0.16140 | -0.15337 * |
| * Ni | 42 | 0.14715 | 0.03241 | 0.13567 * |
| * Ni | 43 | 0.07816 | -0.07513 | 0.00889 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 44 | 0.18081 | 0.27572 | 0.15085 * |
| * Ni | 45 | -0.02843 | 0.14775 | -0.01626 * |
| * Ni | 46 | -0.12500 | -0.12545 | -0.09034 * |
| * Ni | 47 | 0.19200 | 0.30469 | 0.41821 * |
| * Ni | 48 | 0.00057 | 0.07881 | -0.05966 * |
| * Ni | 49 | -0.09257 | -0.11856 | -0.08102 * |
| * Ni | 50 | 0.21960 | 0.20951 | 0.51305 * |
| * Ni | 51 | -0.09246 | -0.11364 | -0.21972 * |
| * Ni | 52 | -0.18523 | -0.06706 | -0.12915 * |
| * Ni | 53 | 0.08168 | 0.09978 | 0.32925 * |
| * Ni | 54 | 0.00352 | -0.01621 | -0.11499 * |
| * Ni | 55 | 0.02592 | -0.05526 | -0.05872 * |
| * Ni | 56 | 0.03127 | 0.04244 | 0.30945 * |
| * Ni | 57 | 0.07235 | 0.09544 | -0.01965 * |
| * Ni | 58 | 0.04365 | 0.02553 | 0.01544 * |
| * Ni | 59 | 0.02402 | 0.01151 | 0.31617 * |
| * Ni | 60 | 0.08283 | 0.01718 | -0.01226 * |
| * Ni | 61 | 0.01912 | 0.04592 | 0.10862 * |
| * Ni | 62 | -0.19203 | -0.31863 | -0.54055 * |
| * Ni | 63 | 0.14619 | 0.09782 | 0.12450 * |
| * Ni | 64 | -0.04866 | -0.09421 | 0.10489 * |
| * Ni | 65 | -0.06237 | 0.02062 | -0.30726 * |
| * Ni | 66 | 0.04438 | 0.14537 | 0.04969 * |
| * Ni | 67 | -0.07502 | -0.07469 | 0.03500 * |
| * Ni | 68 | -0.06800 | -0.10019 | -0.28037 * |
| * Ni | 69 | -0.05889 | -0.03069 | -0.02263 * |
| * Ni | 70 | -0.04310 | 0.02742 | 0.04134 * |
| * Ni | 71 | -0.25811 | -0.21554 | -0.51607 * |
| * Ni | 72 | 0.04787 | 0.01103 | 0.04896 * |
| * Ni | 73 | 0.04886 | 0.00645 | 0.04594 * |
| * Ni | 74 | -0.21459 | -0.24054 | -0.42162 * |
| * Ni | 75 | 0.11301 | 0.09579 | 0.12205 * |

