

## Electronic Supplementary Information

### Structure coordinates

We provide here the coordinates for all the CNT structures used in the current paper. We first report OH, then OOH adsorbate coordinates, considering for each species undoped, N- and B- doped surfaces. The coordinates are given in VASP file format. The first line of structure file refers to the  $(n,m)$  type CNT, the number of KPOINTS used in the calculation and the DFT calculated total energy.

#### 1.1 OH adsorbate

##### 1.1.1 OH adsorbate on undoped CNT

OH\_CNT(5,5) ### KPOINTS: 2x2x3 ### ### E= -471.43640302 eV

```
1.0000000000000000
13.8564000000000007 -8.0000000000000000 0.0000000000000000
0.0000000000000000 16.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.3947799999999999
C O H
60 1 1
```

Selective dynamics

Direct

```
0.5619981129388494 0.4259978572751649 0.0811638298498377 T T T
0.5619282151852838 0.4259936989559501 0.4142061539076427 T T T
0.5619074020211404 0.4258463122554593 0.7476778613203345 T T T
0.4803933288880873 0.5452255445556332 0.0811113234204857 T T T
0.4805245607956649 0.5452827427943987 0.4146205644542985 T T T
0.4790139276551342 0.5444143539273426 0.7479098077465816 T T T
0.3934338874942023 0.5490332740091775 0.0812065586094840 T T T
0.3933602141584583 0.5486470280501632 0.4148454424594662 T T T
0.3927668940801972 0.5491877901714168 0.7480458820838758 T T T
0.1156030286298396 0.3439413434428573 0.0817980497981664 T T T
0.1156382209718684 0.3437916353139578 0.4140657165495632 T T T
```

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1173959533879590 | 0.3439615736491072 | 0.7477783453222527 | T | T | T |
| 0.0784874323687094 | 0.1529767288468286 | 0.0813832910709604 | T | T | T |
| 0.0783901924638178 | 0.1529340667185924 | 0.4140624470798261 | T | T | T |
| 0.0783250909727578 | 0.1527251056950167 | 0.7478100877028642 | T | T | T |
| 0.1177250124693139 | 0.0901660024895117 | 0.0813086591020561 | T | T | T |
| 0.1177710295587601 | 0.0902303043293135 | 0.4139941785841617 | T | T | T |
| 0.1175329453083972 | 0.0895465536152033 | 0.7477215069355028 | T | T | T |
| 0.2873180639984296 | 0.0800468582764585 | 0.0808859156917392 | T | T | T |
| 0.2872883615167628 | 0.0799974102977301 | 0.4139169537272290 | T | T | T |
| 0.2871519583275783 | 0.0796318742908484 | 0.7473857033618588 | T | T | T |
| 0.3899991066188520 | 0.1373037872665912 | 0.0808153508895495 | T | T | T |
| 0.3899807948699828 | 0.1372964725245629 | 0.4137663837272658 | T | T | T |
| 0.3900272229680047 | 0.1372093330332994 | 0.7473161245415409 | T | T | T |
| 0.5410444149543173 | 0.3282877769202164 | 0.0809334176322137 | T | T | T |
| 0.5410089620449979 | 0.3282710031314919 | 0.4140109431545402 | T | T | T |
| 0.5411002886124225 | 0.3282176472417363 | 0.7474725801000009 | T | T | T |
| 0.1929798211031443 | 0.4420710459480532 | 0.0819504267564938 | T | T | T |
| 0.1929248217448062 | 0.4418467376615731 | 0.4142270301574923 | T | T | T |
| 0.1797376200751928 | 0.4535303672111885 | 0.7476054083658733 | T | T | T |
| 0.2416188132138410 | 0.4813801457464528 | 0.2482250611484608 | T | T | T |
| 0.2402260467845348 | 0.4845673135186366 | 0.5790324211685917 | T | T | T |
| 0.2401636209128001 | 0.4849344071473993 | 0.9168154229090096 | T | T | T |
| 0.5565952498441362 | 0.4680284780774149 | 0.2477026184387343 | T | T | T |
| 0.5559566524251356 | 0.4677750059926939 | 0.5812581866925083 | T | T | T |
| 0.5559184265077052 | 0.4677063240270209 | 0.9142162382032567 | T | T | T |
| 0.1503367011902214 | 0.0715401629789280 | 0.2476189273705144 | T | T | T |
| 0.1507088332531832 | 0.0717126001091257 | 0.5810622196865779 | T | T | T |
| 0.1507195778495181 | 0.0716831667791180 | 0.9141988941428904 | T | T | T |
| 0.2370230335931234 | 0.0661939710543390 | 0.2474354010935952 | T | T | T |
| 0.2369838740059713 | 0.0663199783370411 | 0.5809587753466894 | T | T | T |
| 0.2370245699774809 | 0.0663491739467352 | 0.9139368585575576 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5148665676371404 | 0.5288443324260123 | 0.2478080682798406 | T | T | T |
| 0.5143388481950144 | 0.5282158979362939 | 0.5814590599853412 | T | T | T |
| 0.5141153910152388 | 0.5279795343120676 | 0.9142633800060880 | T | T | T |
| 0.0907015657696370 | 0.2922970150714307 | 0.2479020574836571 | T | T | T |
| 0.0941402057511727 | 0.2927728861844823 | 0.5825844931146282 | T | T | T |
| 0.0943168760749947 | 0.2929162337050314 | 0.9130792618666990 | T | T | T |
| 0.4380570515318705 | 0.1783929762908013 | 0.2473155695278706 | T | T | T |
| 0.4379337272313804 | 0.1787133168724509 | 0.5807825416471433 | T | T | T |
| 0.4379626172297070 | 0.1787193880584509 | 0.9138010537571530 | T | T | T |
| 0.5152058468662655 | 0.2763105207483523 | 0.2474519685201081 | T | T | T |
| 0.5149897704473771 | 0.2761813740476697 | 0.5808525006458894 | T | T | T |
| 0.5150224850155213 | 0.2762185470870169 | 0.9139918055470315 | T | T | T |
| 0.0722429429520868 | 0.1944789941253938 | 0.2477497366157446 | T | T | T |
| 0.0738470740035134 | 0.1952200317114999 | 0.5817145887317414 | T | T | T |
| 0.0740321176592167 | 0.1953272738921979 | 0.9138883073391409 | T | T | T |
| 0.3443662510504438 | 0.5368021251915573 | 0.2481121320276172 | T | T | T |
| 0.3416353067195545 | 0.5343172388425359 | 0.5813277076714165 | T | T | T |
| 0.3417368214868590 | 0.5348948806826929 | 0.9147723544209768 | T | T | T |
| 0.1198379736560436 | 0.5001693358231483 | 0.7366057181140347 | T | T | T |
| 0.0787382739663560 | 0.4804851393771710 | 0.8428107258363342 | T | T | T |

OH\_CNT(6,6) #### KPOINTS: 2x2x3 #### E= -567.71322468 eV

1.0000000000000000

14.7224000000000004 -8.5000000000000000 0.0000000000000000

0.0000000000000000 17.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3992800000000001

C O H

72 1 1

Selective dynamics

Direct

0.6161781159717961 0.4961653944355118 0.0835826931695521 T T T

0.6161402089968053 0.4962285337129981 0.4169060748771049 T T T

0.6160360470815374 0.4961211399519172 0.7501616805947938 T T T

0.5330921161030054 0.6034267744494661 0.0834105454091699 T T T

0.5337586735854937 0.6041983443034258 0.4167711170103180 T T T

0.5333287803667613 0.6036922616366968 0.7503324548340188 T T T

0.4531009591441172 0.6102220741301683 0.0833902827168118 T T T

0.4535047713873375 0.6111300349646683 0.4167034158313724 T T T

0.4531969422267275 0.6102143571685222 0.7504225746898652 T T T

0.1719271949063472 0.4562806859057645 0.0853564305540847 T T T

0.1752507638048361 0.4539199772805407 0.4165338864961064 T T T

0.1725556003938473 0.4558907203073879 0.7477260674668045 T T T

0.0681387896608447 0.2661181798209921 0.0820232184861257 T T T

0.0658766622335902 0.2652508554802200 0.4166570594904619 T T T

0.0684760998735130 0.2661124936512609 0.7513960568314582 T T T

0.0619168993766536 0.1791891063231712 0.0829418415829321 T T T

0.0603749497701604 0.1781090982450442 0.4167540703813724 T T T

0.0619787896333937 0.1791011097204182 0.7506055864017306 T T T

0.1405166310716243 0.0676608921749340 0.0833873181530560 T T T

0.1399427245732378 0.0672618983357926 0.4168385734385865 T T T

0.1404789119549119 0.0676348706803129 0.7502711718539209 T T T

0.2191586507889897 0.0581028873526048 0.0833769690275623 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2191485976126576 | 0.0581942326610636 | 0.4169105415333725 | T | T | T |
| 0.2191942671409533 | 0.0582030775223110 | 0.7503303475339971 | T | T | T |
| 0.4094596338815823 | 0.1388695435628894 | 0.0833835576130981 | T | T | T |
| 0.4094430312413027 | 0.1386384338555597 | 0.4168053898637746 | T | T | T |
| 0.4094394253878616 | 0.1388701150090212 | 0.7502591164859124 | T | T | T |
| 0.4970957825095667 | 0.2181761410447644 | 0.0833021785374864 | T | T | T |
| 0.4972448734955774 | 0.2181758325884963 | 0.4168000328820322 | T | T | T |
| 0.4970854116431040 | 0.2181382498889946 | 0.7502305109669932 | T | T | T |
| 0.6074277239895817 | 0.4083816651542447 | 0.0834627797874303 | T | T | T |
| 0.6075306263763154 | 0.4082945237148444 | 0.4168849783520456 | T | T | T |
| 0.6073723557432996 | 0.4084013067076492 | 0.7502037863700799 | T | T | T |
| 0.2616755906707712 | 0.5301576916002285 | 0.0834856226378051 | T | T | T |
| 0.2636999190326968 | 0.5319314361721155 | 0.4167366404798272 | T | T | T |
| 0.2620815518430614 | 0.5297355137226435 | 0.7499989485295112 | T | T | T |
| 0.0699043183040437 | 0.1416301490590575 | 0.2502842244983652 | T | T | T |
| 0.0696966119022531 | 0.1414181789698358 | 0.5831990467695747 | T | T | T |
| 0.0697321509875886 | 0.1415111659094195 | 0.9168636930790542 | T | T | T |
| 0.1096552455082145 | 0.0850602539113236 | 0.2503809573228061 | T | T | T |
| 0.1094558795116935 | 0.0848427503420169 | 0.5832411949976671 | T | T | T |
| 0.1096960216344070 | 0.0848075882222270 | 0.9168644266152579 | T | T | T |
| 0.5654093305721264 | 0.5879060269853278 | 0.2503291446135796 | T | T | T |
| 0.5655738925635709 | 0.5881220062004197 | 0.5832965356132008 | T | T | T |
| 0.5655762230684459 | 0.5879243115893776 | 0.9168973358530412 | T | T | T |
| 0.1362390629217010 | 0.4094209693422800 | 0.2502965132535304 | T | T | T |
| 0.1367358289766709 | 0.4092270610961978 | 0.5827510486134441 | T | T | T |
| 0.1177609076773761 | 0.4143895999007136 | 0.9161115188759095 | T | T | T |
| 0.2649281563167225 | 0.0664539471142218 | 0.2504490270067650 | T | T | T |
| 0.2649861391037964 | 0.0665401442375495 | 0.5833364374102682 | T | T | T |
| 0.2648090266825372 | 0.0661134718286603 | 0.9168423849657316 | T | T | T |
| 0.3613826972465996 | 0.1073540883162501 | 0.2503699998595726 | T | T | T |
| 0.3614103093729432 | 0.1074033323568459 | 0.5832796058317211 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3614697876222996 | 0.1073371535300002 | 0.9168233079879975 | T | T | T |
| 0.0809438979395408 | 0.3126293500309745 | 0.2505377555299312 | T | T | T |
| 0.0813596649365063 | 0.3125827672862581 | 0.5827985486674910 | T | T | T |
| 0.0812441342745241 | 0.3125564379490862 | 0.9166532824386691 | T | T | T |
| 0.3111643235153669 | 0.5616013133891865 | 0.2499197004099146 | T | T | T |
| 0.3113897389430144 | 0.5611890670692636 | 0.5835060624539266 | T | T | T |
| 0.3106334425375898 | 0.5615541245753737 | 0.9168872251079085 | T | T | T |
| 0.5345843072728589 | 0.2639629730282360 | 0.2501967634807365 | T | T | T |
| 0.5346020719575649 | 0.2639417214857058 | 0.5834224623445241 | T | T | T |
| 0.5346219559898606 | 0.2638597502310740 | 0.9167168687287968 | T | T | T |
| 0.5904994633277794 | 0.3602733568492416 | 0.2503058122070194 | T | T | T |
| 0.5904842364220957 | 0.3602590839975514 | 0.5834499514056205 | T | T | T |
| 0.5905450540243465 | 0.3603122053318745 | 0.9167696687234510 | T | T | T |
| 0.6074573200353873 | 0.5334616297700766 | 0.2503830384244836 | T | T | T |
| 0.6073456964497176 | 0.5334197110002150 | 0.5833892367105352 | T | T | T |
| 0.6074930651026863 | 0.5334137542750687 | 0.9168843457682003 | T | T | T |
| 0.4073321391185017 | 0.6017485623049115 | 0.2500218574478343 | T | T | T |
| 0.4075169679934479 | 0.6016627402809971 | 0.5835373630695931 | T | T | T |
| 0.4064223982361434 | 0.6007600994152551 | 0.9169168087236859 | T | T | T |
| 0.0365653647070201 | 0.4258885666414608 | 0.9135321274796492 | T | T | T |
| 0.0582950937691492 | 0.4903911329397789 | 0.9013011968399661 | T | T | T |

OH\_CNT(7,7) #### KPOINTS: 1x1x3 #### E= -663.52351080 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C O H

84 1 1

Selective dynamics

Direct

0.1811926731094392 0.0460409235755771 0.0827636567148626 T T T

0.2643495629485140 0.0549598868106996 0.0827558022826482 T T T

0.0677598271751842 0.1112101615316793 0.0826409249928983 T T T

0.4452651462351372 0.1493000601772829 0.0827234408190456 T T T

0.0485401402556915 0.1789313135091319 0.0824475958829641 T T T

0.5264646627048003 0.2260960370586835 0.0827519451607894 T T T

0.0888753087327842 0.3520665419181896 0.0828445286247001 T T T

0.6359988215892430 0.4057443278607065 0.0827266419111474 T T T

0.1427069160707386 0.4430730904725753 0.0835295109319461 T T T

0.6551645595267649 0.4926009617065868 0.0826379409084448 T T T

0.3005444304023749 0.5982143787455571 0.0798185458139660 T T T

0.6133248096510321 0.6242036518744377 0.0825591813064672 T T T

0.3906723545672534 0.6401404381155680 0.0822153206762915 T T T

0.5555246507589188 0.6563129859758822 0.0825919635878108 T T T

0.0489385754614554 0.2187679225771864 0.2490397938127605 T T T

0.5616759431370416 0.2693006748930947 0.2492688444880890 T T T

0.0693784085332570 0.3063773556577937 0.2489575578442625 T T T

0.6168682581207857 0.3599462733614369 0.2492861005511656 T T T

0.1753602986518369 0.4866467437214163 0.2488657597573629 T T T

0.1447280072068877 0.0520187602310706 0.2492994397838822 T T T

0.3093310846319336 0.0694632328885842 0.2492897155460433 T T T

0.0872016066108337 0.0849348840312870 0.2492485779818985 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4007254028913465 | 0.1171519362406380 | 0.2492642481375859 | T | T | T |
| 0.6547730353492758 | 0.5322511905588110 | 0.2492717580064762 | T | T | T |
| 0.2478602426080257 | 0.5789680817715259 | 0.2487125738275608 | T | T | T |
| 0.6338202429414007 | 0.5986757022687142 | 0.2491725189849509 | T | T | T |
| 0.4364371117531833 | 0.6552015204628643 | 0.2490545933661638 | T | T | T |
| 0.5184029220675913 | 0.6621734819520585 | 0.2490741017587683 | T | T | T |
| 0.1811849308717026 | 0.0460235420906150 | 0.4158420155323849 | T | T | T |
| 0.2643556281181202 | 0.0549689296205211 | 0.4158162269711868 | T | T | T |
| 0.0677578403459190 | 0.1112149844560726 | 0.4157976284789814 | T | T | T |
| 0.4452500762975424 | 0.1492899953850541 | 0.4157720402514097 | T | T | T |
| 0.0485505746734596 | 0.1789590987968205 | 0.4157061945441004 | T | T | T |
| 0.5264601295642911 | 0.2260963208693613 | 0.4157882405894788 | T | T | T |
| 0.0887381212320808 | 0.3520249873460113 | 0.4150370747740130 | T | T | T |
| 0.6359961875956065 | 0.4057151108812985 | 0.4158561842315906 | T | T | T |
| 0.1427906456340847 | 0.4430052758208727 | 0.4142079600887269 | T | T | T |
| 0.6551716931419885 | 0.4925870179731193 | 0.4159045359500245 | T | T | T |
| 0.3005846672741413 | 0.5980876365750837 | 0.4177405097500677 | T | T | T |
| 0.6132908171559706 | 0.6242357869785066 | 0.4156635107748065 | T | T | T |
| 0.3908107880518381 | 0.6404131156229075 | 0.4158548065567508 | T | T | T |
| 0.5556252638573895 | 0.6565603417660599 | 0.4155983047063438 | T | T | T |
| 0.1447788674834969 | 0.0521386741593436 | 0.5827403876688390 | T | T | T |
| 0.3093855929181226 | 0.0695592731513528 | 0.5826688039573333 | T | T | T |
| 0.0874927771866354 | 0.0851224440357534 | 0.5827361612152625 | T | T | T |
| 0.4006810923527255 | 0.1171510174276399 | 0.5826315510877333 | T | T | T |
| 0.0489109884497210 | 0.2190807057849587 | 0.5825968825915969 | T | T | T |
| 0.5616541809581691 | 0.2693454106809685 | 0.5826059337297275 | T | T | T |
| 0.0689791693990072 | 0.3063406739693639 | 0.5824339561687029 | T | T | T |
| 0.6168990785105467 | 0.3599613674066056 | 0.5826792755377410 | T | T | T |
| 0.1751467875877137 | 0.4865095465395691 | 0.5827895471468026 | T | T | T |
| 0.6547585114560301 | 0.5322574866759494 | 0.5825944313584017 | T | T | T |
| 0.2566713330837828 | 0.5636806907716195 | 0.5824289425960981 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6338168048491974 | 0.5987861420483698 | 0.5825144940946252 | T | T | T |
| 0.4366820708076509 | 0.6544845678730739 | 0.5822033201193687 | T | T | T |
| 0.5195067613802540 | 0.6629468572036129 | 0.5822649866071637 | T | T | T |
| 0.0677810083425989 | 0.1112246939974236 | 0.7492353842452805 | T | T | T |
| 0.0482137320682677 | 0.1789948807052358 | 0.7490956294886617 | T | T | T |
| 0.5265300201750356 | 0.2261107180670105 | 0.7492673409706625 | T | T | T |
| 0.0870401256153066 | 0.3517393649913833 | 0.7490563631766323 | T | T | T |
| 0.6361207366508425 | 0.4057221581902744 | 0.7493308581977576 | T | T | T |
| 0.1408972681860787 | 0.4434224131682341 | 0.7491045114628854 | T | T | T |
| 0.1810083110355616 | 0.0458730564500612 | 0.7492972660708332 | T | T | T |
| 0.2643459850964064 | 0.0548388585600569 | 0.7492860525857402 | T | T | T |
| 0.4452202612639584 | 0.1491345734501831 | 0.7492576698566701 | T | T | T |
| 0.6552091822580794 | 0.4927096679345477 | 0.7492990506488562 | T | T | T |
| 0.3013903622232619 | 0.5940143735355243 | 0.7490214579370410 | T | T | T |
| 0.6137904167233901 | 0.6245500114508645 | 0.7491285997862609 | T | T | T |
| 0.3924940245179002 | 0.6409101063529070 | 0.7490770427210065 | T | T | T |
| 0.5560598293146651 | 0.6570820519414247 | 0.7490616550361550 | T | T | T |
| 0.1447857851681065 | 0.0521648875755126 | 0.9158428882780381 | T | T | T |
| 0.3093899099530615 | 0.0695581024213096 | 0.9158864567163735 | T | T | T |
| 0.0874782423166666 | 0.0851192742244943 | 0.9157540247362067 | T | T | T |
| 0.4006939516401539 | 0.1171629207619493 | 0.9158820838243041 | T | T | T |
| 0.0488269381434621 | 0.2190145403381329 | 0.9155531461253081 | T | T | T |
| 0.5616384927919923 | 0.2693319776454776 | 0.9159317339559145 | T | T | T |
| 0.0689427490070264 | 0.3063013130426860 | 0.9155677303188049 | T | T | T |
| 0.6168837366127012 | 0.3599600671378652 | 0.9159640003009479 | T | T | T |
| 0.1750441986974345 | 0.4866884612367333 | 0.9151911442883711 | T | T | T |
| 0.6547829084655008 | 0.5322766382027290 | 0.9158978067297973 | T | T | T |
| 0.2565498055261303 | 0.5639105693012954 | 0.9154654465432605 | T | T | T |
| 0.6339213164914385 | 0.5988543042669068 | 0.9157431466757701 | T | T | T |
| 0.4366171561021396 | 0.6542389192530569 | 0.9159019396657998 | T | T | T |
| 0.5194489352008113 | 0.6627228777311595 | 0.9158886228755142 | T | T | T |