* *



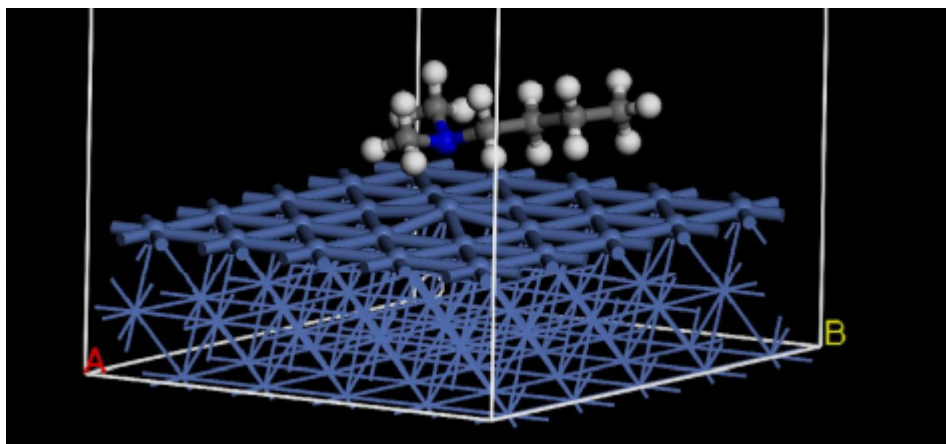
Final energy = -102981.3837423 eV

***** Forces *****

| ***** Forces ***** | | | | |
|---------------------------------|----|----------|----------|----------|
| * Cartesian components (eV/A) * | | | | |
| *-----* | | | | |
| | | x | y | z |
| * H | 1 | -0.00602 | 0.04029 | 0.11047 |
| * H | 2 | 0.01728 | 0.05006 | 0.03185 |
| * H | 3 | 0.01936 | -0.00799 | 0.05810 |
| * H | 4 | 0.03439 | -0.03001 | -0.01588 |
| * H | 5 | -0.01931 | -0.02594 | -0.04938 |
| * H | 6 | 0.02490 | -0.03771 | 0.03030 |
| * H | 7 | 0.01520 | -0.05854 | 0.01383 |
| * H | 8 | -0.02889 | -0.13272 | -0.00548 |
| * H | 9 | -0.03999 | -0.08320 | 0.14670 |
| * H | 10 | -0.21213 | -0.36265 | -0.03095 |
| * H | 11 | 0.60839 | -0.04394 | -0.71916 |
| * H | 12 | -0.00546 | -0.01175 | 0.05387 |
| * H | 13 | 0.17790 | -0.13895 | 0.05541 |
| * H | 14 | 0.14971 | 0.03742 | 0.09536 |
| * H | 15 | 0.15402 | 0.52056 | -0.17508 |
| * C | 1 | 0.02417 | -0.07450 | -0.08370 |
| * C | 2 | -0.06312 | -0.11068 | 0.16109 |
| * C | 3 | 0.06693 | -0.02403 | -0.08058 |
| * C | 4 | 0.08221 | 0.16047 | -0.19021 |
| * C | 5 | -1.02557 | 0.06444 | 0.56143 |
| * C | 6 | -0.39386 | -0.00882 | -0.25391 |
| * N | 1 | 0.12552 | -0.35750 | 0.16746 |
| * Ni | 1 | -0.06292 | 0.04328 | -0.00093 |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 2 | 0.05732 | 0.00765 | 0.02977 | * |
| * Ni | 3 | -0.01738 | 0.00805 | -0.00402 | * |
| * Ni | 4 | 0.02746 | 0.00862 | 0.03008 | * |
| * Ni | 5 | -0.04760 | -0.04136 | -0.05300 | * |
| * Ni | 6 | 0.02264 | -0.00156 | -0.01727 | * |
| * Ni | 7 | 0.06435 | 0.00377 | 0.00299 | * |
| * Ni | 8 | -0.01081 | -0.00064 | -0.00627 | * |
| * Ni | 9 | 0.03445 | 0.03190 | 0.02769 | * |
| * Ni | 10 | 0.00926 | 0.01155 | 0.10047 | * |
| * Ni | 11 | -0.00913 | -0.03617 | -0.00127 | * |
| * Ni | 12 | 0.01987 | 0.00392 | 0.01521 | * |
| * Ni | 13 | -0.00042 | 0.02336 | -0.00655 | * |
| * Ni | 14 | -0.02376 | -0.00199 | 0.05027 | * |
| * Ni | 15 | 0.06876 | -0.01590 | 0.02654 | * |
| * Ni | 16 | -0.03256 | 0.05584 | -0.00587 | * |
| * Ni | 17 | 0.01954 | 0.08087 | 0.03658 | * |
| * Ni | 18 | 0.01425 | 0.02085 | 0.02353 | * |
| * Ni | 19 | -0.04396 | 0.00449 | -0.01057 | * |
| * Ni | 20 | -0.10350 | -0.08648 | -0.08025 | * |
| * Ni | 21 | 0.00436 | -0.03065 | -0.04463 | * |
| * Ni | 22 | -0.04578 | -0.08140 | -0.01575 | * |
| * Ni | 23 | -0.00492 | 0.03073 | -0.00273 | * |
| * Ni | 24 | 0.02887 | 0.00982 | 0.00228 | * |
| * Ni | 25 | -0.08132 | -0.00781 | -0.05419 | * |
| * Ni | 26 | -0.03596 | -0.01608 | -0.03445 | * |
| * Ni | 27 | 0.02055 | 0.00894 | -0.00211 | * |
| * Ni | 28 | 0.06181 | -0.02516 | 0.01477 | * |
| * Ni | 29 | -0.03572 | -0.06960 | 0.01459 | * |
| * Ni | 30 | 0.03056 | 0.00501 | 0.00120 | * |
| * Ni | 31 | -0.01956 | 0.07405 | 0.03727 | * |
| * Ni | 32 | 0.00392 | -0.03940 | 0.00740 | * |
| * Ni | 33 | -0.00918 | 0.04606 | 0.01248 | * |
| * Ni | 34 | -0.05236 | 0.03026 | -0.00231 | * |
| * Ni | 35 | -0.01896 | 0.05795 | -0.00226 | * |
| * Ni | 36 | 0.05592 | -0.01450 | 0.01120 | * |
| * Ni | 37 | -0.00835 | -0.19353 | -0.04490 | * |
| * Ni | 38 | -0.01188 | 0.06081 | 0.07315 | * |
| * Ni | 39 | -0.01312 | 0.01958 | -0.00182 | * |
| * Ni | 40 | 0.13961 | 0.24091 | -0.27527 | * |
| * Ni | 41 | 0.02618 | 0.04045 | 0.07267 | * |
| * Ni | 42 | 0.00414 | -0.00967 | -0.00363 | * |
| * Ni | 43 | 0.01330 | 0.03502 | 0.02197 | * |
| * Ni | 44 | 0.00439 | -0.00699 | -0.00815 | * |
| * Ni | 45 | 0.03043 | 0.01609 | -0.01433 | * |