0.2123830776906727 0.6383384081762633 0.2391545550544046 T T T  
0.1783627904554238 0.6288030113607633 0.3473799011885116 T T T

OH\_CNT (8,8) ### KPOINTS: 1x1x3 ### E= -759.08852703 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C O H

96 1 1

Selective dynamics

Direct

0.2520408899658561 0.0431690513338671 0.0832907745637312 T T T

0.1154278891359535 0.0526346909460476 0.0832576458714676 T T T

0.3326036338558959 0.0693021172643875 0.0833292838796619 T T T

0.0690920177961756 0.0883350933991552 0.0832450790775789 T T T

0.4930391040592429 0.1759413128736605 0.0833826803465855 T T T

0.0386816884277508 0.2119717217006066 0.0832390479735193 T T T

0.5618220274688780 0.2493004061487863 0.0833691600455925 T T T

0.0565930651193277 0.2904862995623441 0.0832509773281937 T T T

0.6533473699648020 0.4121890804391947 0.0832302663714487 T T T

0.1455529287024699 0.4536587240157028 0.0835847004232212 T T T

0.6698280542379782 0.4901591648959084 0.0831861098739693 T T T

0.2143047316607117 0.5273557469477858 0.0833535779257110 T T T

0.6380229462075110 0.6128381861975138 0.0831269775903302 T T T

0.3744698989872138 0.6311348664109500 0.0828780723514988 T T T

0.5915285852853670 0.6482690513715713 0.0831419558494585 T T T

0.4548636871701997 0.6571811307553088 0.0828990524984324 T T T

0.2138541464293476 0.0377009461492709 0.2498886560903897 T T T

0.1449330235033313 0.0423269867153336 0.2498487023975263 T T T

0.3738859417798339 0.0896445058056765 0.2499302890705718 T T T

0.4547252731015324 0.1434001920584945 0.2499376533606931 T T T

0.0375623490157808 0.1757165099891172 0.2497943895279393 T T T

0.6700614389485360 0.5260385137058754 0.2498464082109569 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2530845943848282 | 0.5585209783728692 | 0.2497923125673318 | T | T | T |
| 0.6541201674018121 | 0.5879611275109820 | 0.2498126366283263 | T | T | T |
| 0.5620725086131301 | 0.6585949496989164 | 0.2497964216599642 | T | T | T |
| 0.0532669140249343 | 0.1134525610916286 | 0.2498155207788552 | T | T | T |
| 0.5913045466682948 | 0.2891273721751024 | 0.2499201128743351 | T | T | T |
| 0.0720900500513452 | 0.3312224227568799 | 0.2497854367671027 | T | T | T |
| 0.6373524356944050 | 0.3712104539400700 | 0.2498969817348002 | T | T | T |
| 0.1172046188389298 | 0.4139552677479498 | 0.2497925076714462 | T | T | T |
| 0.3337648935774920 | 0.6115786091798302 | 0.2497929629477189 | T | T | T |
| 0.4932267851774509 | 0.6631739317699282 | 0.2497971636993593 | T | T | T |
| 0.2520401820202749 | 0.0431683745219451 | 0.4164989153136259 | T | T | T |
| 0.1154291953852058 | 0.0526290286818893 | 0.4164359298020878 | T | T | T |
| 0.3326028240485288 | 0.0693016210975998 | 0.4165178815157684 | T | T | T |
| 0.0690982549680758 | 0.0883331044991598 | 0.4163845962803402 | T | T | T |
| 0.4930386224125218 | 0.1759425720972576 | 0.4164865034357054 | T | T | T |
| 0.0386613962406379 | 0.2119730930325296 | 0.4163234920216006 | T | T | T |
| 0.5618222041866158 | 0.2493016642590074 | 0.4164826011982641 | T | T | T |
| 0.0565745269935326 | 0.2904944458788417 | 0.4163209725668872 | T | T | T |
| 0.6533485399952884 | 0.4121895309592964 | 0.4165371439778885 | T | T | T |
| 0.1454769144536246 | 0.4537290098190296 | 0.4159914612400504 | T | T | T |
| 0.6698359259608594 | 0.4901615377627939 | 0.4165230064175898 | T | T | T |
| 0.2142343226311648 | 0.5274520307203719 | 0.4162335530164388 | T | T | T |
| 0.6380103535619659 | 0.6128312463542330 | 0.4164777177078267 | T | T | T |
| 0.3744602046532329 | 0.6312152925494351 | 0.4166985663745377 | T | T | T |
| 0.5915434298897211 | 0.6482899573785312 | 0.4164360975044348 | T | T | T |
| 0.4548625131321686 | 0.6572177075752598 | 0.4166898904999746 | T | T | T |
| 0.2137901817875925 | 0.0377080238490125 | 0.5832960832911600 | T | T | T |
| 0.1450901308392935 | 0.0424814969739219 | 0.5832965648507449 | T | T | T |
| 0.3739475713863299 | 0.0897517255016260 | 0.5833287185229662 | T | T | T |
| 0.0530608777235578 | 0.1132738350811750 | 0.5832659025461683 | T | T | T |
| 0.4547080990917341 | 0.1434167865109551 | 0.5833161946426942 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0379077239811612 | 0.1757094027246743 | 0.5832245384071670 | T | T | T |
| 0.5912834183320932 | 0.2891854499263849 | 0.5832782943262587 | T | T | T |
| 0.0734554886021940 | 0.3315261303793766 | 0.5835136660636282 | T | T | T |
| 0.6372972084257476 | 0.3711604538165309 | 0.5832892518642546 | T | T | T |
| 0.1183717885427508 | 0.4137946610878175 | 0.5843518773312514 | T | T | T |
| 0.6699970796410173 | 0.5260399158925193 | 0.5832788767570939 | T | T | T |
| 0.2514578605323430 | 0.5619171355892866 | 0.5808827578358663 | T | T | T |
| 0.6540101075864629 | 0.5878219391266145 | 0.5831830368979007 | T | T | T |
| 0.3321539585678812 | 0.6111603413567787 | 0.5830237608451903 | T | T | T |
| 0.5618357211474511 | 0.6583933303013136 | 0.5831993775291228 | T | T | T |
| 0.4929758560294287 | 0.6626294301768587 | 0.5833071221667213 | T | T | T |
| 0.2518984176881313 | 0.0430416339632141 | 0.7498888947509439 | T | T | T |
| 0.1155234227299226 | 0.0526751975710790 | 0.7498426700679858 | T | T | T |
| 0.3325982391910923 | 0.0692730559529025 | 0.7499207929665929 | T | T | T |
| 0.4930604450959186 | 0.1759021750299111 | 0.7499377856020345 | T | T | T |
| 0.0388729933022804 | 0.2118477898331547 | 0.7497627037192746 | T | T | T |
| 0.1449286220279087 | 0.4535136568370139 | 0.7497845296908575 | T | T | T |
| 0.2034201036214872 | 0.5388576503136518 | 0.7498378856073556 | T | T | T |
| 0.6380079760405492 | 0.6128627669708043 | 0.7497968299765293 | T | T | T |
| 0.5917725026879836 | 0.6484959877749571 | 0.7497869216756556 | T | T | T |
| 0.0688076308720781 | 0.0881015965486418 | 0.7498151276195804 | T | T | T |
| 0.5618849074930199 | 0.2493534096142478 | 0.7499283260894789 | T | T | T |
| 0.0570343253010661 | 0.2906643551844983 | 0.7497531433387040 | T | T | T |
| 0.6533566324158357 | 0.4121671492700724 | 0.7498828588233888 | T | T | T |
| 0.6698567707416525 | 0.4901594711310608 | 0.7498495741334749 | T | T | T |
| 0.3741425830088733 | 0.6319028171749114 | 0.7497797788340860 | T | T | T |
| 0.4540304145386442 | 0.6566226216230482 | 0.7497806696558140 | T | T | T |
| 0.2137921806480838 | 0.0377083588062166 | 0.9164723552327286 | T | T | T |
| 0.1450897356101068 | 0.0424830741711616 | 0.9164138108234540 | T | T | T |
| 0.3739448100905380 | 0.0897509193403239 | 0.9165218395976673 | T | T | T |
| 0.0530436487229267 | 0.1132673294902083 | 0.9163358939144095 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4547069520655382 | 0.1434158986360021 | 0.9165596011205416 | T | T | T |
| 0.0379005537421827 | 0.1757048777112218 | 0.9163217949844246 | T | T | T |
| 0.5912837332559400 | 0.2891854612215219 | 0.9165600032061360 | T | T | T |
| 0.0734506227626696 | 0.3314976554062463 | 0.9160213966980834 | T | T | T |
| 0.6372971309616623 | 0.3711612386324788 | 0.9164915464537688 | T | T | T |
| 0.1184207443332495 | 0.4137494193310406 | 0.9152013793864737 | T | T | T |
| 0.6699900933725561 | 0.5260355459529613 | 0.9163908176465704 | T | T | T |
| 0.2515183494062960 | 0.5618027929193872 | 0.9186975942163434 | T | T | T |
| 0.6540232896916160 | 0.5878330005033907 | 0.9164311195020216 | T | T | T |
| 0.3321742113083714 | 0.6110610382121658 | 0.9165649356468287 | T | T | T |
| 0.5618330790733134 | 0.6583829988171832 | 0.9163744138769524 | T | T | T |
| 0.4929809026236796 | 0.6626275417322161 | 0.9162547079785031 | T | T | T |
| 0.1562344274329860 | 0.5780057045724678 | 0.7503328624213162 | T | T | T |
| 0.1922655465440666 | 0.6330562693318587 | 0.7428275640311123 | T | T | T |

OH\_CNT(9,9) #### KPOINTS: 1x1x3 #### E= -854.48010460 eV

1.000000000000000

18.1865334800000014 -10.500000000000000 0.000000000000000

0.000000000000000 21.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.4005503900000003

C O H

108 1 1

Selective dynamics

Direct

0.1977386849122746 0.0296608629361326 0.0831987955116355 T T T

0.1349713053876886 0.0388190209941593 0.0832214546684018 T T T

0.3469183375831293 0.0653480415876046 0.0832632605583381 T T T

0.4250999561778844 0.1081926302404842 0.0832869227383430 T T T

0.0502704165279511 0.1096180927706773 0.0831662373420944 T T T

0.0333363142321236 0.1673483696508289 0.0831711404155202 T T T

0.5684546463696549 0.2327735706439890 0.0833009258530203 T T T

0.6256828967328175 0.3076755919067050 0.0833185508579993 T T T

0.0538450485971797 0.3113207156991498 0.0828503494859032 T T T

0.0878396082994083 0.3895789922510636 0.0820706868280216 T T T

0.6956658997738580 0.4631698072043036 0.0833254157030676 T T T

0.7051655882896106 0.5351997869873019 0.0832438751357091 T T T

0.1988480551101686 0.5394994759750225 0.0856164918044271 T T T

0.2720437797855932 0.5981071324585571 0.0835586532498850 T T T

0.6718010843012776 0.6503310286369824 0.0832707202471868 T T T

0.6295215269361660 0.6862274272774314 0.0833368658439802 T T T

0.4284254299173571 0.6832812450960052 0.0831570038468342 T T T

0.5036184107207230 0.7025796253638109 0.0832018369230342 T T T

0.2328846300958551 0.0318741775752374 0.2499775849915178 T T T

0.3078600819342612 0.0498415447319357 0.2500472036643539 T T T

0.4634209930213509 0.1351136228900337 0.2501250775155846 T T T

0.5354557029274466 0.1977146919296318 0.2501355856037291 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0417395325096428 | 0.2729229398842078 | 0.2500934252009751 | T | T | T |
| 0.1094096088031596 | 0.4283042817220543 | 0.2504665767467856 | T | T | T |
| 0.1672074151203667 | 0.5031689380703582 | 0.2501188512578625 | T | T | T |
| 0.3114460532082634 | 0.6247294179391230 | 0.2498662405852669 | T | T | T |
| 0.3894713740873366 | 0.6675833094048451 | 0.2497991023640361 | T | T | T |
| 0.1080966750388762 | 0.0502689314955918 | 0.2501157953087999 | T | T | T |
| 0.0653668874823369 | 0.0857510793479111 | 0.2501157423967941 | T | T | T |
| 0.0315625239916001 | 0.2005484496344449 | 0.2500827960756031 | T | T | T |
| 0.6492317347473708 | 0.3467105405164093 | 0.2500702933432891 | T | T | T |
| 0.6843766263632973 | 0.4248714062419425 | 0.2500092745866934 | T | T | T |
| 0.7034253740427592 | 0.5683492661271925 | 0.2499565264376896 | T | T | T |
| 0.6867591767070257 | 0.6262849222730247 | 0.2499971096860739 | T | T | T |
| 0.6024839804373412 | 0.6975344738661398 | 0.2499112919108166 | T | T | T |
| 0.5392675749082528 | 0.7059364965926456 | 0.2498922645007718 | T | T | T |
| 0.1977785313454919 | 0.0295807420048781 | 0.4166665124633374 | T | T | T |
| 0.1349703269973268 | 0.0388850319732414 | 0.4166664992895334 | T | T | T |
| 0.3468781559174814 | 0.0652591545614174 | 0.4166665335343678 | T | T | T |
| 0.4251510797475977 | 0.1081911941966844 | 0.4166665651057492 | T | T | T |
| 0.0500881651647894 | 0.1094805859320429 | 0.4166664853037461 | T | T | T |
| 0.0329036377229639 | 0.1672548714348763 | 0.4166665434097125 | T | T | T |
| 0.5684537542085099 | 0.2327133626037589 | 0.4166665086562785 | T | T | T |
| 0.6256928871192420 | 0.3076608853289342 | 0.4166664998130197 | T | T | T |
| 0.0523546169793425 | 0.3108680892959240 | 0.4166667812554681 | T | T | T |
| 0.0867244117984031 | 0.3895472216053355 | 0.4166671536529392 | T | T | T |
| 0.6957095764138291 | 0.4631273702357484 | 0.4166664434268607 | T | T | T |
| 0.7051846751780640 | 0.5352213155924236 | 0.4166664185247990 | T | T | T |
| 0.2012592687800973 | 0.5368870276599725 | 0.4166673802625915 | T | T | T |
| 0.2735166276948525 | 0.5985979110055653 | 0.4166670800645796 | T | T | T |
| 0.6717014708087251 | 0.6502311989230860 | 0.4166664091904138 | T | T | T |
| 0.6293150537859227 | 0.6860732007922546 | 0.4166663756264180 | T | T | T |
| 0.4285722905848567 | 0.6838383783255438 | 0.4166670181200773 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5039600478372163 | 0.7032237051640169 | 0.4166666496119230 | T | T | T |
| 0.2328846131900237 | 0.0318741731602443 | 0.5833554195429765 | T | T | T |
| 0.3078600678521223 | 0.0498415397924277 | 0.5832858416036352 | T | T | T |
| 0.1080966711704947 | 0.0502689114019399 | 0.5832171191148749 | T | T | T |
| 0.0653669545223021 | 0.0857510993901722 | 0.5832171339663325 | T | T | T |
| 0.4634209994640435 | 0.1351136231651452 | 0.5832080097053366 | T | T | T |
| 0.5354557103838273 | 0.1977147003928371 | 0.5831974660071737 | T | T | T |
| 0.0315624986239755 | 0.2005484430677609 | 0.5832503396233566 | T | T | T |
| 0.0417394540127623 | 0.2729229590342685 | 0.5832400206916895 | T | T | T |
| 0.6492317331493627 | 0.3467105363578633 | 0.5832627534171494 | T | T | T |
| 0.6843766341589258 | 0.4248714196565703 | 0.5833236771187064 | T | T | T |
| 0.1094090305945042 | 0.4283046762432564 | 0.5828675934795758 | T | T | T |
| 0.1672065575947291 | 0.5031696879149480 | 0.5832161063430316 | T | T | T |
| 0.7034253933410366 | 0.5683492604752667 | 0.5833763205027385 | T | T | T |
| 0.6867592065130144 | 0.6262849382654806 | 0.5833357046452646 | T | T | T |
| 0.3114458099644075 | 0.6247299561494513 | 0.5834679513413380 | T | T | T |
| 0.3894712417669738 | 0.6675835697196280 | 0.5835347564256744 | T | T | T |
| 0.6024839793011305 | 0.6975344740556637 | 0.5834215123167354 | T | T | T |
| 0.5392675833980066 | 0.7059365173246929 | 0.5834408120653461 | T | T | T |
| 0.1977386726098733 | 0.0296608527643609 | 0.7501341016544725 | T | T | T |
| 0.1349712770958977 | 0.0388189599414802 | 0.7501113777820585 | T | T | T |
| 0.3469183125911783 | 0.0653480326144778 | 0.7500698087465001 | T | T | T |
| 0.4250999382641627 | 0.1081926166328216 | 0.7500461466781499 | T | T | T |
| 0.5684546419763998 | 0.2327735717743621 | 0.7500321652608405 | T | T | T |
| 0.0538450131545959 | 0.3113208372102506 | 0.7504832380226008 | T | T | T |
| 0.0878392825644812 | 0.3895792256857988 | 0.7512630934081557 | T | T | T |
| 0.1988467892104004 | 0.5395007065710959 | 0.7477181038307592 | T | T | T |
| 0.2720432784207319 | 0.5981078977854456 | 0.7497754949328187 | T | T | T |
| 0.4284253967963999 | 0.6832813561700603 | 0.7501764593443875 | T | T | T |
| 0.0502704972706951 | 0.1096181243564961 | 0.7501666197713559 | T | T | T |
| 0.0333363478212020 | 0.1673483462038596 | 0.7501616905730139 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6256828882524693 | 0.3076755849185622 | 0.7500144816897035 | T | T | T |
| 0.6956659000507823 | 0.4631698193683447 | 0.7500075357154589 | T | T | T |
| 0.7051655873513701 | 0.5351997881773776 | 0.7500890000466267 | T | T | T |
| 0.6718010779208111 | 0.6503310383820928 | 0.7500620884805016 | T | T | T |
| 0.6295214869870516 | 0.6862274036689634 | 0.7499959327986445 | T | T | T |
| 0.5036183722281979 | 0.7025795957459595 | 0.7501312437492174 | T | T | T |
| 0.2327953209653871 | 0.0318278298624428 | 0.9166664808832207 | T | T | T |
| 0.3078850295951359 | 0.0498204544872372 | 0.9166665368116391 | T | T | T |
| 0.1079893519403909 | 0.0500743030473707 | 0.9166664235649832 | T | T | T |
| 0.0653411041868034 | 0.0857541384877530 | 0.9166664739532236 | T | T | T |
| 0.4633826813894928 | 0.1350239404506168 | 0.9166665251116155 | T | T | T |
| 0.5354729903219365 | 0.1976989134924706 | 0.9166665492490929 | T | T | T |
| 0.0317529100155747 | 0.2004378935990512 | 0.9166664026980825 | T | T | T |
| 0.0421928211142450 | 0.2731019456520322 | 0.9166665224536538 | T | T | T |
| 0.6492764108806173 | 0.3467035747643507 | 0.9166664964916600 | T | T | T |
| 0.6844092448261411 | 0.4249326213894225 | 0.9166664621340916 | T | T | T |
| 0.1085948845351780 | 0.4280618706046002 | 0.9166670352895764 | T | T | T |
| 0.1536477520622269 | 0.5109746288587868 | 0.9166684646081571 | T | T | T |
| 0.7033902010674746 | 0.5683785174850575 | 0.9166664378905894 | T | T | T |
| 0.6867075936236212 | 0.6262563742339304 | 0.9166663879969037 | T | T | T |
| 0.3109833710601901 | 0.6253056447233450 | 0.9166668867815690 | T | T | T |
| 0.3887718309152096 | 0.6669499612411605 | 0.9166667657372717 | T | T | T |
| 0.6024094394872144 | 0.6973882271884031 | 0.9166664397278641 | T | T | T |
| 0.5391683914197909 | 0.7054988276680935 | 0.9166665358044834 | T | T | T |
| 0.0975378114453897 | 0.5354178794143267 | 0.9166780088246024 | T | T | T |
| 0.1245804812594585 | 0.5887771675294718 | 0.9166652570906475 | T | T | T |

OH\_CNT(10,10) #### KPOINTS: 1x1x3 #### E= -949.73471481 eV

1.0000000000000000

19.0525588799999994 -11.0000000000000000 0.0000000000000000

0.0000000000000000 22.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4010841699999999

C O H

120 1 1

Selective dynamics

Direct

0.1873354162685884 0.0242405265649450 0.0833314975256133 T T T

0.2542045657841909 0.0286110972938201 0.0833315814920609 T T T

0.0819715158154247 0.0625048328725686 0.0833312902608184 T T T

0.4013108671824758 0.0831849079873211 0.0833320076077595 T T T

0.0478211469991050 0.1031711071695134 0.0833306319742209 T T T

0.4750480516513133 0.1310295532446328 0.0833326250947800 T T T

0.0252204375228829 0.2191346360786529 0.0833301337345801 T T T

0.6065581490236047 0.2570289289569505 0.0833327415638620 T T T

0.0372935175168777 0.2893002006195809 0.0833305028675751 T T T

0.6586169445104889 0.3295811371751790 0.0833326898414634 T T T

0.1004411325871012 0.4373383300617098 0.0833305036993015 T T T

0.7247822635358770 0.4781225820754010 0.0833322621821928 T T T

0.1409211543808029 0.5165301389842820 0.0833284532551692 T T T

0.7360402148319395 0.5477324029944709 0.0833319701358901 T T T

0.2871596953315596 0.6344039015015661 0.0833312296891755 T T T

0.7124097321558496 0.6632512462939782 0.0833314160805563 T T T

0.3604087266030922 0.6820422792307184 0.0833310429533164 T T T

0.6792288311464534 0.7046720598670196 0.0833313728112231 T T T

0.5086893322870616 0.7407305621956374 0.0833305110464253 T T T

0.5754962306100281 0.7453228020544079 0.0833307675934571 T T T

0.0365037361466824 0.1284187635541096 0.2499312396980732 T T T

0.5765490769128583 0.2225414375122799 0.2499670146296868 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0488890153764465 | 0.3258970328458827 | 0.2495265843304941 | T | T | T |
| 0.0812747177647166 | 0.4006079656717798 | 0.2488065652467349 | T | T | T |
| 0.1836819837749409 | 0.5454119936883252 | 0.2522229682698747 | T | T | T |
| 0.7358226025254363 | 0.5801162759536275 | 0.2498855072022885 | T | T | T |
| 0.2511918705112024 | 0.6054377297695982 | 0.2502631463645810 | T | T | T |
| 0.3984170678361959 | 0.7024175614027487 | 0.2499292572636824 | T | T | T |
| 0.6576721548892248 | 0.7205344833167597 | 0.2500284459165583 | T | T | T |
| 0.6057083416702732 | 0.7410224143572933 | 0.2500420522944555 | T | T | T |
| 0.1569916046321086 | 0.0281154526550632 | 0.2498561029139421 | T | T | T |
| 0.2899595730968632 | 0.0367251192352359 | 0.2499013201001462 | T | T | T |
| 0.1040563406309578 | 0.0473559359273117 | 0.2499383268882783 | T | T | T |
| 0.3638564217921166 | 0.0641474369086773 | 0.2499240799855407 | T | T | T |
| 0.5104980162876225 | 0.1592558154498274 | 0.2499789083104814 | T | T | T |
| 0.0251159605910122 | 0.1867178164101320 | 0.2498731071641081 | T | T | T |
| 0.6801999636112296 | 0.3668908600968771 | 0.2499650306855208 | T | T | T |
| 0.7134265220754314 | 0.4414878197787140 | 0.2499595179881995 | T | T | T |
| 0.7238849136861842 | 0.6380647807165980 | 0.2499379090279858 | T | T | T |
| 0.4725042614986341 | 0.7317134623949416 | 0.2498795194128985 | T | T | T |
| 0.1874089348283355 | 0.0243187107797488 | 0.4167327619486672 | T | T | T |
| 0.2541904036851923 | 0.0286285297614255 | 0.4167234889977556 | T | T | T |
| 0.0819960548541210 | 0.0625911347784588 | 0.4167941383739414 | T | T | T |
| 0.4013545784601101 | 0.0832554445642851 | 0.4166792065703701 | T | T | T |
| 0.0481792431194247 | 0.1033954585542880 | 0.4167906216655445 | T | T | T |
| 0.4750065479654468 | 0.1310194950210682 | 0.4167157437156790 | T | T | T |
| 0.0252606036920629 | 0.2193442985868947 | 0.4168285979312988 | T | T | T |
| 0.6065531689890155 | 0.2570635112173776 | 0.4166979031305564 | T | T | T |
| 0.0369857199083084 | 0.2892091183897643 | 0.4168129369506882 | T | T | T |
| 0.6585749501938490 | 0.3295431413657881 | 0.4166862066001498 | T | T | T |
| 0.1016230752672030 | 0.4376018144465826 | 0.4170592470738733 | T | T | T |
| 0.7247748409873431 | 0.4781283451312294 | 0.4167081965302618 | T | T | T |
| 0.1550239154442670 | 0.5098604878817827 | 0.4167345829233609 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7360280685990684 | 0.5477450531684284 | 0.4166800125919322 | T | T | T |
| 0.2877560428812851 | 0.6335170244813135 | 0.4165285437145079 | T | T | T |
| 0.7124100521416735 | 0.6632597811168531 | 0.4166527616180148 | T | T | T |
| 0.3610210514323762 | 0.6822903053338422 | 0.4164399929521422 | T | T | T |
| 0.6792187395823321 | 0.7046776291459569 | 0.4166573251221775 | T | T | T |
| 0.5084912023186822 | 0.7404168270135180 | 0.4166641441516882 | T | T | T |
| 0.5754174174570267 | 0.7450511480166454 | 0.4166883670158349 | T | T | T |
| 0.1569872413141026 | 0.0280688110956942 | 0.5833311838742408 | T | T | T |
| 0.2898947537503078 | 0.0366468827251582 | 0.5833315886719398 | T | T | T |
| 0.1039031718522795 | 0.0472395085418096 | 0.5833312806484084 | T | T | T |
| 0.3638975622011376 | 0.0641446264610483 | 0.5833320202667606 | T | T | T |
| 0.0365693441962396 | 0.1284572530174955 | 0.5833303758555006 | T | T | T |
| 0.5104900091066266 | 0.1592043143630923 | 0.5833326169534681 | T | T | T |
| 0.0248144225517438 | 0.1867014972463424 | 0.5833297999923031 | T | T | T |
| 0.5765984226783641 | 0.2225697655581149 | 0.5833328309897112 | T | T | T |
| 0.0475960704984195 | 0.3255034807636553 | 0.5833309635455818 | T | T | T |
| 0.6802059516687309 | 0.3668494799258133 | 0.5833326560121526 | T | T | T |
| 0.0804139886042167 | 0.4006292419223561 | 0.5833311293614447 | T | T | T |
| 0.7134545869832762 | 0.4415010831627106 | 0.5833324363726686 | T | T | T |
| 0.1863523090630524 | 0.5430128675276745 | 0.5833293502020462 | T | T | T |
| 0.7358330157515069 | 0.5801128946700591 | 0.5833317348780549 | T | T | T |
| 0.2526671501779031 | 0.6056581847932577 | 0.5833305837317886 | T | T | T |
| 0.7239061338436910 | 0.6380860964812937 | 0.5833314661029043 | T | T | T |
| 0.3984554226995868 | 0.7023699238472791 | 0.5833308236300868 | T | T | T |
| 0.6577665991633648 | 0.7206206562278620 | 0.5833313250956595 | T | T | T |
| 0.4726196876634648 | 0.7317991223221122 | 0.5833301572470062 | T | T | T |
| 0.6056913217411646 | 0.7410275289630133 | 0.5833306567811696 | T | T | T |
| 0.0819961674480304 | 0.0625910707075886 | 0.7498679795400762 | T | T | T |
| 0.0481794830953880 | 0.1033955020484592 | 0.7498706343618615 | T | T | T |
| 0.6065531741472354 | 0.2570635234412708 | 0.7499676906501727 | T | T | T |
| 0.1016216698168726 | 0.4376025335112364 | 0.7496020235078749 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7360281489892496 | 0.5477450751921088 | 0.7499837066571289 | T | T | T |
| 0.2877557701896813 | 0.6335189305623719 | 0.7501325064391205 | T | T | T |
| 0.3610212972170752 | 0.6822910256087428 | 0.7502213778817680 | T | T | T |
| 0.6792187921144762 | 0.7046776880122447 | 0.7500052521023349 | T | T | T |
| 0.5754176231311618 | 0.7450517164431072 | 0.7499728029782363 | T | T | T |
| 0.1874088920713965 | 0.0243188461301392 | 0.7499299234049290 | T | T | T |
| 0.2541903430107196 | 0.0286286402690783 | 0.7499398138829465 | T | T | T |
| 0.4013546420995637 | 0.0832556135942622 | 0.7499850089505550 | T | T | T |
| 0.4750065937936859 | 0.1310195664821377 | 0.7499493077713842 | T | T | T |
| 0.0252596740396569 | 0.2193438504165420 | 0.7498316085496359 | T | T | T |
| 0.0369854636547072 | 0.2892088534771297 | 0.7498479343078529 | T | T | T |
| 0.6585749669732734 | 0.3295431332248120 | 0.7499791523113039 | T | T | T |
| 0.7247748204283880 | 0.4781283561666679 | 0.7499562117064881 | T | T | T |
| 0.1550229378927376 | 0.5098613943358467 | 0.7499243120141321 | T | T | T |
| 0.7124101345087070 | 0.6632598886963441 | 0.7500103417575400 | T | T | T |
| 0.5084915281030133 | 0.7404179784853613 | 0.7499965243154411 | T | T | T |
| 0.1569915960516629 | 0.0281154992284911 | 0.9168066304942368 | T | T | T |
| 0.2899596995248611 | 0.0367254333689246 | 0.9167615984927184 | T | T | T |
| 0.1040563065339504 | 0.0473560042395835 | 0.9167241559773160 | T | T | T |
| 0.3638565087641638 | 0.0641476256672583 | 0.9167396529121494 | T | T | T |
| 0.0365040260669835 | 0.1284188804909142 | 0.9167299176909485 | T | T | T |
| 0.5104979583818334 | 0.1592557776255471 | 0.9166864290922506 | T | T | T |
| 0.0251155611111063 | 0.1867175380561621 | 0.9167875885507802 | T | T | T |
| 0.5765490260973930 | 0.2225413938910838 | 0.9166984916812736 | T | T | T |
| 0.0488889693136712 | 0.3258970649880667 | 0.9171344998069013 | T | T | T |
| 0.6801999894221487 | 0.3668908702098153 | 0.9167001271488062 | T | T | T |
| 0.0812740952613432 | 0.4006081009972250 | 0.9178544308110831 | T | T | T |
| 0.7134265320755321 | 0.4414878585633882 | 0.9167050586484685 | T | T | T |
| 0.1836827275019806 | 0.5454124239868415 | 0.9144354908310950 | T | T | T |
| 0.7358227145062350 | 0.5801163351223048 | 0.9167781801365767 | T | T | T |
| 0.2511919186040708 | 0.6054393993413693 | 0.9163976148207904 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7238849893476229 | 0.6380647408292619 | 0.9167250829318225 | T | T | T |
| 0.3984171013192867 | 0.7024176470438754 | 0.9167326524837369 | T | T | T |
| 0.6576719505269056 | 0.7205342577104917 | 0.9166338275324930 | T | T | T |
| 0.4725044308350216 | 0.7317140454392363 | 0.9167813068492738 | T | T | T |
| 0.6057082386100315 | 0.7410223262036143 | 0.9166193157395013 | T | T | T |
| 0.0848420907191429 | 0.5367139810760256 | 0.0833180237301750 | T | T | T |
| 0.1087896665127477 | 0.5875937798818818 | 0.0832542156555042 | T | T | T |

OH\_CNT(8,0) #### KPOINTS: 2x2x2 #### E= -500.33641137 eV

1.000000000000000

12.9903810600000007 -7.500000000000000 0.000000000000000

0.000000000000000 15.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 8.5305455000000006

C O H

64 1 1

Selective dynamics

Direct

0.0765620419424461 0.1914099968539201 0.0835676641281699 T T T

0.4965020824336276 0.2637285863220668 0.0845764640723339 T T T

0.1348381200885198 0.3754250021241738 0.0823878173108412 T T T

0.5586872493013187 0.4479447871165604 0.0847249675484320 T T T

0.1526325091706090 0.0811379555617063 0.0847728172685528 T T T

0.3270863228666213 0.1092974954195756 0.0844815052084610 T T T

0.3041959061544208 0.5282755874554874 0.0825212535502018 T T T

0.4786285485826038 0.5545681784399884 0.0836169654427835 T T T

0.2326095917315485 0.0761392887912025 0.1682161919818976 T T T

0.0970607820605278 0.1207076107881227 0.1679370242837126 T T T

0.4194648309549206 0.1763977419103254 0.1680544647794218 T T T

0.2101484272794116 0.4645988695095115 0.1672406155683676 T T T

0.5364139567594763 0.5173441614678251 0.1680141578429590 T T T

0.3977329722547556 0.5576168254181769 0.1663957246392902 T T T

0.0902834017585425 0.2798338140086808 0.1663860742205091 T T T

0.5452874170416862 0.3594956192636071 0.1681628027031369 T T T

0.0896435621155651 0.2796352496385906 0.3333834701788144 T T T

0.5453102302623883 0.3595429313509633 0.3346719997276884 T T T

0.2326149001204287 0.0762382034926352 0.3346065775664506 T T T

0.0969136499527213 0.1209621072559594 0.3339646595678711 T T T

0.4195375939430171 0.1763205951625136 0.3350728968132495 T T T

0.2107809300671223 0.4636328736420399 0.3315302302998840 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5362524371130867 | 0.5175228453494318 | 0.3339142959200690 | T | T | T |
| 0.3979511780876571 | 0.5581291889165328 | 0.3334104250962301 | T | T | T |
| 0.1530180828280858 | 0.0818364951703171 | 0.4177587318247466 | T | T | T |
| 0.3271848456048544 | 0.1094705184369879 | 0.4185035571314972 | T | T | T |
| 0.3043086616284272 | 0.5276242916577563 | 0.4161786652801002 | T | T | T |
| 0.4787161217201100 | 0.5550874609825597 | 0.4172341234428554 | T | T | T |
| 0.0758081217075429 | 0.1913282608688260 | 0.4172818145331380 | T | T | T |
| 0.4963836492357527 | 0.2636276650886638 | 0.4183686847921591 | T | T | T |
| 0.1353329087912948 | 0.3750586887171674 | 0.4162510172875364 | T | T | T |
| 0.5582625083171631 | 0.4477825051274256 | 0.4177548711141724 | T | T | T |
| 0.0765657220571562 | 0.1923539946041255 | 0.5843778566346053 | T | T | T |
| 0.4964860175462973 | 0.2636146433958142 | 0.5845581549606101 | T | T | T |
| 0.1354412815363730 | 0.3763793295608353 | 0.5823345663258118 | T | T | T |
| 0.5580510080543042 | 0.4477348374613391 | 0.5847667681470511 | T | T | T |
| 0.1530930828955789 | 0.0820486212607288 | 0.5848581907180375 | T | T | T |
| 0.3271966037072276 | 0.1093256926739934 | 0.5844840017106681 | T | T | T |
| 0.3030677842880405 | 0.5276063785034705 | 0.5824346164508472 | T | T | T |
| 0.4776095042700062 | 0.5543855921306716 | 0.5843168238736610 | T | T | T |
| 0.2328163545260913 | 0.0764014233488156 | 0.6682545844848055 | T | T | T |
| 0.0979402413144997 | 0.1217671944508013 | 0.6680440617705867 | T | T | T |
| 0.4197161315359788 | 0.1760698393709025 | 0.6681472163171974 | T | T | T |
| 0.2094166782122284 | 0.4653164499757801 | 0.6633828069792442 | T | T | T |
| 0.5353874271251198 | 0.5166011802667480 | 0.6680465366384091 | T | T | T |
| 0.3971304022094939 | 0.5574679411953581 | 0.6670960361431153 | T | T | T |
| 0.0901600764556949 | 0.2804399629746799 | 0.6671003115689843 | T | T | T |
| 0.5449542690753121 | 0.3593143542732020 | 0.6681644895904663 | T | T | T |
| 0.0931059582933006 | 0.2819393908591767 | 0.8347460584854915 | T | T | T |
| 0.5451180658036106 | 0.3592635594400442 | 0.8344910725772477 | T | T | T |
| 0.2327900807107155 | 0.0760677052394413 | 0.8344487337310390 | T | T | T |
| 0.0980585639658264 | 0.1216386250934537 | 0.8339334612588478 | T | T | T |
| 0.4198376745556285 | 0.1759548673183096 | 0.8350458613275336 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1999877452096849 | 0.4780238342662576 | 0.8355490368340183 | T | T | T |
| 0.5354642062845834 | 0.5165197850994179 | 0.8338399744050082 | T | T | T |
| 0.3952700221078069 | 0.5546900341038946 | 0.8347028937930254 | T | T | T |
| 0.1530087887001743 | 0.0814180824200604 | 0.9177401777333778 | T | T | T |
| 0.3272625662265993 | 0.1091963355255377 | 0.9184323640393321 | T | T | T |
| 0.3039122249445608 | 0.5290998387247189 | 0.9178581210235999 | T | T | T |
| 0.4775784580938073 | 0.5533580966694733 | 0.9174783980573972 | T | T | T |
| 0.0778192809277972 | 0.1923147767438455 | 0.9174521336043443 | T | T | T |
| 0.4964907540800170 | 0.2635359201566211 | 0.9183578959384859 | T | T | T |
| 0.1339276588751175 | 0.3758077958820066 | 0.9179345960086206 | T | T | T |
| 0.5583561773641220 | 0.4476025651647385 | 0.9177759538228918 | T | T | T |
| 0.1475024495955310 | 0.5385613192281765 | 0.8544616419845015 | T | T | T |
| 0.1923812114434703 | 0.6058425598462340 | 0.8090320719356199 | T | T | T |

OH\_CNT(9,0) #### KPOINTS: 2x2x2 #### E= -564.55034530 eV

1.000000000000000

13.8564064600000005 -8.000000000000000 0.000000000000000

0.000000000000000 16.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 8.5367054200000005