| | | | | | |
|------|----|----------|----------|----------|---|
| * Ni | 46 | -0.06604 | 0.01787 | 0.01985 | * |
| * Ni | 47 | -0.03856 | -0.01187 | -0.01727 | * |
| * Ni | 48 | -0.02957 | 0.03077 | -0.01569 | * |
| * Ni | 49 | 0.01286 | 0.03233 | 0.02646 | * |
| * Ni | 50 | -0.02653 | -0.01433 | -0.00388 | * |
| * Ni | 51 | 0.03554 | 0.02199 | 0.00092 | * |
| * Ni | 52 | 0.04386 | -0.02340 | -0.00255 | * |
| * Ni | 53 | 0.03342 | 0.07595 | 0.01488 | * |
| * Ni | 54 | 0.02214 | 0.01996 | -0.00150 | * |
| * Ni | 55 | -0.02269 | 0.02031 | 0.05403 | * |
| * Ni | 56 | -0.00951 | -0.01853 | 0.00893 | * |
| * Ni | 57 | -0.00447 | -0.01237 | -0.03597 | * |
| * Ni | 58 | 0.01109 | 0.04229 | 0.04696 | * |
| * Ni | 59 | 0.07696 | 0.02152 | 0.04789 | * |
| * Ni | 60 | 0.00791 | -0.02266 | -0.02952 | * |
| * Ni | 61 | -0.07670 | 0.01130 | -0.00189 | * |
| * Ni | 62 | 0.01469 | 0.06620 | 0.07552 | * |
| * Ni | 63 | -0.01051 | 0.00157 | 0.00223 | * |
| * Ni | 64 | 0.00465 | 0.00017 | 0.00505 | * |
| * Ni | 65 | -0.05364 | 0.03373 | -0.01690 | * |
| * Ni | 66 | 0.00798 | 0.01090 | -0.03682 | * |
| * Ni | 67 | 0.06997 | 0.00489 | 0.01831 | * |
| * Ni | 68 | -0.01156 | -0.00255 | -0.02840 | * |
| * Ni | 69 | 0.02563 | 0.02321 | 0.01229 | * |
| * Ni | 70 | -0.02386 | 0.01172 | 0.03028 | * |
| * Ni | 71 | 0.05334 | 0.04138 | 0.04578 | * |
| * Ni | 72 | 0.03700 | -0.01625 | -0.00663 | * |
| * Ni | 73 | 0.04291 | 0.00203 | -0.01672 | * |
| * Ni | 74 | 0.07983 | 0.01253 | 0.03272 | * |
| * Ni | 75 | 0.01543 | -0.04589 | -0.02949 | * |
| * | | | | | * |