C O H

72 1 1

Selective dynamics

Direct

0.1948699838841918 0.0653484591572292 0.0834065128064446 T T T

0.0830557354611345 0.1274424231422659 0.0832994317199829 T T T

0.3683947340929360 0.1253872450653410 0.0831776722917581 T T T

0.0843355529986128 0.2811233339194214 0.0839193317754360 T T T

0.5214207507796653 0.2779515588170195 0.0831773840223407 T T T

0.1933631469020495 0.4562102079333608 0.0872164999436656 T T T

0.5843928493293553 0.4519536584677030 0.0834419039555352 T T T

0.3692970386699992 0.5624989130588340 0.0838611664832744 T T T

0.5233512884463231 0.5644018614126444 0.0833021208343657 T T T

0.1270522109967841 0.0818820619284983 0.1670129741232718 T T T

0.2786505539249967 0.0799971319621063 0.1671616040364653 T T T

0.4521224555773505 0.1944377396249218 0.1666698172100959 T T T

0.0692110138374884 0.1976788857687944 0.1666641482867763 T T T

0.5678535250212234 0.3676505741443161 0.1670844548389699 T T T

0.1274675052977010 0.3712043166401449 0.1684282977360913 T T T

0.5692533257794379 0.5207542625388215 0.1671846551567726 T T T

0.2790897277354597 0.5203478771088579 0.1681946599604556 T T T

0.4525991128050363 0.5773715537526579 0.1666311058538952 T T T

0.1269317421495479 0.0814849720861851 0.3334472855029964 T T T

0.2787228585737115 0.0801056537244740 0.3329607691943808 T T T

0.4520909852400593 0.1945727331036636 0.3334619818890012 T T T

0.0684628214867442 0.1965335704466966 0.3339252916268178 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5678462577085822 | 0.3676804836920745 | 0.3330765007638714 | T | T | T |
| 0.1275886021778028 | 0.3699171067776538 | 0.3344921126053297 | T | T | T |
| 0.5695901131166219 | 0.5208885958842439 | 0.3333269345028374 | T | T | T |
| 0.2804042575695009 | 0.5203563325867610 | 0.3345017184996110 | T | T | T |
| 0.4536600774275511 | 0.5780876200910545 | 0.3339773731678532 | T | T | T |
| 0.1947794760972163 | 0.0652349717798118 | 0.4167458545711135 | T | T | T |
| 0.0824417229249605 | 0.1268735584539502 | 0.4173224302019625 | T | T | T |
| 0.3683710193597338 | 0.1256616699671464 | 0.4169748970515382 | T | T | T |
| 0.0845751380223281 | 0.2804658262131489 | 0.4177551052553854 | T | T | T |
| 0.5213673160707811 | 0.2781366074921175 | 0.4169395192085690 | T | T | T |
| 0.1955963207451164 | 0.4539936829691155 | 0.4192398137366525 | T | T | T |
| 0.5845400677108719 | 0.4521978257312688 | 0.4167528381209184 | T | T | T |
| 0.3697492684268210 | 0.5621670528415315 | 0.4177790814435853 | T | T | T |
| 0.5237543009749167 | 0.5649796391564077 | 0.4173571818463773 | T | T | T |
| 0.1947961767418202 | 0.0651192624171283 | 0.5834857102887668 | T | T | T |
| 0.0826282337414450 | 0.1267712046532519 | 0.5832590754163032 | T | T | T |
| 0.3683782083757968 | 0.1255443179306948 | 0.5831266730990928 | T | T | T |
| 0.0851363729312908 | 0.2806993771328279 | 0.5845400706282218 | T | T | T |
| 0.5213813080712645 | 0.2780103834605035 | 0.5830991888863127 | T | T | T |
| 0.1948296053640676 | 0.4548523907379186 | 0.5837183583140283 | T | T | T |
| 0.5845572918033086 | 0.4520497026153567 | 0.5834691098263729 | T | T | T |
| 0.3695807293487412 | 0.5617890486391972 | 0.5845927887429819 | T | T | T |
| 0.5238826970234765 | 0.5647942220447719 | 0.5833008309628684 | T | T | T |
| 0.1267230447717067 | 0.0811808860084878 | 0.6670429240300768 | T | T | T |
| 0.2785699425753051 | 0.0797660268063684 | 0.6671236766365127 | T | T | T |
| 0.4520356380759915 | 0.1945301459789960 | 0.6665734265059882 | T | T | T |
| 0.0695351322428683 | 0.1968982044098833 | 0.6675937238783195 | T | T | T |
| 0.5679988409593609 | 0.3677163375114408 | 0.6669937376245570 | T | T | T |
| 0.1270823322977805 | 0.3701370697949812 | 0.6687333606002096 | T | T | T |
| 0.5697803217349556 | 0.5210032410489251 | 0.6672078506502718 | T | T | T |
| 0.2801412513329886 | 0.5211084464204596 | 0.6686220096696541 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4532956319581291 | 0.5770988289042300 | 0.6676049831099677 | T | T | T |
| 0.1267982183180544 | 0.0811570305128422 | 0.8334405003337393 | T | T | T |
| 0.2785901808920264 | 0.0796926132711187 | 0.8329993463314055 | T | T | T |
| 0.4520134932101100 | 0.1943745322902295 | 0.8334604999297749 | T | T | T |
| 0.0706742617509940 | 0.1977300824311555 | 0.8339013223154061 | T | T | T |
| 0.5679502389732131 | 0.3675805943839246 | 0.8330974106374265 | T | T | T |
| 0.1258656858782766 | 0.3705652226615891 | 0.8330669695736466 | T | T | T |
| 0.5698199982556765 | 0.5209308460057840 | 0.8333085134017530 | T | T | T |
| 0.2795575035317914 | 0.5223232745992361 | 0.8332394468605409 | T | T | T |
| 0.4524845491893106 | 0.5760437884616371 | 0.8340131907790674 | T | T | T |
| 0.1947856862068769 | 0.0649655323096973 | 0.9167707060733750 | T | T | T |
| 0.0834690869484013 | 0.1274870524122702 | 0.9176325221034055 | T | T | T |
| 0.3683358917095874 | 0.1252941589475883 | 0.9169759718180410 | T | T | T |
| 0.0873469766268382 | 0.2825640507315270 | 0.9167516708872880 | T | T | T |
| 0.5213923903765521 | 0.2779281671101085 | 0.9169376759588515 | T | T | T |
| 0.1826525096086722 | 0.4669170725165006 | 0.9152667988179974 | T | T | T |
| 0.5846573545520576 | 0.4520343843483267 | 0.9167985784949684 | T | T | T |
| 0.3677359159873463 | 0.5596666796646260 | 0.9168357316302277 | T | T | T |
| 0.5231788507758617 | 0.5639998602709944 | 0.9176837110684574 | T | T | T |
| 0.1253092306861696 | 0.5159939510550572 | 0.8955501442558643 | T | T | T |
| 0.1666022240973138 | 0.5828639408160782 | 0.9255313596338813 | T | T | T |

OH\_CNT(10,0) ### KPOINTS: 2x2x2 ### E= -628.90946342 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C O H

80 1 1

Selective dynamics

Direct

0.2396845975332158 0.0617873065718006 0.0835080551440288 T T T

0.1081973020714247 0.0836851898452233 0.0834703661263518 T T T

0.4057180997540802 0.1426814276604082 0.0837536471674075 T T T

0.5434037438120397 0.2924367715556773 0.0837511132532200 T T T

0.1129574965776685 0.3610244288425421 0.0818417025906080 T T T

0.2495234021520658 0.5108158418896054 0.0819650976016648 T T T

0.5490943480099613 0.5671758839422651 0.0835434413701146 T T T

0.4152672316470638 0.5856145754286027 0.0826668763560982 T T T

0.0622971473227244 0.1988762834029572 0.0825912952793659 T T T

0.6000031449781743 0.4558440329931074 0.0835945000609594 T T T

0.1658316386679064 0.0597117639596458 0.1667834817556392 T T T

0.4817844213947450 0.2119128035330276 0.1672482721927526 T T T

0.1724060764443243 0.4426218396415093 0.1664417609497095 T T T

0.4900129369187086 0.5893721535201836 0.1666191385208699 T T T

0.3226832340011873 0.0909973168160423 0.1669066166456900 T T T

0.0723365920134132 0.1315152566428423 0.1666415414542877 T T T

0.0765653442737975 0.2774052767284416 0.1655714574457923 T T T

0.5842907506186296 0.3762871717097215 0.1669436784699379 T T T

0.5872175167049839 0.5214739685329264 0.1669251702941155 T T T

0.3331279466224617 0.5587903578399430 0.1655756244652593 T T T

0.3227844780408907 0.0912781295238004 0.3336939192445323 T T T

0.0719942665079483 0.1315463109895699 0.3332270450816844 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0762793628824942 | 0.2772828953380027 | 0.3326577266341521 | T | T | T |
| 0.5841636376052910 | 0.3761575179327639 | 0.3336864156594713 | T | T | T |
| 0.5869396352826618 | 0.5214826408340342 | 0.3335415541117073 | T | T | T |
| 0.3332316297658864 | 0.5591199261288374 | 0.3327303759012330 | T | T | T |
| 0.1657226725802830 | 0.0598575003532248 | 0.3334722354046802 | T | T | T |
| 0.4820681200509022 | 0.2117575510161941 | 0.3336547152867121 | T | T | T |
| 0.1733003277688886 | 0.4419400714768793 | 0.3309729076734679 | T | T | T |
| 0.4898681899538845 | 0.5896470911090919 | 0.3332649223308767 | T | T | T |
| 0.0615041589461051 | 0.1986044038070766 | 0.4163323130801226 | T | T | T |
| 0.5992267611141361 | 0.4553360038972772 | 0.4171055992398724 | T | T | T |
| 0.2399854399921435 | 0.0624295110767869 | 0.4170984581064185 | T | T | T |
| 0.1082802338279910 | 0.0838453897341806 | 0.4165922185219362 | T | T | T |
| 0.4058797619604693 | 0.1427424777794495 | 0.4169319647066552 | T | T | T |
| 0.5437411593963238 | 0.2922367168553850 | 0.4169317635914760 | T | T | T |
| 0.1137479402774767 | 0.3609103638692933 | 0.4154720487382572 | T | T | T |
| 0.2497745826669037 | 0.5102321120979216 | 0.4154148775297713 | T | T | T |
| 0.5488762242970401 | 0.5670387342599648 | 0.4165795576494037 | T | T | T |
| 0.4154784490338264 | 0.5865490096463700 | 0.4163143303434365 | T | T | T |
| 0.2397830853452759 | 0.0619683053668121 | 0.5834219848655404 | T | T | T |
| 0.1084687267499384 | 0.0841751869419576 | 0.5835862583546758 | T | T | T |
| 0.4057544817912617 | 0.1427127304555821 | 0.5837521760145370 | T | T | T |
| 0.5437075979151226 | 0.2924034157721834 | 0.5837084618484121 | T | T | T |
| 0.1132246758743480 | 0.3621513539169664 | 0.5821173981493202 | T | T | T |
| 0.2483312361187416 | 0.5101465024856325 | 0.5822297164365936 | T | T | T |
| 0.5486067250215534 | 0.5668089484434905 | 0.5835778082729401 | T | T | T |
| 0.4143803308565492 | 0.5854754185639975 | 0.5834924614837212 | T | T | T |
| 0.0621221171187330 | 0.1996712194625291 | 0.5834793176607848 | T | T | T |
| 0.5997525380003009 | 0.4556289978644288 | 0.5833901833280826 | T | T | T |
| 0.1657489375092373 | 0.0595962904665563 | 0.6668179528206405 | T | T | T |
| 0.4816822996254584 | 0.2121115611822970 | 0.6671294112958136 | T | T | T |
| 0.1705629838809554 | 0.4438574601173615 | 0.6629017069119929 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4891184466089433 | 0.5882857752553839 | 0.6668832814322574 | T | T | T |
| 0.3226394547654304 | 0.0908427809228358 | 0.6668626913901727 | T | T | T |
| 0.0731182338704810 | 0.1324224597892029 | 0.6669084963758565 | T | T | T |
| 0.0754551678048663 | 0.2777774693799944 | 0.6659799030888792 | T | T | T |
| 0.5845996239658958 | 0.3763993837098677 | 0.6668711996062791 | T | T | T |
| 0.5872918068585915 | 0.5215136166859274 | 0.6667797581852037 | T | T | T |
| 0.3325612826591908 | 0.5592687142832320 | 0.6660499790871360 | T | T | T |
| 0.3226413556458353 | 0.0907139758658440 | 0.8337677549915555 | T | T | T |
| 0.0734037725294175 | 0.1324675478520885 | 0.8330546991634458 | T | T | T |
| 0.0778971983789237 | 0.2790521408021856 | 0.8336516058682149 | T | T | T |
| 0.5846879971563713 | 0.3765183549557169 | 0.8337895583723111 | T | T | T |
| 0.5876236523905466 | 0.5217699081874331 | 0.8333729887596724 | T | T | T |
| 0.3316238055193676 | 0.5568691381145020 | 0.8336575811493236 | T | T | T |
| 0.1656565474198065 | 0.0593251133129539 | 0.8334117267665057 | T | T | T |
| 0.4816495972967406 | 0.2121507267970273 | 0.8336347052105555 | T | T | T |
| 0.1590145601024222 | 0.4523776052426077 | 0.8349155490674532 | T | T | T |
| 0.4890811751739022 | 0.5879668241406677 | 0.8330849862013127 | T | T | T |
| 0.0633330440633410 | 0.1996809941677490 | 0.9163648218642753 | T | T | T |
| 0.6001725492290906 | 0.4558824997192861 | 0.9171847460820696 | T | T | T |
| 0.2397426649518196 | 0.0616615524908417 | 0.9171180399901202 | T | T | T |
| 0.1084658809259878 | 0.0838384780880750 | 0.9164860171108857 | T | T | T |
| 0.4057192738156374 | 0.1427883489216924 | 0.9169479107399905 | T | T | T |
| 0.5433985223792172 | 0.2925239544181462 | 0.9169777137163819 | T | T | T |
| 0.1114014057493756 | 0.3611539464693498 | 0.9170891987861279 | T | T | T |
| 0.2489669100717545 | 0.5118995688635247 | 0.9169700163381819 | T | T | T |
| 0.5490304120841797 | 0.5669449672964963 | 0.9165244071326712 | T | T | T |
| 0.4145686543101950 | 0.5843669872397170 | 0.9164155932814565 | T | T | T |
| 0.0980531917230338 | 0.4909206402325620 | 0.8558538723753932 | T | T | T |
| 0.1309573885620685 | 0.5531925928567371 | 0.8190085744454995 | T | T | T |

OH\_CNT(11,0) ### KPOINTS: 2x2x2 ### E= -692.89362120 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C O H

88 1 1

Selective dynamics

Direct

0.1507531464709771 0.0536869980100364 0.0834312303811418 T T T

0.2959942154316948 0.0744422929329632 0.0837322354544233 T T T

0.0642796140305279 0.1239776719127907 0.0835532730857757 T T T

0.4506114015729804 0.1762482047393927 0.0840688461212832 T T T

0.0629857595391007 0.2594032545536179 0.0825048561918377 T T T

0.5666553447373979 0.3261066680833360 0.0837142937281488 T T T

0.1400629672247282 0.4165603439133352 0.0814616258651384 T T T

0.6085980681874795 0.4782313738768325 0.0834116189713393 T T T

0.2806617444621750 0.5470004140336097 0.0816727011958518 T T T

0.5595436449344104 0.5828284904537985 0.0835343996291163 T T T

0.4363346665295769 0.6056322800164972 0.0826083601664121 T T T

0.2191237401129527 0.0528908102516963 0.1669291311805854 T T T

0.0976451625858868 0.0783625965804116 0.1668704048445025 T T T

0.3754186778814805 0.1168861858350752 0.1673073665961000 T T T

0.0521733341332610 0.1858327842429781 0.1666667326297532 T T T

0.5160649793939862 0.2477428366616906 0.1672954542046412 T T T

0.0931474272923369 0.3376895659122346 0.1654709610408522 T T T

0.5981472875100152 0.4048459334736271 0.1669009961250298 T T T

0.2043497638808645 0.4892961109117309 0.1659510734749477 T T T

0.5952575654220786 0.5393966194582108 0.1668660275090628 T T T

0.3600430871411763 0.5852609581330891 0.1655735816041767 T T T

0.5052703971425564 0.6057961876460325 0.1666866519833954 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2190596605597597 | 0.0527997387147686 | 0.3339580924309422 | T | T | T |
| 0.0976676769400707 | 0.0784890259388209 | 0.3334775121118570 | T | T | T |
| 0.3753502320500257 | 0.1168342433911217 | 0.3337147048324934 | T | T | T |
| 0.0520724892290632 | 0.1860924019437366 | 0.3330008810248473 | T | T | T |
| 0.5160897403719762 | 0.2478292330423693 | 0.3336824165613917 | T | T | T |
| 0.0926972486933051 | 0.3377296181585449 | 0.3324509620468042 | T | T | T |
| 0.5982596946910425 | 0.4049258404692517 | 0.3339563635082594 | T | T | T |
| 0.2049378554141801 | 0.4885966070039847 | 0.3307201686830431 | T | T | T |
| 0.5951529742988796 | 0.5393479118951453 | 0.3335117658518017 | T | T | T |
| 0.3601202084173226 | 0.5856141960568070 | 0.3325526576310238 | T | T | T |
| 0.5051040788746594 | 0.6059112101937721 | 0.3330137808538946 | T | T | T |
| 0.1508153897437925 | 0.0537205302852734 | 0.4171420327407341 | T | T | T |
| 0.2959686903571760 | 0.0744198826069552 | 0.4171971321296953 | T | T | T |
| 0.0646540109847965 | 0.1243349544097310 | 0.4165085112255901 | T | T | T |
| 0.4505191654076439 | 0.1763777976385705 | 0.4170471614971704 | T | T | T |
| 0.0622662838069702 | 0.2594237126629944 | 0.4161609757990359 | T | T | T |
| 0.5666252319602446 | 0.3261392949236120 | 0.4171957743735926 | T | T | T |
| 0.1405598920680061 | 0.4163832022549381 | 0.4152883953257360 | T | T | T |
| 0.6085936516025318 | 0.4781615953377185 | 0.4172047618119158 | T | T | T |
| 0.2808090391485230 | 0.5463204092663919 | 0.4152424031497137 | T | T | T |
| 0.5592564429473942 | 0.5824850901455291 | 0.4166058158883967 | T | T | T |
| 0.4364942227113177 | 0.6062544745867904 | 0.4161673241246592 | T | T | T |
| 0.1508875112627951 | 0.0539198034063086 | 0.5834362943384248 | T | T | T |
| 0.2960238972258168 | 0.0743846725783930 | 0.5836432300250336 | T | T | T |
| 0.0648152956411698 | 0.1246415134880023 | 0.5836406303306382 | T | T | T |
| 0.4506191939936910 | 0.1762373348049057 | 0.5839934605432223 | T | T | T |
| 0.0628749878937033 | 0.2602122439620773 | 0.5833661868147574 | T | T | T |
| 0.5666408227159959 | 0.3260663093359525 | 0.5836953477311683 | T | T | T |
| 0.1403630286820469 | 0.4176539801098086 | 0.5816218295393321 | T | T | T |
| 0.6084260680486625 | 0.4781477411409026 | 0.5834841781681089 | T | T | T |
| 0.2796040376398264 | 0.5465776438271108 | 0.5816995229582721 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5589215532939789 | 0.5823964310844520 | 0.5837159129662727 | T | T | T |
| 0.4356364960975491 | 0.6057427517061695 | 0.5833936385958763 | T | T | T |
| 0.2192149200465980 | 0.0530546160487660 | 0.6669207546125581 | T | T | T |
| 0.0979433827682605 | 0.0787532174095018 | 0.6669404604806557 | T | T | T |
| 0.3754737801566534 | 0.1167669590817305 | 0.6672325733694615 | T | T | T |
| 0.0529134568338563 | 0.1864978670196502 | 0.6666836328107258 | T | T | T |
| 0.5161474879932013 | 0.2476313461640099 | 0.6672595582934018 | T | T | T |
| 0.0925161904183957 | 0.3383188737841714 | 0.6657575023134178 | T | T | T |
| 0.5979697610205780 | 0.4047616279213878 | 0.6669570997960846 | T | T | T |
| 0.2030110982048007 | 0.4908603865426869 | 0.6628076186758276 | T | T | T |
| 0.5948948221243394 | 0.5391637175336558 | 0.6670151097254603 | T | T | T |
| 0.3595884437586872 | 0.5858209078054816 | 0.6657578174977518 | T | T | T |
| 0.5045995996900602 | 0.6051705731037135 | 0.6667826004219477 | T | T | T |
| 0.2191517366607285 | 0.0530104475183797 | 0.8338762850748128 | T | T | T |
| 0.0976973428792514 | 0.0783946813216655 | 0.8334034681829328 | T | T | T |
| 0.3754311593547758 | 0.1166814002143305 | 0.8336892234535179 | T | T | T |
| 0.0532787474716617 | 0.1865650080907897 | 0.8328687098867811 | T | T | T |
| 0.5162050093501999 | 0.2476072306313148 | 0.8336753824529815 | T | T | T |
| 0.0947688191647107 | 0.3391421474896404 | 0.8335124162107621 | T | T | T |
| 0.5980133763551223 | 0.4047782800996232 | 0.8339058805951473 | T | T | T |
| 0.1942055579897874 | 0.5015538364921924 | 0.8346545796870120 | T | T | T |
| 0.5951427435038559 | 0.5392900783694246 | 0.8334727430777366 | T | T | T |
| 0.3584062302572715 | 0.5836763945145662 | 0.8334869993599416 | T | T | T |
| 0.5043750331125987 | 0.6048030381157465 | 0.8329264227112305 | T | T | T |
| 0.1508292346889670 | 0.0537413080725828 | 0.9171166249168295 | T | T | T |
| 0.2959871117622630 | 0.0745022293164253 | 0.9171926611786628 | T | T | T |
| 0.0646048760123749 | 0.1241467723462440 | 0.9165660092265425 | T | T | T |
| 0.4506307093301206 | 0.1761559873063951 | 0.9170751891152744 | T | T | T |
| 0.0641200298264380 | 0.2600150175035888 | 0.9162175244689492 | T | T | T |
| 0.5665595841464186 | 0.3260335416998352 | 0.9171627218926679 | T | T | T |
| 0.1387061406821863 | 0.4169541729312745 | 0.9168332580733686 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6085220174411672 | 0.4781149556221614 | 0.9171266982216124 | T | T | T |
| 0.2802576100542185 | 0.5483617762256658 | 0.9167993481553403 | T | T | T |
| 0.5592569805462499 | 0.5824704227498511 | 0.9166102737141266 | T | T | T |
| 0.4355484042841631 | 0.6045808773718904 | 0.9162657777742417 | T | T | T |
| 0.1475935084669144 | 0.5500960396358131 | 0.8530982851395312 | T | T | T |
| 0.1867870908055551 | 0.6088255957220062 | 0.8217671418374859 | T | T | T |

OH\_CNT(12,0) ### KPOINTS: 1x1x2 ### E= -756.29798061 eV

1.0000000000000000

15.588499999999998 -9.000000000000000 0.000000000000000

0.0000000000000000 18.000000000000000 0.000000000000000

0.0000000000000000 0.000000000000000 8.457919999999997

C O H

96 1 1

Selective dynamics

Direct

0.6531160045195787 0.5368952463033169 0.4170451826439481 T T T

0.6532992557697136 0.5369435632210386 0.9169983715298160 T T T

0.4650744723096003 0.6503015527353159 0.4162721561899868 T T T

0.4639798444759786 0.6482920004727832 0.9163065587593844 T T T

0.3915127288595223 0.1097794725675649 0.4173419775476128 T T T

0.3914253181220180 0.1099421020343188 0.9173541969202151 T T T

0.1089774400115265 0.0666609361863145 0.4170827194117047 T T T

0.1088318239628753 0.0664371720438981 0.9170232984098264 T T T

0.6327944426381145 0.3914551916022816 0.4169358281934600 T T T

0.6329171613167308 0.3914334278562275 0.9169321854336444 T T T

0.5912640842642047 0.6314345302199905 0.4166199795965969 T T T

0.5911065278363408 0.6311113231229187 0.9165835977692534 T T T

0.1647742166449176 0.4664542210786942 0.4159870708669878 T T T

0.1627230709925818 0.4679517443121405 0.9168591826156058 T T T

0.0718384447333511 0.3098513720675207 0.4162821130677303 T T T

0.0735666679903314 0.3105817155781208 0.9163413459555895 T T T

0.2350211147580771 0.0478252928619661 0.4169892116173148 T T T

0.2348008770880837 0.0474538927428064 0.9169607848414897 T T T

0.5368175135855713 0.2351859058120451 0.4173338562236616 T T T

0.5368771632097142 0.2351768142616068 0.9173550614254582 T T T

0.3091804026155980 0.5914527676437504 0.4159968537977083 T T T

0.3088025939213494 0.5939112992893547 0.9170464275370852 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0498578368054193 | 0.1634727272411207 | 0.4166843314328069 | T | T | T |
| 0.0505332094604029 | 0.1639110142109151 | 0.9166461148672650 | T | T | T |
| 0.5913522783804395 | 0.6314125387216035 | 0.0835625469056245 | T | T | T |
| 0.5907436677435532 | 0.6310776594905202 | 0.5836563501616739 | T | T | T |
| 0.0500509909747195 | 0.1635796627873393 | 0.0835313772683082 | T | T | T |
| 0.0504729903356886 | 0.1640679133827802 | 0.5837135265971729 | T | T | T |
| 0.3090813387890212 | 0.5918244137103581 | 0.0819971655334400 | T | T | T |
| 0.3080465350877796 | 0.5923310898584134 | 0.5826721456217206 | T | T | T |
| 0.1088421428313692 | 0.0665204009103377 | 0.0836060921490860 | T | T | T |
| 0.1089184045721669 | 0.0665856320564340 | 0.5836105059473293 | T | T | T |
| 0.6532687057468708 | 0.5369748745420503 | 0.0835377682961180 | T | T | T |
| 0.6531017615738701 | 0.5369039106302184 | 0.5835472163175027 | T | T | T |
| 0.2348587055872956 | 0.0476039005553929 | 0.0841371898829568 | T | T | T |
| 0.2349017040239767 | 0.0476779755491638 | 0.5840933540963129 | T | T | T |
| 0.1643000930036622 | 0.4666921037037231 | 0.0820984218306882 | T | T | T |
| 0.1645114292127611 | 0.4680560005244449 | 0.5828327952568605 | T | T | T |
| 0.3914337625787513 | 0.1098870887747595 | 0.0840713191711960 | T | T | T |
| 0.3914391127526957 | 0.1098034227075796 | 0.5840602526641224 | T | T | T |
| 0.4647586369424311 | 0.6492503608153959 | 0.0830958272121104 | T | T | T |
| 0.4641903585407234 | 0.6500041545352597 | 0.5838876565054496 | T | T | T |
| 0.5368706143429270 | 0.2351401967254960 | 0.0840983112187852 | T | T | T |
| 0.5368121874809624 | 0.2352041643677704 | 0.5840686146744105 | T | T | T |
| 0.0724913488099347 | 0.3099034723004929 | 0.0831599621734450 | T | T | T |
| 0.0724363474911563 | 0.3107937855578816 | 0.5839307631433210 | T | T | T |
| 0.6328553200068029 | 0.3914400436424387 | 0.0841177629223299 | T | T | T |
| 0.6328858800540882 | 0.3914579615406982 | 0.5840651859148444 | T | T | T |
| 0.2319035655159260 | 0.5366835171879324 | 0.1664200637218136 | T | T | T |
| 0.2305107198208309 | 0.5392004289423989 | 0.6637521655038700 | T | T | T |
| 0.0507078571712062 | 0.2327941623449392 | 0.1666937335007362 | T | T | T |
| 0.0516557489212556 | 0.2335087892139817 | 0.6668601745439312 | T | T | T |
| 0.3118521261018568 | 0.0690839161855108 | 0.1673197269647666 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3118067465014317 | 0.0690268655953685 | 0.6672907379586788 | T | T | T |
| 0.3884144604417771 | 0.6288460027198816 | 0.1659422079324013 | T | T | T |
| 0.3882035939194860 | 0.6309244591651793 | 0.6661183210829880 | T | T | T |
| 0.6318121984995749 | 0.5925046232878354 | 0.1665955455431971 | T | T | T |
| 0.6314286004570019 | 0.5922936438489729 | 0.6666434593238008 | T | T | T |
| 0.4679739420327680 | 0.1665287619835923 | 0.1671717794141779 | T | T | T |
| 0.4679208999802988 | 0.1666038474271257 | 0.6671404263549223 | T | T | T |
| 0.0696540779565182 | 0.1067592839739029 | 0.1666434626644610 | T | T | T |
| 0.0699785704366962 | 0.1070978210238951 | 0.6667388233813014 | T | T | T |
| 0.1111709298086298 | 0.3890064127393736 | 0.1659816410893869 | T | T | T |
| 0.1097206170038230 | 0.3897540655734288 | 0.6661754599051628 | T | T | T |
| 0.5932890303578486 | 0.3119571722088635 | 0.1673380508460157 | T | T | T |
| 0.5933399837226961 | 0.3119965107357197 | 0.6673024232064700 | T | T | T |
| 0.5345224333165680 | 0.6511481862583952 | 0.1667488125527244 | T | T | T |
| 0.5337637737131999 | 0.6505580342218154 | 0.6668144533376804 | T | T | T |
| 0.1656838408955770 | 0.0465921718358184 | 0.1670469747795789 | T | T | T |
| 0.1655653871107013 | 0.0464161677338563 | 0.6670298959452624 | T | T | T |
| 0.6534031502239305 | 0.4680810220244978 | 0.1669578565835992 | T | T | T |
| 0.6534630021853409 | 0.4681241195262458 | 0.6669739739876317 | T | T | T |
| 0.0695697642836499 | 0.1068674631351427 | 0.3338700462428155 | T | T | T |
| 0.0699384478845856 | 0.1070464151717894 | 0.8337553200599952 | T | T | T |
| 0.5343875127991617 | 0.6513511177910741 | 0.3333332024582716 | T | T | T |
| 0.5336270162294805 | 0.6501105468803322 | 0.8331455773462503 | T | T | T |
| 0.6316538883681996 | 0.5925772170228675 | 0.3338211979313865 | T | T | T |
| 0.6316714126784249 | 0.5923929914937930 | 0.8336888247746513 | T | T | T |
| 0.4680123801308143 | 0.1664951435607782 | 0.3343193045523897 | T | T | T |
| 0.4679265461842251 | 0.1666343432559704 | 0.8343372885056861 | T | T | T |
| 0.0505847222029405 | 0.2329474122643336 | 0.3334012447708266 | T | T | T |
| 0.0520297814821708 | 0.2336294114909067 | 0.8332281086070576 | T | T | T |
| 0.1657443126213732 | 0.0467327876923703 | 0.3338419994468285 | T | T | T |
| 0.1654427863160276 | 0.0462581825846208 | 0.8338121710867686 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3885536782329033 | 0.6295159461168078 | 0.3330633315585972 | T | T | T |
| 0.3869741343798579 | 0.6283456064513707 | 0.8338388863558770 | T | T | T |
| 0.5932458951472203 | 0.3119999221053587 | 0.3339191662829203 | T | T | T |
| 0.5933873473741447 | 0.3119812423390618 | 0.8339014561533641 | T | T | T |
| 0.1107798966438874 | 0.3890449806748480 | 0.3331022117279016 | T | T | T |
| 0.1120226834052006 | 0.3905304659403827 | 0.8338158344769285 | T | T | T |
| 0.2324020996271798 | 0.5360061958538669 | 0.3316537570028179 | T | T | T |
| 0.2228502876331315 | 0.5515681512966710 | 0.8351258494836508 | T | T | T |
| 0.3119068424655265 | 0.0691087291511022 | 0.3339634715580103 | T | T | T |
| 0.3117901635096349 | 0.0690108587392970 | 0.8339638212294885 | T | T | T |
| 0.6533490630318747 | 0.4681212783878341 | 0.3338183384484773 | T | T | T |
| 0.6535076999789817 | 0.4681410140588212 | 0.8338180264350935 | T | T | T |
| 0.1904948253705170 | 0.6132424276305646 | 0.8539965577445997 | T | T | T |
| 0.1448950231687254 | 0.5968021502949764 | 0.7771543175158276 | T | T | T |

OH\_CNT(13,0) ### KPOINTS: 1x1x2 ### E= -1227.62729967 eV

1.0000000000000000

24.248699999999995 -14.000000000000000 0.0000000000000000

0.0000000000000000 28.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 12.838699999999993

C O H

156 1 1

Selective dynamics

Direct

0.4407632987387974 0.4066998822552825 0.0278249827420900 T T T

0.4527621876034867 0.3697455771726260 0.1946632944333130 T T T

0.4527736451802130 0.3697313206858530 0.3055424614316536 T T T

0.3829915820862153 0.4497100627223465 0.0276987957436375 T T T

0.4405459309377331 0.4065920355574714 0.1389499210883225 T T T

0.4165949550753025 0.4334690206036778 0.1944475291847639 T T T

0.4161498722109649 0.4331155685585664 0.3056398085346422 T T T

0.2931207225077574 0.4448421977130831 0.0271273056993355 T T T

0.3826938514324149 0.4495605073598085 0.1387684957658224 T T T

0.3405006717018693 0.4532368269843229 0.1942001417530137 T T T

0.3398084423617211 0.4529284228756482 0.3056449896553977 T T T

0.1920694416524890 0.3941236546526201 0.0268597202824294 T T T

0.2930117339528271 0.4448721679731362 0.1381790317264796 T T T

0.2424374587801644 0.4250095274984532 0.1933999034060699 T T T

0.2418525612423065 0.4260022405208626 0.3044926387437185 T T T

0.1028031729597795 0.3083940905369686 0.0271170085443133 T T T

0.1920645624752143 0.3942161770625897 0.1375208759734447 T T T

0.1446672668956351 0.3547773656973549 0.1933783719082127 T T T

0.1447060843206515 0.3560147230950618 0.3045664186279146 T T T

0.0442855543072793 0.2077039887945085 0.0277632819157531 T T T

0.1028798658574936 0.3085736650264380 0.1382170317288108 T T T

0.0690176210242964 0.2589403256196892 0.1942509162989185 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0697847605132404 | 0.2594865714420695 | 0.3057024798647173 | T | T | T |
| 0.0317916731460234 | 0.1145753315367880 | 0.0278909922180996 | T | T | T |
| 0.0445862185874467 | 0.2079692004668918 | 0.1388462725443036 | T | T | T |
| 0.0321100168617595 | 0.1588465296661726 | 0.1945167234147830 | T | T | T |
| 0.0324922806027858 | 0.1590494252323807 | 0.3056819668637873 | T | T | T |
| 0.0687166908322606 | 0.0513996643589476 | 0.0280127733079000 | T | T | T |
| 0.0319148504000151 | 0.1147166665710932 | 0.1389828866485127 | T | T | T |
| 0.0443784747794250 | 0.0780369549392450 | 0.1946869869121522 | T | T | T |
| 0.0441650964461041 | 0.0778438593679201 | 0.3055520328534277 | T | T | T |
| 0.1444985041184056 | 0.0312033672891223 | 0.0282833585750650 | T | T | T |
| 0.0686050753519576 | 0.0513023583638261 | 0.1391114220292519 | T | T | T |
| 0.1025009290518286 | 0.0353198251204413 | 0.1947918772435208 | T | T | T |
| 0.1023757129958169 | 0.0352363573456776 | 0.3057760117083114 | T | T | T |
| 0.2427044845478023 | 0.0593965347868455 | 0.0282331814892430 | T | T | T |
| 0.1444514927356528 | 0.0311929733326861 | 0.1391892456162925 | T | T | T |
| 0.1921138213808715 | 0.0394040520923685 | 0.1949066655899108 | T | T | T |
| 0.1921256568764370 | 0.0394604414289267 | 0.3059643325471705 | T | T | T |
| 0.3410098960089105 | 0.1296106218648324 | 0.0282061441027907 | T | T | T |
| 0.2426773889820235 | 0.0593838708598016 | 0.1393075212281086 | T | T | T |
| 0.2933293141578999 | 0.0900857177761482 | 0.1949893033701387 | T | T | T |
| 0.2933225151494973 | 0.0900740789676402 | 0.3059547619935050 | T | T | T |
| 0.4166216808684122 | 0.2255969159589372 | 0.0282182031189755 | T | T | T |
| 0.3410330305597931 | 0.1296320701554349 | 0.1392829127279655 | T | T | T |
| 0.3829035092360163 | 0.1756764307918480 | 0.1948512722442744 | T | T | T |
| 0.3828663930106144 | 0.1756570235893714 | 0.3059082676276436 | T | T | T |
| 0.4525597812486516 | 0.3255080717122409 | 0.0279611367266825 | T | T | T |
| 0.4166543652869450 | 0.2256160695319679 | 0.1391236805893936 | T | T | T |
| 0.4402990797018434 | 0.2765461829364966 | 0.1947089124886515 | T | T | T |
| 0.4403813052865112 | 0.2765755854957260 | 0.3057026403815862 | T | T | T |
| 0.4525780012710954 | 0.3255101727485665 | 0.1390636545441881 | T | T | T |
| 0.4402833981976174 | 0.4062825716965763 | 0.3612215199716034 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4528669838055436 | 0.3696925384809402 | 0.5279879924095930 | T | T | T |
| 0.4529107403684513 | 0.3697289725655621 | 0.6389043043633428 | T | T | T |
| 0.3820074663579421 | 0.4487195487368080 | 0.3612346114761024 | T | T | T |
| 0.4403009920900882 | 0.4062298479482508 | 0.4721580445173554 | T | T | T |
| 0.4161950077633080 | 0.4329706989642652 | 0.5276357023103652 | T | T | T |
| 0.4164403474772716 | 0.4331670871083158 | 0.6387270358647279 | T | T | T |
| 0.2926631344338020 | 0.4456054911027094 | 0.3606128979027635 | T | T | T |
| 0.3818824489184672 | 0.4484615574172671 | 0.4720066047897984 | T | T | T |
| 0.3396271360538647 | 0.4520091643725629 | 0.5276285066615984 | T | T | T |
| 0.3402191224353585 | 0.4527029605811728 | 0.6383640107260142 | T | T | T |
| 0.1911872788759965 | 0.3971830911141601 | 0.3583226584522123 | T | T | T |
| 0.2918446640881581 | 0.4443753168250574 | 0.4723761919863081 | T | T | T |
| 0.2425773312243247 | 0.4277620112941038 | 0.5282320443085824 | T | T | T |
| 0.2424786048209019 | 0.4264562438960335 | 0.6380833301545543 | T | T | T |
| 0.1030777190074852 | 0.3092587181332201 | 0.3606821307006876 | T | T | T |
| 0.1879558422156521 | 0.4066476846000618 | 0.4727297122673840 | T | T | T |
| 0.1436485421569131 | 0.3560738355799691 | 0.5282164775573760 | T | T | T |
| 0.1442328771183256 | 0.3554423598929486 | 0.6382122108854430 | T | T | T |
| 0.0456098382143773 | 0.2081667049006339 | 0.3613053329695943 | T | T | T |
| 0.1043370844598544 | 0.3093716702707350 | 0.4724228272925755 | T | T | T |
| 0.0704847316807743 | 0.2590530552407734 | 0.5276908533634806 | T | T | T |
| 0.0697765031806310 | 0.2588399717380311 | 0.6383966012731944 | T | T | T |
| 0.0318567187462554 | 0.1145351005794707 | 0.3612474641294545 | T | T | T |
| 0.0458264033802259 | 0.2081041335772830 | 0.4720677283722025 | T | T | T |
| 0.0324824086513427 | 0.1588085874172161 | 0.5276700748943465 | T | T | T |
| 0.0322493925260700 | 0.1586879321117796 | 0.6387471630918504 | T | T | T |
| 0.0682399233050127 | 0.0509412790614393 | 0.3612865993674425 | T | T | T |
| 0.0317733532800233 | 0.1143949322377026 | 0.4721757387353147 | T | T | T |
| 0.0439068322178028 | 0.0775237871681353 | 0.5280277519721299 | T | T | T |
| 0.0439279175408895 | 0.0775638050698457 | 0.6389742686989730 | T | T | T |
| 0.1444441395921587 | 0.0312886920282691 | 0.3615364686518635 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0680962211467176 | 0.0507831108090732 | 0.4723977955972221 | T | T | T |
| 0.1023026877819754 | 0.0351586817235464 | 0.5280876532937517 | T | T | T |
| 0.1023313597549088 | 0.0351707107005449 | 0.6391637788041491 | T | T | T |
| 0.2426918136576619 | 0.0594396524850944 | 0.3615975194595131 | T | T | T |
| 0.1444503054299577 | 0.0313024210781539 | 0.4724871596432703 | T | T | T |
| 0.1921469967663549 | 0.0395349122121056 | 0.5281812348805480 | T | T | T |
| 0.1921335610323222 | 0.0395128886739280 | 0.6392268493845122 | T | T | T |
| 0.3409746560510942 | 0.1296262111630395 | 0.3615713756574659 | T | T | T |
| 0.2426875110602638 | 0.0594533361515420 | 0.4726174139416263 | T | T | T |
| 0.2933023646818418 | 0.0901037287516325 | 0.5282528394233957 | T | T | T |
| 0.2933091986973085 | 0.0900931464396337 | 0.6392074092154587 | T | T | T |
| 0.4166478358196727 | 0.2256138576832389 | 0.3614703195520618 | T | T | T |
| 0.3409604497938339 | 0.1296280165108050 | 0.4725974191069183 | T | T | T |
| 0.3828195238012770 | 0.1756526454876646 | 0.5281630885892661 | T | T | T |
| 0.3828397011321703 | 0.1756656529109584 | 0.6392073250993232 | T | T | T |
| 0.4527121155986792 | 0.3255370095261602 | 0.3612631831270914 | T | T | T |
| 0.4166516067971900 | 0.2255923382917166 | 0.4724214674184042 | T | T | T |
| 0.4404730749515148 | 0.2765765992231982 | 0.5280594866344822 | T | T | T |
| 0.4404710474298719 | 0.2765726769211018 | 0.6391241427733203 | T | T | T |
| 0.4528275490696334 | 0.3255665551459308 | 0.4723623484855350 | T | T | T |
| 0.4405560711215680 | 0.4063872342378323 | 0.6944632529834789 | T | T | T |
| 0.4528101804325217 | 0.3697286153456163 | 0.8613188667001138 | T | T | T |
| 0.4528872919172321 | 0.3698503589203645 | 0.9722734087752488 | T | T | T |
| 0.3826399277890082 | 0.4491746977400359 | 0.6942307945858239 | T | T | T |
| 0.4406155961203171 | 0.4065022570053582 | 0.8054753435915715 | T | T | T |
| 0.4169486303803432 | 0.4337362301010650 | 0.8609593958695473 | T | T | T |
| 0.4170267635069461 | 0.4338659592346306 | 0.9721239535026999 | T | T | T |
| 0.2928227644368171 | 0.4447578101498788 | 0.6939407675161946 | T | T | T |
| 0.3829283878891890 | 0.4495673166793181 | 0.8051051397551025 | T | T | T |
| 0.3408012978105743 | 0.4533805731030182 | 0.8606882769423156 | T | T | T |
| 0.3408012719929454 | 0.4533260658634797 | 0.9716664254357436 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1916083464968734 | 0.3959019009606430 | 0.6946507727031382 | T | T | T |
| 0.2930694545803031 | 0.4449560541238367 | 0.8050729774832569 | T | T | T |
| 0.2426615164589376 | 0.4251876951741237 | 0.8606111809258520 | T | T | T |
| 0.2426084893589018 | 0.4248459843330571 | 0.9712740073760827 | T | T | T |
| 0.1034336084021995 | 0.3086048801209267 | 0.6939592353692225 | T | T | T |
| 0.1918835474584282 | 0.3948946196428111 | 0.8044842049318112 | T | T | T |
| 0.1444886436886682 | 0.3545942808640211 | 0.8605752074541843 | T | T | T |
| 0.1445969797892005 | 0.3544312985824737 | 0.9712847674011793 | T | T | T |
| 0.0450378314987010 | 0.2077261523484668 | 0.6942199542666827 | T | T | T |
| 0.1029929058690811 | 0.3084810459047527 | 0.8050918542354573 | T | T | T |
| 0.0688198229239592 | 0.2586384135643520 | 0.8606855641223776 | T | T | T |
| 0.0687147643944552 | 0.2586200855383974 | 0.9716878067033283 | T | T | T |
| 0.0316185487037548 | 0.1142786426264286 | 0.6945323875243250 | T | T | T |
| 0.0445878506265590 | 0.2076668213164038 | 0.8051096630765987 | T | T | T |
| 0.0317623483446538 | 0.1585811969004511 | 0.8610133879613217 | T | T | T |
| 0.0316714520760485 | 0.1586252199940260 | 0.9721754967135239 | T | T | T |
| 0.0682462167223617 | 0.0509014356300573 | 0.6946778519076714 | T | T | T |
| 0.0317002879670472 | 0.1144088191100865 | 0.8055524526432324 | T | T | T |
| 0.0443802480784237 | 0.0779830697498417 | 0.8613853366552963 | T | T | T |
| 0.0444410705622602 | 0.0781094438658958 | 0.9723454598675808 | T | T | T |
| 0.1444497108227462 | 0.0312795691289392 | 0.6948633157387234 | T | T | T |
| 0.0684295073973764 | 0.0510829593375069 | 0.8058201501938297 | T | T | T |
| 0.1025023230871063 | 0.0353038193195878 | 0.8614331327620781 | T | T | T |
| 0.1025874263163860 | 0.0354229819205234 | 0.9725202623171013 | T | T | T |
| 0.2426858448939447 | 0.0594597924263593 | 0.6948428178755889 | T | T | T |
| 0.1444462277070728 | 0.0312297554003776 | 0.8058249254396923 | T | T | T |
| 0.1921175640871569 | 0.0394092797593590 | 0.8615006517773707 | T | T | T |
| 0.1921283236319019 | 0.0393419585388903 | 0.9725910356794947 | T | T | T |
| 0.3409680158639552 | 0.1296487598819552 | 0.6948432253949312 | T | T | T |
| 0.2426761662143697 | 0.0594201472623303 | 0.8059299485956254 | T | T | T |
| 0.2933260898134347 | 0.0901132689481046 | 0.8616161599412892 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2933256827168724 | 0.0900857134249146 | 0.9725908466979593 | T | T | T |
| 0.4166659660144622 | 0.2256074379983213 | 0.6948649735640412 | T | T | T |
| 0.3410040086089932 | 0.1296572854446087 | 0.8059196587565646 | T | T | T |
| 0.3828981671403378 | 0.1756820820815824 | 0.8614850445314033 | T | T | T |
| 0.3829136170462710 | 0.1756375583024875 | 0.9725679271050134 | T | T | T |
| 0.4527768272084142 | 0.3255193878392239 | 0.6946390723398953 | T | T | T |
| 0.4166890381285828 | 0.2256280515266015 | 0.8058156758402372 | T | T | T |
| 0.4403624067566190 | 0.2765443299576682 | 0.8614133710636034 | T | T | T |
| 0.4402633104546883 | 0.2765658873574509 | 0.9724877032819667 | T | T | T |
| 0.4527102430362474 | 0.3255219625999530 | 0.8057618751187232 | T | T | T |
| 0.1751698835228491 | 0.4522907503276666 | 0.4824902757969766 | T | T | T |
| 0.1383545841921121 | 0.4385273041867411 | 0.4546275392438554 | T | T | T |