Final energy = -102982.1717836 eV

```

***** Forces *****
*
* Cartesian components (eV/A) *
* ----- *
* x y z *
*
* H 1 0.00188 0.03302 0.01907 *
* H 2 0.00662 0.02999 0.01959 *
* H 3 0.00731 0.00251 0.00869 *
* H 4 0.04267 0.06747 0.05288 *
* H 5 -0.03380 0.00426 0.02185 *
* H 6 -0.01718 0.01351 0.02789 *
* H 7 0.05156 0.02904 0.03372 *
* H 8 0.04405 0.03428 0.04632 *
* H 9 0.03132 0.01598 0.06309 *
* H 10 0.04424 0.02611 0.06077 *
* H 11 -0.02525 -0.01137 -0.00095 *
* H 12 -0.01856 -0.00198 0.03403 *
* H 13 0.02589 0.00641 0.03554 *
* H 14 0.00467 0.03572 0.03355 *
* H 15 -0.01798 0.01883 -0.01287 *
* C 1 0.06286 -0.13042 0.01470 *
* C 2 -0.13344 0.04565 0.02732 *
* C 3 0.15990 -0.03363 -0.12236 *
* C 4 -0.12940 0.05580 0.00778 *
* C 5 -0.13002 -0.02709 0.02480 *
* C 6 0.01465 0.08729 -0.04801 *
* N 1 0.00502 0.00960 0.02994 *
* Ni 1 0.08656 -0.00366 0.03931 *
* Ni 2 -0.15984 -0.25720 -0.20681 *
* Ni 3 0.08099 0.11058 0.10320 *
* Ni 4 -0.00455 -0.06702 -0.02123 *
* Ni 5 -0.42355 -0.01530 -0.03170 *
* Ni 6 0.11735 0.13717 0.03252 *
* Ni 7 -0.02345 -0.07962 -0.04162 *
* Ni 8 0.47056 0.17005 0.18398 *
* Ni 9 -0.09901 -0.03824 -0.03386 *
* Ni 10 -0.12868 -0.08354 -0.08867 *
* Ni 11 0.13302 0.21049 0.17709 *
* Ni 12 -0.09715 -0.06514 -0.01506 *
* Ni 13 -0.07819 0.04257 0.04475 *
* Ni 14 -0.04070 -0.25819 -0.31386 *
* Ni 15 0.02068 -0.01181 0.03555 *