### 1.1.2 OH adsorbate on N-doped CNT

OH\_N-CNT(5,5) ### KPOINTS: 2x2x3 ### ### E= -470.64475701 eV

1.0000000000000000

13.8564000000000007 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3947799999999999

C N O H

59 1 1 1

Selective dynamics

Direct

0.5658034051999178 0.4266749864405554 0.0848618241839205 T T T

0.5658112622941405 0.4266812348803790 0.4174127877420364 T T T

0.5657578120248604 0.4265794048117231 0.7511328663165132 T T T

0.4843261531009354 0.5459709420607569 0.0841638562423976 T T T

0.4842656228514742 0.5459252002795199 0.4173514943751266 T T T

0.4850472279894191 0.5458334541543707 0.7507602127064731 T T T

0.3962983015536776 0.5480554853061372 0.0839411323047856 T T T

0.3962783348478417 0.5480544397721464 0.4168075147244718 T T T

0.3965252807065044 0.5460241187221559 0.7503870122803709 T T T

0.1146586503303325 0.3447029952386502 0.0831633405736690 T T T

0.1150359154976270 0.3447617756590848 0.4161696571514087 T T T

0.0976405911995522 0.3488362043559450 0.7491844644648258 T T T

0.0785267060306368 0.1554604404711690 0.0830017677554007 T T T

0.0785771371592985 0.1554196288345489 0.4166212098950196 T T T

0.0778329048988091 0.1556184551198690 0.7499282600041356 T T T

0.1180390570446699 0.0932516884571064 0.0833887304818230 T T T

0.1179775377666434 0.0931729939260916 0.4169001687695598 T T T

0.1183380612072188 0.0942633643231447 0.7502163830193376 T T T

0.2873434542883363 0.0827757054586764 0.0841550227162404 T T T

0.2873452391897169 0.0827953942626980 0.4174110968353923 T T T

0.2874591331962015 0.0828293463729594 0.7507356894733281 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3899623611994935 | 0.1388817164894716 | 0.0843944908432534 | T | T | T |
| 0.3899756447026589 | 0.1388895402346907 | 0.4176542830604941 | T | T | T |
| 0.3899973266059574 | 0.1390642281299665 | 0.7510335186125877 | T | T | T |
| 0.5435310676910385 | 0.3286526053019287 | 0.0847927877138737 | T | T | T |
| 0.5435032801025356 | 0.3286537060303719 | 0.4176212730535760 | T | T | T |
| 0.5438400633445595 | 0.3286166507159018 | 0.7511966589904332 | T | T | T |
| 0.1938525978269210 | 0.4423451541609119 | 0.0818431597332719 | T | T | T |
| 0.1939054052105003 | 0.4423238085434685 | 0.4179593430958743 | T | T | T |
| 0.2433777888778016 | 0.4818009860984034 | 0.2499910929800823 | T | T | T |
| 0.2438844124599468 | 0.4779261118449671 | 0.5854390280867359 | T | T | T |
| 0.2439044543436659 | 0.4777955521048364 | 0.9145184662566028 | T | T | T |
| 0.5606645676351080 | 0.4690565770114804 | 0.2510676675856126 | T | T | T |
| 0.5606299059137145 | 0.4688838204100412 | 0.5842743796798557 | T | T | T |
| 0.5605979499092301 | 0.4688509270531037 | 0.9179045257777568 | T | T | T |
| 0.1506952551344122 | 0.0745564675174235 | 0.2502346302083051 | T | T | T |
| 0.1513216924981129 | 0.0753785649517564 | 0.5838613471359976 | T | T | T |
| 0.1513426489224637 | 0.0753891157771644 | 0.9166988896431969 | T | T | T |
| 0.2370289568256557 | 0.0692210662345618 | 0.2506805907491385 | T | T | T |
| 0.2372096186247354 | 0.0697774372642393 | 0.5842232976771385 | T | T | T |
| 0.2372133770819054 | 0.0697347253416229 | 0.9171452708331674 | T | T | T |
| 0.5189226859956710 | 0.5296696260096717 | 0.2508553345330156 | T | T | T |
| 0.5191018721498515 | 0.5293578969850009 | 0.5840028763631471 | T | T | T |
| 0.5191088624937151 | 0.5293646359884752 | 0.9177058850742368 | T | T | T |
| 0.0908469488280028 | 0.2930940731534502 | 0.2498087521843874 | T | T | T |
| 0.0879884198877718 | 0.2928942470736043 | 0.5801961551023658 | T | T | T |
| 0.0871757414698429 | 0.2927921671665344 | 0.9188189240804718 | T | T | T |
| 0.4384000041696449 | 0.1795604387869005 | 0.2510780868548567 | T | T | T |
| 0.4384310852244874 | 0.1798636479571130 | 0.5844993609979658 | T | T | T |
| 0.4384065171278561 | 0.1798778757196136 | 0.9177296939105661 | T | T | T |
| 0.5165606517378802 | 0.2765311343388782 | 0.2511770073378244 | T | T | T |
| 0.5168077941550391 | 0.2765842495985050 | 0.5844649585938424 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5167939696272246 | 0.2765753886835491 | 0.9178816942702995 | T | T | T |
| 0.0720835048108687 | 0.1963880274390922 | 0.2498613596244380 | T | T | T |
| 0.0736134745162106 | 0.1986787238353466 | 0.5832096215654567 | T | T | T |
| 0.0731751173029942 | 0.1984981671295121 | 0.9163104205777278 | T | T | T |
| 0.3462503584418518 | 0.5354437581546282 | 0.2502577794599460 | T | T | T |
| 0.3459802688638151 | 0.5323701860407869 | 0.5845318370605590 | T | T | T |
| 0.3459831927670284 | 0.5323708265190926 | 0.9160586426070900 | T | T | T |
| 0.1968710718023618 | 0.4406672804872003 | 0.7499243049047952 | T | T | T |
| 0.0255282837227724 | 0.3777263775146394 | 0.7375212612447839 | T | T | T |
| 0.0101940116168579 | 0.3886952512944132 | 0.8588968499190341 | T | T | T |

OH\_N-CNT(6,6) ### KPOINTS: 2x2x3 ### E= -566.85745221 eV

1.000000000000000

14.722400000000000 -8.500000000000000 0.000000000000000

0.000000000000000 17.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.399280000000001

C N O H

71 1 1 1

Selective dynamics

Direct

0.6144880539652904 0.4957048392845949 0.0833974610292178 T T T

0.6144333764515653 0.4956632773049538 0.4165968804592335 T T T

0.6143566736234575 0.4954626928494745 0.7499812661114100 T T T

0.5290659527560677 0.6007982247393507 0.0831956275796014 T T T

0.5290955498458564 0.6008677332052439 0.4166997980873542 T T T

0.5280961937213323 0.6001616071743849 0.7499472008790781 T T T

0.4493979451948318 0.6079905960652794 0.0830530451308485 T T T

0.4494509688590879 0.6081120188405011 0.4168073822678962 T T T

0.4492620102169433 0.6086927788510301 0.7499463465816442 T T T

0.1726417741304822 0.4547825196404989 0.0820764764341538 T T T

0.1726104388042768 0.4548240175579394 0.4178556303333900 T T T

0.0696525161951419 0.2638072114334046 0.0835323265521451 T T T

0.0696786974726602 0.2638255556971205 0.4164290732891338 T T T

0.0718572889812764 0.2635533021365130 0.7499637542335535 T T T

0.0606569611364565 0.1759442519919230 0.0833460138473502 T T T

0.0607102237090081 0.1759778110868010 0.4166480715572110 T T T

0.0609933075638328 0.1753904853383716 0.7499930857006175 T T T

0.1389819837949642 0.0641639673044631 0.0836505297700299 T T T

0.1389760151808555 0.0641521000743837 0.4164137682176682 T T T

0.1388799631336882 0.0640052047403719 0.7500368492801470 T T T

0.2182751695747507 0.0559938049090599 0.0836131387903319 T T T

0.2182739194580863 0.0559959424411941 0.4165263963142741 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2181066835587105 | 0.0557325340278078 | 0.7500678144373372 | T | T | T |
| 0.4087338667922460 | 0.1392287358380747 | 0.0835964513611240 | T | T | T |
| 0.4087327210428322 | 0.1392312287556746 | 0.4166017386604413 | T | T | T |
| 0.4087262895653435 | 0.1392600789453073 | 0.7500858427379029 | T | T | T |
| 0.4962986220313249 | 0.2183657473064591 | 0.0835405334356045 | T | T | T |
| 0.4962943204887055 | 0.2183672328538496 | 0.4166139754482792 | T | T | T |
| 0.4964153880779771 | 0.2184086564903191 | 0.7500703267451144 | T | T | T |
| 0.6068961565555836 | 0.4084883235385782 | 0.0834560724996069 | T | T | T |
| 0.6069060310427262 | 0.4084787665135242 | 0.4165894987509481 | T | T | T |
| 0.6070976700388484 | 0.4084442138567614 | 0.7500214289830407 | T | T | T |
| 0.2607682827854239 | 0.5342821407893081 | 0.0834228485059982 | T | T | T |
| 0.2607500586135033 | 0.5343278908431015 | 0.4164260986580935 | T | T | T |
| 0.2528689391938111 | 0.5476792882047582 | 0.7498823577865247 | T | T | T |
| 0.0681749711532842 | 0.1379286546029563 | 0.2500021983503055 | T | T | T |
| 0.0686471593026217 | 0.1378357185833223 | 0.5830929368252463 | T | T | T |
| 0.0686217210597768 | 0.1378246393367620 | 0.9169122117897828 | T | T | T |
| 0.1076958728442588 | 0.0811218314881550 | 0.2500289425327777 | T | T | T |
| 0.1079111431373504 | 0.0811366695417835 | 0.5832402237919303 | T | T | T |
| 0.1079228278189131 | 0.0811597855297034 | 0.9168069281884883 | T | T | T |
| 0.5616843992372638 | 0.5857185314386834 | 0.2499753219628688 | T | T | T |
| 0.5610497526278092 | 0.5849662618013839 | 0.5834453313804445 | T | T | T |
| 0.5610565222235604 | 0.5849491588117530 | 0.9164521588614778 | T | T | T |
| 0.1364514468789149 | 0.4080053589640076 | 0.2499715193309132 | T | T | T |
| 0.1403873832359471 | 0.4076525491399974 | 0.5851082252748915 | T | T | T |
| 0.1404238538097891 | 0.4076162935817478 | 0.9148176271489845 | T | T | T |
| 0.2643876878119475 | 0.0649941617038653 | 0.2500828776759695 | T | T | T |
| 0.2643380742480037 | 0.0650857565334224 | 0.5834143164734468 | T | T | T |
| 0.2643383389247353 | 0.0650836737336589 | 0.9167370284900165 | T | T | T |
| 0.3608105977972858 | 0.1072527926919270 | 0.2501007192674230 | T | T | T |
| 0.3606888864371680 | 0.1074454699207358 | 0.5833804440011399 | T | T | T |
| 0.3606917386740454 | 0.1074486857812091 | 0.9168066897063600 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0844094566106821 | 0.3113884761258062 | 0.2499682863651354 | T | T | T |
| 0.0877690851319081 | 0.3117029629066919 | 0.5841794998273748 | T | T | T |
| 0.0877753010976436 | 0.3116869290250247 | 0.9157635184852767 | T | T | T |
| 0.3088726900235579 | 0.5630540981324474 | 0.2499163351765243 | T | T | T |
| 0.3083198897508577 | 0.5659325426231512 | 0.5807855522173737 | T | T | T |
| 0.3082903418578394 | 0.5658248205875395 | 0.9190366757866341 | T | T | T |
| 0.5340968591834767 | 0.2640770738675434 | 0.2500669473119014 | T | T | T |
| 0.5340076043698244 | 0.2641725252939786 | 0.5834043728039399 | T | T | T |
| 0.5339987803369144 | 0.2641776752772257 | 0.9167289071856801 | T | T | T |
| 0.5902444478592824 | 0.3603626988670939 | 0.2500240612623795 | T | T | T |
| 0.5901971079981108 | 0.3602950244194161 | 0.5833873066754652 | T | T | T |
| 0.5901658786934607 | 0.3603000600992374 | 0.9166794186636050 | T | T | T |
| 0.6050352850850776 | 0.5324875907430773 | 0.2499997241294917 | T | T | T |
| 0.6044732444132086 | 0.5320671030864865 | 0.5834748790504773 | T | T | T |
| 0.6045310395772341 | 0.5321015784673009 | 0.9164799922878976 | T | T | T |
| 0.4046534811660096 | 0.6010969894887128 | 0.2499294561064728 | T | T | T |
| 0.4027966553930832 | 0.5997318261952367 | 0.5835295832590128 | T | T | T |
| 0.4027421970412934 | 0.5996064199472180 | 0.9163367233335876 | T | T | T |
| 0.1746399020941813 | 0.4520390656309042 | 0.7499540711088016 | T | T | T |
| 0.2064383189852357 | 0.6007673712801846 | 0.7499167401881448 | T | T | T |
| 0.2528500425515131 | 0.6643063941203077 | 0.7430071372660564 | T | T | T |

OH\_N-CNT(7,7) #### KPOINTS: 1x1x3 #### E= -662.68828967 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C N O H