```

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 16 | -0.01561 | 0.00422 | -0.08324 * |
| * Ni | 17 | -0.18357 | -0.14088 | -0.19698 * |
| * Ni | 18 | 0.10720 | 0.05552 | 0.06636 * |
| * Ni | 19 | 0.07432 | 0.23960 | 0.10707 * |
| * Ni | 20 | -0.20227 | -0.22410 | -0.26635 * |
| * Ni | 21 | 0.14922 | 0.09514 | 0.10550 * |
| * Ni | 22 | 0.09823 | -0.14780 | 0.15287 * |
| * Ni | 23 | 0.41080 | 0.22424 | 0.03156 * |
| * Ni | 24 | 0.00956 | 0.15486 | 0.05899 * |
| * Ni | 25 | -0.08427 | -0.10425 | -0.10155 * |
| * Ni | 26 | 0.12688 | 0.33543 | 0.20445 * |
| * Ni | 27 | -0.03162 | -0.01800 | 0.00829 * |
| * Ni | 28 | -0.15402 | -0.10716 | -0.03661 * |
| * Ni | 29 | 0.03548 | -0.23975 | -0.07347 * |
| * Ni | 30 | -0.04457 | -0.10427 | -0.01719 * |
| * Ni | 31 | -0.05574 | -0.01765 | -0.06126 * |
| * Ni | 32 | 0.03071 | -0.10643 | -0.01454 * |
| * Ni | 33 | 0.03026 | -0.06143 | -0.09776 * |
| * Ni | 34 | -0.01787 | 0.01386 | 0.03863 * |
| * Ni | 35 | -0.21922 | -0.24389 | -0.06701 * |
| * Ni | 36 | 0.03468 | -0.00982 | 0.00844 * |
| * Ni | 37 | 0.10500 | -0.00470 | -0.00315 * |
| * Ni | 38 | 0.17402 | 0.04738 | 0.02948 * |
| * Ni | 39 | 0.01415 | 0.06951 | 0.08510 * |
| * Ni | 40 | -0.08413 | -0.13066 | 0.00239 * |
| * Ni | 41 | 0.01394 | -0.05826 | 0.03460 * |
| * Ni | 42 | 0.00322 | 0.06127 | 0.04817 * |
| * Ni | 43 | -0.12193 | -0.09804 | -0.02645 * |
| * Ni | 44 | 0.09745 | 0.41147 | 0.22677 * |
| * Ni | 45 | 0.03009 | 0.07719 | 0.02477 * |
| * Ni | 46 | -0.08650 | -0.14186 | -0.08011 * |
| * Ni | 47 | 0.11565 | 0.04796 | -0.06331 * |
| * Ni | 48 | 0.06223 | 0.00362 | -0.01774 * |
| * Ni | 49 | -0.00343 | 0.00991 | -0.05920 * |
| * Ni | 50 | -0.33397 | -0.19839 | -0.04937 * |
| * Ni | 51 | 0.01752 | -0.07156 | -0.08367 * |
| * Ni | 52 | 0.04127 | 0.05523 | -0.07398 * |
| * Ni | 53 | 0.26454 | 0.12466 | 0.07717 * |
| * Ni | 54 | -0.09951 | 0.02327 | 0.00048 * |
| * Ni | 55 | -0.09164 | 0.01951 | -0.05894 * |
| * Ni | 56 | 0.00376 | 0.00786 | 0.15014 * |
| * Ni | 57 | -0.00631 | 0.07467 | -0.02358 * |
| * Ni | 58 | -0.06265 | -0.03147 | -0.03902 * |
| * Ni | 59 | -0.05597 | 0.03739 | 0.17989 * |

| | | | | |
|------|----|----------|----------|------------|
| * Ni | 60 | 0.03252 | 0.03679 | -0.01082 * |
| * Ni | 61 | 0.01691 | 0.02520 | 0.08787 * |
| * Ni | 62 | -0.06139 | -0.21168 | -0.26204 * |
| * Ni | 63 | 0.20579 | 0.15930 | 0.13583 * |
| * Ni | 64 | 0.03263 | -0.06073 | 0.03550 * |
| * Ni | 65 | -0.28876 | 0.01264 | -0.07127 * |
| * Ni | 66 | 0.03511 | 0.05579 | -0.00491 * |
| * Ni | 67 | 0.05133 | -0.10847 | -0.05264 * |
| * Ni | 68 | 0.53176 | 0.13569 | 0.22083 * |
| * Ni | 69 | -0.12987 | 0.00074 | -0.00707 * |
| * Ni | 70 | -0.06988 | 0.01699 | -0.02410 * |
| * Ni | 71 | -0.16266 | 0.11438 | -0.01588 * |
| * Ni | 72 | -0.06354 | -0.03182 | -0.01642 * |
| * Ni | 73 | -0.06160 | 0.02021 | 0.01945 * |
| * Ni | 74 | -0.09188 | -0.30164 | -0.38872 * |
| * Ni | 75 | 0.07711 | 0.10112 | 0.06685 * |

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