83 1 1 1

Selective dynamics

Direct

0.1817217093393183 0.0451519485977431 0.0833704185611173 T T T

0.2646907454120945 0.0537891507658509 0.0834305072783679 T T T

0.0691525169401009 0.1113741084839132 0.0831619624450919 T T T

0.4455637048868519 0.1497253551367710 0.0834771703372799 T T T

0.0500799438650686 0.1790079379505134 0.0829325387578779 T T T

0.5263340951195309 0.2268331102504575 0.0834638324043521 T T T

0.0892658634872133 0.3517424810574125 0.0837651304213081 T T T

0.6367778265764276 0.4063921503601469 0.0833869043642351 T T T

0.1414235918396759 0.4422318648570285 0.0846019450583889 T T T

0.6556559708159027 0.4930855205344893 0.0832658409719325 T T T

0.2971884996168275 0.5971989701280063 0.0800866169636026 T T T

0.6106812448340557 0.6224295793977906 0.0831995943839685 T T T

0.3874383916893674 0.6381937805979536 0.0830209695640480 T T T

0.5519242721907617 0.6533415287143352 0.0831293174448414 T T T

0.0504752781888744 0.2187977904067350 0.2497197582314676 T T T

0.5616574730199986 0.2701011517765529 0.2500695512559139 T T T

0.0711204608444857 0.3057605607972482 0.2496048196625593 T T T

0.6175269165517508 0.3605561806593129 0.2500364087388607 T T T

0.1453636282339235 0.0514765914856801 0.2499788189186155 T T T

0.3098738242608380 0.0687095241270745 0.2500550137241366 T T T

0.0887129127886404 0.0850940386721782 0.2498962292490123 T T T

0.4011029527716318 0.1170721907509305 0.2500538960271098 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6547047134199866 | 0.5324965485055766 | 0.2498675169541900 | T | T | T |
| 0.2446123321189165 | 0.5772463456512150 | 0.2496371516262967 | T | T | T |
| 0.6319610757942236 | 0.5976164505832102 | 0.2497250453970102 | T | T | T |
| 0.4329668287955606 | 0.6525675548445697 | 0.2495384263136108 | T | T | T |
| 0.5147877155432301 | 0.6590077928190954 | 0.2495622610292604 | T | T | T |
| 0.1817093969529447 | 0.0451837776402209 | 0.4166371390290953 | T | T | T |
| 0.2646817973702835 | 0.0538334778453997 | 0.4166266345536528 | T | T | T |
| 0.0690522312996163 | 0.1112740522079594 | 0.4166139103916174 | T | T | T |
| 0.4455561062054119 | 0.1497093128091175 | 0.4165902722270881 | T | T | T |
| 0.0501353576813468 | 0.1790146111335269 | 0.4165557715297482 | T | T | T |
| 0.5263230291972840 | 0.2268262070232369 | 0.4166353665990405 | T | T | T |
| 0.0893990780282146 | 0.3516507340334371 | 0.4154714971149607 | T | T | T |
| 0.6368139955802975 | 0.4064006505402042 | 0.4166253635139353 | T | T | T |
| 0.1416322133464134 | 0.4420785979555219 | 0.4144985684761716 | T | T | T |
| 0.6557062307935525 | 0.4930993962068680 | 0.4165571799721091 | T | T | T |
| 0.2973243997655622 | 0.5968103349596683 | 0.4189401503742239 | T | T | T |
| 0.6104962427815104 | 0.6222454702644031 | 0.4162139164867142 | T | T | T |
| 0.3876036299327559 | 0.6382672848598190 | 0.4161547290498890 | T | T | T |
| 0.5518200881642177 | 0.6532255764470016 | 0.4161020641355835 | T | T | T |
| 0.1454792908313470 | 0.0516922831726616 | 0.5834811298957236 | T | T | T |
| 0.3099197621256377 | 0.0686179595136199 | 0.5833840318753841 | T | T | T |
| 0.0884603276680639 | 0.0848823715926239 | 0.5835081024962265 | T | T | T |
| 0.4010858773723445 | 0.1170939872524377 | 0.5833610188385824 | T | T | T |
| 0.0503084592893212 | 0.2192533839501560 | 0.5829266645155257 | T | T | T |
| 0.5616578595142319 | 0.2700749810190812 | 0.5834476598313619 | T | T | T |
| 0.0695041515402379 | 0.3061757286080471 | 0.5831066835960900 | T | T | T |
| 0.6173198717056755 | 0.3604812514617363 | 0.5834799287458391 | T | T | T |
| 0.1718467660263272 | 0.4866225285846389 | 0.5815963644383428 | T | T | T |
| 0.6546743071912662 | 0.5325170057984717 | 0.5832542360126713 | T | T | T |
| 0.2533530578784944 | 0.5641506805648814 | 0.5830096331062383 | T | T | T |
| 0.6318778702249437 | 0.5976259990355903 | 0.5830825996040866 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4331935896391008 | 0.6518502381523037 | 0.5827441976087346 | T | T | T |
| 0.5156161675828099 | 0.6595546677464895 | 0.5828273858691754 | T | T | T |
| 0.0687729154742924 | 0.1111881334483991 | 0.7499144465924299 | T | T | T |
| 0.0497081557459485 | 0.1791208953884520 | 0.7497810478390645 | T | T | T |
| 0.5265112538249495 | 0.2267821537591286 | 0.7500317844831257 | T | T | T |
| 0.0866256901610030 | 0.3515999389726228 | 0.7496484218031035 | T | T | T |
| 0.6368078517717708 | 0.4063891799733859 | 0.7500505641905760 | T | T | T |
| 0.1380633172665506 | 0.4425489976406306 | 0.7497809331289945 | T | T | T |
| 0.1818609894113561 | 0.0453814292159054 | 0.7499914622421591 | T | T | T |
| 0.2647824655930676 | 0.0537427373876374 | 0.7499838436599692 | T | T | T |
| 0.4455573489694682 | 0.1496761097101632 | 0.7500253074774513 | T | T | T |
| 0.6557962775866701 | 0.4932538088142772 | 0.7499742991955464 | T | T | T |
| 0.2980681637372987 | 0.5941746124927059 | 0.7497907767221664 | T | T | T |
| 0.6108697185923064 | 0.6226054634080127 | 0.7496735243981154 | T | T | T |
| 0.3889824037276722 | 0.6389746225327374 | 0.7496865774052509 | T | T | T |
| 0.5522884721461658 | 0.6539212340015561 | 0.7496378556292024 | T | T | T |
| 0.1455160297388388 | 0.0517203339836297 | 0.9165142621982771 | T | T | T |
| 0.3098993922133442 | 0.0685846017163495 | 0.9166100807494681 | T | T | T |
| 0.0885830888020191 | 0.0850094017074032 | 0.9163748973966397 | T | T | T |
| 0.4010786783460831 | 0.1170921568025106 | 0.9166635450555587 | T | T | T |
| 0.0501797389175779 | 0.2192432403266031 | 0.9165426180820767 | T | T | T |
| 0.5616657181483913 | 0.2700582241110500 | 0.9166056319582474 | T | T | T |
| 0.0692886473096897 | 0.3061675155637273 | 0.9162153236319006 | T | T | T |
| 0.6173088285138799 | 0.3604798778697371 | 0.9166230235511706 | T | T | T |
| 0.1717831871780784 | 0.4867917591969604 | 0.9176735426836246 | T | T | T |
| 0.6546442666357085 | 0.5325333455539157 | 0.9165428841674789 | T | T | T |
| 0.2531567698121208 | 0.5644198436691571 | 0.9163907287814004 | T | T | T |
| 0.6320122493770458 | 0.5977515921431225 | 0.9163610446999980 | T | T | T |
| 0.4331188650056208 | 0.6517102594161582 | 0.9165586534645466 | T | T | T |
| 0.5155928092842568 | 0.6595210995999850 | 0.9164584286473150 | T | T | T |
| 0.1741093562837298 | 0.4840809443891260 | 0.2495948200511139 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2034636927134876 | 0.6290957462099440 | 0.2417103054956887 | T | T | T |
| 0.1817680130771258 | 0.6295979827040504 | 0.3614395186460664 | T | T | T |

OH\_N-CNT(8,8) #### KPOINTS: 1x1x3 #### E= -758.23208953 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C N O H

95 1 1 1

Selective dynamics

Direct

0.2514306243187343 0.0418950710439734 0.0835400291467592 T T T

0.1159465752244493 0.0528026043406352 0.0839385672811232 T T T

0.3320439628897165 0.0686487052499964 0.0833520970130409 T T T

0.0719211032463456 0.0908230210904189 0.0841140716736542 T T T

0.4924840325078285 0.1759695249906209 0.0829531005436591 T T T

0.0435088107215230 0.2158914189453452 0.0840999140223962 T T T

0.5613404715552915 0.2491362621462115 0.0828672034137691 T T T

0.0589659085493430 0.2933075270959224 0.0840698847427219 T T T

0.6531052272846107 0.4119453034694264 0.0829219852486478 T T T

0.1438979878478482 0.4554489269731814 0.0841820088134487 T T T

0.6703688597219383 0.4901037310971147 0.0832049244123455 T T T

0.2132916136085162 0.5289416011579835 0.0829617867997101 T T T

0.6402596098599376 0.6138931436254390 0.0835893684822839 T T T

0.3748930950030335 0.6289878165812047 0.0841282926396157 T T T

0.5937983488077293 0.6492907024677751 0.0839267556305834 T T T

0.4555699753062308 0.6556796506582547 0.0839093217646570 T T T

0.2131358776918309 0.0363436624522344 0.2502386635795704 T T T

0.1447223848233800 0.0414854882236108 0.2505065442980756 T T T

0.3734217206533272 0.0894599956043407 0.2498024272260284 T T T

0.4540471480334092 0.1434265675976621 0.2496214373633440 T T T

0.0430180675306498 0.1798636028311912 0.2509077304237864 T T T

0.6710540510708919 0.5262121946514294 0.2498262868317287 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2525688021765385 | 0.5600117566898783 | 0.2508459477580797 | T | T | T |
| 0.6559047390647603 | 0.5885451163248827 | 0.2500647766216312 | T | T | T |
| 0.5639182627372974 | 0.6592206873929358 | 0.2504460763594947 | T | T | T |
| 0.0571656870804871 | 0.1169153667940280 | 0.2507849513150790 | T | T | T |
| 0.5908482100976638 | 0.2889412832859547 | 0.2495515573052447 | T | T | T |
| 0.0733781570801683 | 0.3335713766360164 | 0.2510108494729808 | T | T | T |
| 0.6369109551806036 | 0.3708989412384107 | 0.2495894089785090 | T | T | T |
| 0.1166778649328675 | 0.4152673846511981 | 0.2509618257581619 | T | T | T |
| 0.3337964294525388 | 0.6102147152921591 | 0.2508173191414886 | T | T | T |
| 0.4942368107377561 | 0.6622286324255456 | 0.2506232865684392 | T | T | T |
| 0.2514237809459110 | 0.0418743388851796 | 0.4167667960226109 | T | T | T |
| 0.1159766758730342 | 0.0528163704130451 | 0.4172339155114327 | T | T | T |
| 0.3320402223309975 | 0.0687252805371559 | 0.4163901781592296 | T | T | T |
| 0.0720833882634231 | 0.0909607843645397 | 0.4173971845475132 | T | T | T |
| 0.4924764857007872 | 0.1759627826324485 | 0.4162383161191000 | T | T | T |
| 0.0436772508830148 | 0.2159451308361766 | 0.4178132436670558 | T | T | T |
| 0.5613365798542329 | 0.2491244924638453 | 0.4162332646141030 | T | T | T |
| 0.0591060271548278 | 0.2933271703703147 | 0.4180431215624477 | T | T | T |
| 0.6531019729721829 | 0.4119406606943301 | 0.4162993910697029 | T | T | T |
| 0.1439915560631015 | 0.4553427067709146 | 0.4178590604131550 | T | T | T |
| 0.6703632813412201 | 0.4900866036324125 | 0.4163047616465487 | T | T | T |
| 0.2133830152495111 | 0.5289339815106916 | 0.4190092769504007 | T | T | T |
| 0.6402767392625293 | 0.6139230981034802 | 0.4166418143677705 | T | T | T |
| 0.3748796764277983 | 0.6289467180887436 | 0.4174830697486617 | T | T | T |
| 0.5938617405239712 | 0.6493623545599558 | 0.4168311452081780 | T | T | T |
| 0.4555463633276040 | 0.6555553396138277 | 0.4174284504943078 | T | T | T |
| 0.2130410452823061 | 0.0360309623335733 | 0.5836175920553882 | T | T | T |
| 0.1449747917160962 | 0.0416984632943528 | 0.5838681383822388 | T | T | T |
| 0.3734401379747052 | 0.0895586037045959 | 0.5830257671670540 | T | T | T |
| 0.0575753836952984 | 0.1172674051204370 | 0.5842639116330374 | T | T | T |
| 0.4540467912237803 | 0.1434050680763395 | 0.5829778001981606 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0433262962767076 | 0.1800665786047909 | 0.5844644546912862 | T | T | T |
| 0.5908131575609135 | 0.2889893702815694 | 0.5829741229977888 | T | T | T |
| 0.0735261775598997 | 0.3347310800309089 | 0.5846281447557287 | T | T | T |
| 0.6368830077247657 | 0.3708646706478098 | 0.5829991728134422 | T | T | T |
| 0.1139262311170478 | 0.4161488585619765 | 0.5818814643254793 | T | T | T |
| 0.6710524073181252 | 0.5263070907897404 | 0.5829986350821168 | T | T | T |
| 0.2528759469801748 | 0.5572060283091773 | 0.5860866443953066 | T | T | T |
| 0.6561344035279888 | 0.5887684398085467 | 0.5832551439734585 | T | T | T |
| 0.3337976843660405 | 0.6077760826760055 | 0.5850545702740122 | T | T | T |
| 0.5637715053132225 | 0.6587840634615870 | 0.5836182045149548 | T | T | T |
| 0.4941930628811472 | 0.6615386058165259 | 0.5837194876048432 | T | T | T |
| 0.2513769193921859 | 0.0417091509450022 | 0.7501648349400998 | T | T | T |
| 0.1162783782467282 | 0.0531959364446847 | 0.7505965114063868 | T | T | T |
| 0.3320657341416318 | 0.0687986874726708 | 0.7498853095377896 | T | T | T |
| 0.4924399166269559 | 0.1758985931339762 | 0.7496248031053867 | T | T | T |
| 0.0437333633615967 | 0.2165075306797871 | 0.7509701388216065 | T | T | T |
| 0.1319309080046454 | 0.4636125513642560 | 0.7511949073346564 | T | T | T |
| 0.6403770047552964 | 0.6139308625162571 | 0.7501412282009082 | T | T | T |
| 0.5935951192589290 | 0.6489263981684422 | 0.7504253358779741 | T | T | T |
| 0.0722456714516056 | 0.0910771321349756 | 0.7507667999931208 | T | T | T |
| 0.5612840128045343 | 0.2491120525519578 | 0.7495751590856272 | T | T | T |
| 0.0577115191139655 | 0.2933390267805051 | 0.7510883046010766 | T | T | T |
| 0.6530687660318678 | 0.4119199553837972 | 0.7496326266351416 | T | T | T |
| 0.6702361741095428 | 0.4900827123426792 | 0.7497491092401867 | T | T | T |
| 0.3753347093578471 | 0.6271307892029792 | 0.7507854115829979 | T | T | T |
| 0.4557637977859968 | 0.6548762713993418 | 0.7506525261649065 | T | T | T |
| 0.2131189949864169 | 0.0361697716530872 | 0.9168670972575748 | T | T | T |
| 0.1450397202660616 | 0.0417893316400633 | 0.9172002050837216 | T | T | T |
| 0.3734484241552660 | 0.0895352049456769 | 0.9165659929603851 | T | T | T |
| 0.0574324305170068 | 0.1171752238866721 | 0.9173866000619535 | T | T | T |
| 0.4540369235301367 | 0.1434115112190020 | 0.9163083709501293 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0432100668715698 | 0.1800125552413207 | 0.9174092965972634 | T | T | T |
| 0.5907996191901029 | 0.2889923662262723 | 0.9161553254106501 | T | T | T |
| 0.0735078361198181 | 0.3348407272368630 | 0.9175508072642664 | T | T | T |
| 0.6368756385965999 | 0.3708563369231013 | 0.9162008178855441 | T | T | T |
| 0.1138938767791487 | 0.4161732845352976 | 0.9205354264697065 | T | T | T |
| 0.6710734262396792 | 0.5263177554074437 | 0.9165930092690362 | T | T | T |
| 0.2528172048949773 | 0.5573034106057547 | 0.9159386940807988 | T | T | T |
| 0.6561654738553625 | 0.5887765036783540 | 0.9168216184190536 | T | T | T |
| 0.3337507234537193 | 0.6077248771202721 | 0.9166722997105033 | T | T | T |
| 0.5637684002836661 | 0.6587868455792374 | 0.9173207884583254 | T | T | T |
| 0.4942510651347202 | 0.6616869782618641 | 0.9175323560230202 | T | T | T |
| 0.2153869010744511 | 0.5270618704343818 | 0.7510147758896190 | T | T | T |
| 0.0847064446436325 | 0.5002259480396426 | 0.7609086235233693 | T | T | T |
| 0.0794406734747606 | 0.5154508788243642 | 0.6395202425606358 | T | T | T |

OH\_N-CNT(9,9) #### KPOINTS: 1x1x3 #### E= -853.61364053 eV

1.0000000000000000

18.1865334800000014 -10.5000000000000000 0.0000000000000000

0.0000000000000000 21.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4005503900000003

C N O H

107 1 1 1

Selective dynamics

Direct

0.1979236280963909 0.0284115162329239 0.0823882765461846 T T T

0.1363083385353001 0.0392572107380435 0.0823616703675854 T T T

0.3469756859551121 0.0640020684511494 0.0826137999760354 T T T

0.4250185652093404 0.1073693730292818 0.0827556289611173 T T T

0.0562197887704713 0.1148624319649959 0.0819891783395928 T T T

0.0398666677651045 0.1728166906963377 0.0819608137460522 T T T

0.5675255375824309 0.2330506848445251 0.0828740220686873 T T T

0.6243095659655539 0.3080019884516514 0.0828805709502188 T T T

0.0528498060390296 0.3142784093140597 0.0820040739345578 T T T

0.0811388726213397 0.3909215769784455 0.0848364595001745 T T T

0.6960264623785799 0.4637193128962660 0.0828813733377897 T T T

0.7071488384518958 0.5363280230403070 0.0828044264490228 T T T

0.1979195562409177 0.5362368102034211 0.0804849080633335 T T T

0.2713368292818270 0.5954322088122702 0.0813553963333039 T T T

0.6732112957161888 0.6508511457944667 0.0825872567358809 T T T

0.6294196375128399 0.6850659330416040 0.0825143576469907 T T T

0.4268418393055371 0.6792076272754549 0.0824604558353784 T T T

0.5021302941864965 0.6988676919842185 0.0824482490423185 T T T

0.2329374497759051 0.0303443654790200 0.2491719949520879 T T T

0.3078406386577346 0.0482939171081523 0.2492742226872495 T T T

0.4632406753048237 0.1346135372546844 0.2494885359464321 T T T

0.5348185728701604 0.1977463492219483 0.2495865568801441 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0439071949619121 | 0.2760511074392342 | 0.2484395052528714 | T | T | T |
| 0.1049315578860606 | 0.4294949926791034 | 0.2487502437653951 | T | T | T |
| 0.1625966815600795 | 0.5046706574494753 | 0.2474336430483068 | T | T | T |
| 0.3093385044623928 | 0.6221454161177573 | 0.2488736441672471 | T | T | T |
| 0.3875608922410401 | 0.6637932953344247 | 0.2488126828768425 | T | T | T |
| 0.1103119359040015 | 0.0518988312729078 | 0.2489623290702275 | T | T | T |
| 0.0702678613309686 | 0.0900516034275423 | 0.2487576040875977 | T | T | T |
| 0.0372842721124202 | 0.2053991965127433 | 0.2485500461864759 | T | T | T |
| 0.6479072324771288 | 0.3470698969309749 | 0.2495833206817641 | T | T | T |
| 0.6840035619025989 | 0.4252081817641633 | 0.2495942760343589 | T | T | T |
| 0.7057340438115512 | 0.5696490155598716 | 0.2494526435790364 | T | T | T |
| 0.6887478563358338 | 0.6272669015309537 | 0.2492893451843420 | T | T | T |
| 0.6017072728287988 | 0.6953869997207671 | 0.2492122071549030 | T | T | T |
| 0.5377756176661098 | 0.7024305478168679 | 0.2492107001934363 | T | T | T |
| 0.1979103042630809 | 0.0284347533473887 | 0.4157824388157415 | T | T | T |
| 0.1362298329283644 | 0.0392437686366320 | 0.4156164929667046 | T | T | T |
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| 0.4250019224608444 | 0.1074200433877330 | 0.4161272849597967 | T | T | T |
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| 0.6242847947641040 | 0.3080728280591274 | 0.4162513521640631 | T | T | T |
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| 0.0838308022601478 | 0.3906017834442634 | 0.4157150566524118 | T | T | T |
| 0.6962078711441337 | 0.4637436413985899 | 0.4162006266918889 | T | T | T |
| 0.7071180186971752 | 0.5362950056081748 | 0.4161420839097996 | T | T | T |
| 0.1968020086042096 | 0.5385579916841479 | 0.4157009471576483 | T | T | T |
| 0.2706718034226923 | 0.5975034103195997 | 0.4156044543902325 | T | T | T |
| 0.6731949233283170 | 0.6507673856304893 | 0.4159810300550265 | T | T | T |
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|--------------------|--------------------|--------------------|---|---|---|
| 0.5021050554820159 | 0.6991611234457970 | 0.4156506005532161 | T | T | T |
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| 0.4632409626098100 | 0.1346077628546742 | 0.5828237737150247 | T | T | T |
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| 0.0371956191366369 | 0.2054064876525721 | 0.5824196646412703 | T | T | T |
| 0.0437019321502288 | 0.2760409605021264 | 0.5825482067380384 | T | T | T |
| 0.6479072072969357 | 0.3470726625065630 | 0.5829156958011639 | T | T | T |
| 0.6840020723432488 | 0.4252104364176595 | 0.5828371667547524 | T | T | T |
| 0.1045066511947876 | 0.4296079672878010 | 0.5825737823292850 | T | T | T |
| 0.1623404033052598 | 0.5047100027797947 | 0.5836751514322385 | T | T | T |
| 0.7057426496453396 | 0.5696519349931799 | 0.5827661763813973 | T | T | T |
| 0.6887461577123254 | 0.6272685984565374 | 0.5827301491336689 | T | T | T |
| 0.3093362049369187 | 0.6221361246412970 | 0.5822985067932516 | T | T | T |
| 0.3875435189596749 | 0.6637651167844257 | 0.5823411269069613 | T | T | T |
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| 0.3469754893641530 | 0.0640009079864379 | 0.7494109179214039 | T | T | T |
| 0.4250204171828560 | 0.1073658140453714 | 0.7495046292227615 | T | T | T |
| 0.5675226838633519 | 0.2330520637605537 | 0.7495928191239835 | T | T | T |
| 0.0526234903723395 | 0.3143630122936975 | 0.7489076195002728 | T | T | T |
| 0.0805880085499355 | 0.3909568806418626 | 0.7460392454393554 | T | T | T |
| 0.1977082696019849 | 0.5363362638763520 | 0.7504375816512816 | T | T | T |
| 0.2712190828571370 | 0.5953609265376030 | 0.7496619671022200 | T | T | T |
| 0.4268491715017907 | 0.6791984745999806 | 0.7486080440108420 | T | T | T |
| 0.0562718524972068 | 0.1149075735969116 | 0.7489100166373722 | T | T | T |
| 0.0398403950942499 | 0.1728100409993414 | 0.7489075909427491 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.6243106138226594 | 0.3080055659511233 | 0.7496252683425720 | T | T | T |
| 0.6960221382623056 | 0.4637210431493551 | 0.7495209079199002 | T | T | T |
| 0.7071495987783235 | 0.5363289755648978 | 0.7494596337229413 | T | T | T |
| 0.6732017085751243 | 0.6508539233876413 | 0.7493408280226181 | T | T | T |
| 0.6294155944224575 | 0.6850617050975065 | 0.7491672582095471 | T | T | T |
| 0.5021467194407472 | 0.6988736807171496 | 0.7487958226123623 | T | T | T |
| 0.2328815911117334 | 0.0302333765305705 | 0.9158057825954072 | T | T | T |
| 0.3078060638741193 | 0.0482636296885534 | 0.9159689995962765 | T | T | T |
| 0.1104791902027104 | 0.0520474516652009 | 0.9155712617382821 | T | T | T |
| 0.0704678292885524 | 0.0901257446528328 | 0.9154747407427547 | T | T | T |
| 0.4632122331657221 | 0.1346356795552600 | 0.9161571828919755 | T | T | T |
| 0.5347514919758792 | 0.1977822628474955 | 0.9162195317347185 | T | T | T |
| 0.0373691881877639 | 0.2059346374555233 | 0.9154130869073546 | T | T | T |
| 0.0427868974528418 | 0.2759898828900560 | 0.9153691129194037 | T | T | T |
| 0.6480072124201682 | 0.3470602123264225 | 0.9162468492387036 | T | T | T |
| 0.6839061783730085 | 0.4252154384608446 | 0.9162188578594074 | T | T | T |
| 0.0909363615856521 | 0.4345083878958974 | 0.9155692896063919 | T | T | T |
| 0.7057773578019624 | 0.5696934747944290 | 0.9161102808186162 | T | T | T |
| 0.6887358925631917 | 0.6272818443479958 | 0.9160073955018985 | T | T | T |
| 0.3102630828952044 | 0.6207930276574412 | 0.9154980417025755 | T | T | T |
| 0.3879753892019517 | 0.6631515577096709 | 0.9154965350575803 | T | T | T |
| 0.6018558496188644 | 0.6955817526988525 | 0.9158105613917626 | T | T | T |
| 0.5377297841444327 | 0.7022082441636135 | 0.9156630292574590 | T | T | T |
| 0.1652680242920610 | 0.5034742169334794 | 0.9155223360512305 | T | T | T |
| 0.0356890059563520 | 0.4571024954637302 | 0.9072736567417047 | T | T | T |
| 0.0316022827501268 | 0.4737529509199111 | 0.0267300870070256 | T | T | T |

OH\_N-CNT(10,10) #### KPOINTS: 1x1x3 #### E= -948.87187048 eV

1.0000000000000000

19.0525588799999994 -11.0000000000000000 0.0000000000000000

0.0000000000000000 22.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4010841699999999

C N O H

119 1 1 1

Selective dynamics

Direct

0.1872127516408682 0.0228266986989858 0.0826347008706203 T T T

0.2540392989042279 0.0273662576931148 0.0828061820427928 T T T

0.0839261330978743 0.0637714624362163 0.0822723811063085 T T T

0.4014879209606503 0.0837593643314022 0.0829449645629728 T T T

0.0523569512014897 0.1065814784765388 0.0821163696285549 T T T

0.4749960970093429 0.1318388400529599 0.0831555645102201 T T T

0.0305380301713518 0.2231894544577322 0.0818401107244340 T T T

0.6069889435726332 0.2574458000330077 0.0831672375926182 T T T

0.0395182765953832 0.2917549437679615 0.0816444623669134 T T T

0.6591455527198387 0.3297830780505609 0.0831633899804202 T T T

0.0975276960030389 0.4382829946491674 0.0818808312411508 T T T

0.7236298868073728 0.4781392364164232 0.0831443481872683 T T T

0.1500941282339579 0.5109820874059781 0.0806150301200111 T T T

0.7345317386158881 0.5475325773503051 0.0831984042157608 T T T

0.2851116430766500 0.6315397702021815 0.0820232028946674 T T T

0.7133402270383913 0.6645611270084610 0.0828867820599799 T T T

0.3588751581939013 0.6787808342375364 0.0819668868708855 T T T

0.6804924482726498 0.7061969251494523 0.0827897085559100 T T T

0.5066058356579282 0.7365818860885619 0.0825243238367165 T T T

0.5742553643178625 0.7430839769167000 0.0825494879077204 T T T

0.0419248405972876 0.1325510990693393 0.2488284238601500 T T T

0.5767699324228371 0.2230255159281314 0.2498553954217014 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0486029669435753 | 0.3273910311851608 | 0.2488195031539574 | T | T | T |
| 0.0781716485584324 | 0.4011686288877879 | 0.2489484543769827 | T | T | T |
| 0.1812748074067984 | 0.5445663802851554 | 0.2489445407386872 | T | T | T |
| 0.7346335272894885 | 0.5800801751764870 | 0.2497645748192574 | T | T | T |
| 0.2491595403284600 | 0.6050647126315635 | 0.2487790974971452 | T | T | T |
| 0.3963338816856127 | 0.6982391990773914 | 0.2488469206027384 | T | T | T |
| 0.6586635430366455 | 0.7216738533682407 | 0.2494506003797064 | T | T | T |
| 0.6052117304958823 | 0.7401276144828932 | 0.2492636930346921 | T | T | T |
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| 0.2899127356333577 | 0.0357137823980284 | 0.2495133793335521 | T | T | T |
| 0.1051030260988923 | 0.0475498281131465 | 0.2490111611796025 | T | T | T |
| 0.3639567240432177 | 0.0641889506648306 | 0.2496426904053238 | T | T | T |
| 0.5105272874522276 | 0.1600088027381206 | 0.2497941503117063 | T | T | T |
| 0.0310336863772302 | 0.1910173278974332 | 0.2488175628254780 | T | T | T |
| 0.6805971798928215 | 0.3671338538805528 | 0.2498840408150212 | T | T | T |
| 0.7128216164283753 | 0.4416076092799536 | 0.2498602302560990 | T | T | T |
| 0.7241496066469686 | 0.6388693218369071 | 0.2496741665272001 | T | T | T |
| 0.4704383717697805 | 0.7272670876366188 | 0.2489914056497830 | T | T | T |
| 0.1871937420717690 | 0.0227913210182552 | 0.4159104390330530 | T | T | T |
| 0.2540238418710215 | 0.0273329355108960 | 0.4161355921976218 | T | T | T |
| 0.0839739443782019 | 0.0637996961054247 | 0.4156613481567891 | T | T | T |
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| 0.0305384971433210 | 0.2232394812997564 | 0.4156764938048001 | T | T | T |
| 0.6069865656352406 | 0.2574445886531568 | 0.4165645342429790 | T | T | T |
| 0.0392427275245920 | 0.2917341576621704 | 0.4159442299627546 | T | T | T |
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| 0.0969372357163022 | 0.4383723275672918 | 0.4158527914317239 | T | T | T |
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| 0.1497283360516037 | 0.5110351232933944 | 0.4169185225068461 | T | T | T |

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| 0.7345312127206107 | 0.5475346895678758 | 0.4163853997797304 | T | T | T |
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| 0.5066128824804520 | 0.7365695287145301 | 0.4155209369073199 | T | T | T |
| 0.5742699640986357 | 0.7430998066441851 | 0.4158652960299117 | T | T | T |
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| 0.0417918236473717 | 0.1325057000339247 | 0.5821892629941305 | T | T | T |
| 0.5105416805375904 | 0.1600548711132341 | 0.5830641348774409 | T | T | T |
| 0.0309086994854123 | 0.1909858503952200 | 0.5821633512920906 | T | T | T |
| 0.5767901198948908 | 0.2230203065877632 | 0.5831924188608023 | T | T | T |
| 0.0479295764146820 | 0.3283032622136183 | 0.5823741283989629 | T | T | T |
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| 0.0744498945816803 | 0.4014604090562336 | 0.5793255950325434 | T | T | T |
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| 0.4706710479112675 | 0.7274933109062588 | 0.5820877206634431 | T | T | T |
| 0.6051942574451037 | 0.7401869517730618 | 0.5825835804935072 | T | T | T |
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| 0.0521689020965579 | 0.1063533606063728 | 0.7488000510526513 | T | T | T |
| 0.6069664805768855 | 0.2573978350476133 | 0.7498585733546466 | T | T | T |
| 0.0828987677381380 | 0.4426592861561308 | 0.7489651218107483 | T | T | T |

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| 0.7345340670438865 | 0.5475266481816798 | 0.7497880251585199 | T | T | T |
| 0.2862167350752190 | 0.6305178909570690 | 0.7486563488438137 | T | T | T |
| 0.3593524875282768 | 0.6785129626138416 | 0.7487668786828022 | T | T | T |
| 0.6802934126931917 | 0.7060062310582887 | 0.7494832253510506 | T | T | T |
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| 0.4750125895710693 | 0.1318531965017020 | 0.7497741355413351 | T | T | T |
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| 0.7236158889001482 | 0.4781230744836275 | 0.7498505034850161 | T | T | T |
| 0.7131531730513064 | 0.6643968178703746 | 0.7496306949358131 | T | T | T |
| 0.5067219625924545 | 0.7366705386630759 | 0.7490061063550761 | T | T | T |
| 0.1568517427835473 | 0.0268070636839658 | 0.9159186647267101 | T | T | T |
| 0.2899556591544750 | 0.0359379836847288 | 0.9161553487976603 | T | T | T |
| 0.1049317157958221 | 0.0473138904327874 | 0.9157113858054635 | T | T | T |
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| 0.5767907018816235 | 0.2230215710334604 | 0.9165205528408820 | T | T | T |
| 0.0482866365256499 | 0.3282421944228544 | 0.9151452299004492 | T | T | T |
| 0.6805803797918406 | 0.3671707940071148 | 0.9164676041167660 | T | T | T |
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| 0.7347489450987824 | 0.5801359963058665 | 0.9165075509267090 | T | T | T |
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| 0.7241557762199498 | 0.6388497274382069 | 0.9163098258601444 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3966328377282082 | 0.6982827574235454 | 0.9157287462749467 | T | T | T |
| 0.6584674970634233 | 0.7215370866200762 | 0.9161279909971162 | T | T | T |
| 0.4706636863664418 | 0.7275236993383150 | 0.9158100717537105 | T | T | T |
| 0.6051676939173888 | 0.7401568298969632 | 0.9159466037539110 | T | T | T |
| 0.1522808466772961 | 0.5102391700092822 | 0.7487057544764585 | T | T | T |
| 0.0279221901136306 | 0.4613210691975563 | 0.7412223678395012 | T | T | T |
| 0.0210701764157112 | 0.4737218920912120 | 0.8623525677390804 | T | T | T |

OH\_N-CNT(8,0) #### KPOINTS: 2x2x2 #### E= -499.54860755 eV

1.0000000000000000

12.9903810600000007 -7.5000000000000000 0.0000000000000000

0.0000000000000000 15.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5305455000000006

C N O H

63 1 1 1

Selective dynamics

Direct

0.0791309539999637 0.1943520044845621 0.0829549735419632 T T T

0.4981318144023143 0.2614667157064224 0.0829389956434583 T T T

0.1363286828841450 0.3782660561627494 0.0817168580960211 T T T

0.5591839822427772 0.4456194623880915 0.0832966536318726 T T T

0.1539495656646718 0.0823090450748228 0.0832565372443269 T T T

0.3279279204591905 0.1085508822742993 0.0829120560182919 T T T

0.3043252644018923 0.5285604794945894 0.0817437416587272 T T T

0.4776172049512808 0.5514601119666751 0.0830470268525897 T T T

0.2336210234142617 0.0765123369059201 0.1666528552148689 T T T

0.0999269191567417 0.1236492824162153 0.1666280402371448 T T T

0.4209081611764937 0.1741334612844777 0.1665284984610606 T T T

0.2099141993680876 0.4679751963851582 0.1676561657459746 T T T

0.5350629680695212 0.5136839381940459 0.1667392863536322 T T T

0.3973109763569244 0.5558975190446407 0.1656341833056700 T T T

0.0923826642558357 0.2827741757017742 0.1656395681977730 T T T

0.5464650379200486 0.3573115378644284 0.1666916677331864 T T T

0.0927825036801321 0.2835342781906138 0.3333990869307816 T T T

0.5464100293018326 0.3571503853666650 0.3330024058273514 T T T

0.2337496877131254 0.0764425228592768 0.3328803599592305 T T T

0.1003283486350235 0.1240977503484191 0.3326172098538217 T T T

0.4210650206624630 0.1738428778534004 0.3332782783726632 T T T

0.2092447229892977 0.4689322791205544 0.3314174767566609 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5346387743658774 | 0.5134028937486375 | 0.3326511537332151 | T | T | T |
| 0.3966091964969689 | 0.5556976933466589 | 0.3333867988508655 | T | T | T |
| 0.1545624225187567 | 0.0830700879939992 | 0.4163753879025692 | T | T | T |
| 0.3280171148909436 | 0.1085077259269010 | 0.4166862649622825 | T | T | T |
| 0.3041712074152945 | 0.5303164855531576 | 0.4173797875291074 | T | T | T |
| 0.4764246545105282 | 0.5502639611948552 | 0.4163442021755329 | T | T | T |
| 0.0804935028166485 | 0.1954296729699097 | 0.4163378320721481 | T | T | T |
| 0.4979393110945483 | 0.2613327936835678 | 0.4167120796250265 | T | T | T |
| 0.1349052178530489 | 0.3788603301265650 | 0.4174678085131863 | T | T | T |
| 0.5583993305026423 | 0.4451269532136387 | 0.4164961908062328 | T | T | T |
| 0.0820301429340242 | 0.1962470957656968 | 0.5824563665689221 | T | T | T |
| 0.4980787363185292 | 0.2613361029201287 | 0.5829708444616896 | T | T | T |
| 0.1346426766003778 | 0.3790497001125436 | 0.5827550860829676 | T | T | T |
| 0.5585612396243553 | 0.4450826132362473 | 0.5831834414179211 | T | T | T |
| 0.1545898961834793 | 0.0829786576184423 | 0.5831322442246533 | T | T | T |
| 0.3279685602951678 | 0.1083806563070681 | 0.5829020121266687 | T | T | T |
| 0.3040975005747542 | 0.5305009968289282 | 0.5828400867434421 | T | T | T |
| 0.4755084636623099 | 0.5487967687028716 | 0.5825487945616433 | T | T | T |
| 0.2338008704809057 | 0.0764797887949033 | 0.6667268985726016 | T | T | T |
| 0.1016272627788661 | 0.1251348955269339 | 0.6666179547406953 | T | T | T |
| 0.4209576669196196 | 0.1739172183367197 | 0.6665675075756602 | T | T | T |
| 0.1995789757921855 | 0.4822880566816921 | 0.6654654726042947 | T | T | T |
| 0.5336694308073830 | 0.5122889738399964 | 0.6667197478779985 | T | T | T |
| 0.3938233942064943 | 0.5507247389645208 | 0.6652569472112936 | T | T | T |
| 0.0976137175968155 | 0.2857118203133798 | 0.6651092784734186 | T | T | T |
| 0.5464490884973122 | 0.3570622975668974 | 0.6667428820985494 | T | T | T |
| 0.0953677218610058 | 0.2842836812881768 | 0.8327654204528333 | T | T | T |
| 0.5464350642779369 | 0.3571712300622106 | 0.8330038318160501 | T | T | T |
| 0.2337540969439932 | 0.0765748228754647 | 0.8329247044883615 | T | T | T |
| 0.1006864460444527 | 0.1244768836868232 | 0.8328500457638732 | T | T | T |
| 0.4210548358890941 | 0.1738910499244119 | 0.8332081610073525 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5343546483319096 | 0.5130974419026101 | 0.8328865903724765 | T | T | T |
| 0.3954088314928254 | 0.5527280451717366 | 0.8328354735066728 | T | T | T |
| 0.1542554633996347 | 0.0828320782346049 | 0.9165366820162174 | T | T | T |
| 0.3279826100467482 | 0.1086296537488981 | 0.9167175337856726 | T | T | T |
| 0.3037895573461775 | 0.5253945387628435 | 0.9163318852922360 | T | T | T |
| 0.4766699359224612 | 0.5504792223748581 | 0.9166385688758040 | T | T | T |
| 0.0801791989020556 | 0.1952859844490073 | 0.9165500884468615 | T | T | T |
| 0.4980391643383778 | 0.2613857974548859 | 0.9166954015412228 | T | T | T |
| 0.1390483788209987 | 0.3782580909796155 | 0.9163037125219397 | T | T | T |
| 0.5587044370733814 | 0.4453618195780740 | 0.9166412890954008 | T | T | T |
| 0.2090133545341960 | 0.4693193207442247 | 0.8371314718237007 | T | T | T |
| 0.1495401411522877 | 0.5421358529106786 | 0.6440373202186419 | T | T | T |
| 0.2004501061786386 | 0.6139632074882319 | 0.6602868218250274 | T | T | T |

OH\_N-CNT(9,0) #### KPOINTS: 2x2x2 #### E= -563.66036329 eV

1.0000000000000000

13.8564064600000005 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5367054200000005

C N O H

71 1 1 1

Selective dynamics

Direct

0.1972753287127094 0.0666168048361014 0.0832553962313324 T T T

0.0877820888709865 0.1311302448761151 0.0828594630645633 T T T

0.3704866865057285 0.1241380690033874 0.0832580436520238 T T T

0.0919965850714420 0.2860431771765638 0.0842353206809464 T T T

0.5241023147795880 0.2755313252254619 0.0831469442972911 T T T

0.1794868598293648 0.4706109252726919 0.0834653449515139 T T T

0.5821023393976966 0.4486168561035163 0.0832759320619146 T T T

0.3644362423473431 0.5576156573937053 0.0840187409017598 T T T

0.5176453647479270 0.5583039996970095 0.0829161059785094 T T T

0.1299019720519322 0.0837491417040587 0.1668790979465133 T T T

0.2807202325134319 0.0801673860334475 0.1670364629702896 T T T

0.4547986692886439 0.1920080542889058 0.1665480488596363 T T T

0.0759093316566024 0.2019484898340833 0.1668459343084485 T T T

0.5689122856563472 0.3653065819815619 0.1671145287090204 T T T

0.1250668804699151 0.3733924668409817 0.1670252383854197 T T T

0.5644745186329830 0.5156546843923036 0.1668141993600687 T T T

0.2770203547852757 0.5256807136114792 0.1668555516135210 T T T

0.4478285401714625 0.5717663746015658 0.1667349816286622 T T T

0.1297110816445744 0.0835867956718877 0.3333217852994381 T T T

0.2805457323974513 0.0801289338098137 0.3330764206768033 T T T

0.4545929933259872 0.1922323434601742 0.3334058227683214 T T T

0.0744880909879100 0.2011372628970507 0.3332946338992697 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5689937852574375 | 0.3655164668705097 | 0.3329602738814783 | T | T | T |
| 0.1253429539315372 | 0.3734547419018344 | 0.3317040724537961 | T | T | T |
| 0.5646505017226583 | 0.5158520898333517 | 0.3332823732705177 | T | T | T |
| 0.2771091134940041 | 0.5254368154558838 | 0.3316202883094083 | T | T | T |
| 0.4485747079922530 | 0.5731364345403365 | 0.3333360765286111 | T | T | T |
| 0.1968643233592668 | 0.0661427434077099 | 0.4167076592201953 | T | T | T |
| 0.0866321018604953 | 0.1302342793003731 | 0.4171683169867454 | T | T | T |
| 0.3702397397509110 | 0.1242965226561741 | 0.4168900427697537 | T | T | T |
| 0.0879335987327553 | 0.2842980751192873 | 0.4160927601451154 | T | T | T |
| 0.5240125943606256 | 0.2758238478251192 | 0.4169685015824809 | T | T | T |
| 0.1905053240591296 | 0.4601002636791399 | 0.4180111731869680 | T | T | T |
| 0.5825470662198171 | 0.4490333712080225 | 0.4166265687490091 | T | T | T |
| 0.3662031821395988 | 0.5617426601880018 | 0.4161568641729188 | T | T | T |
| 0.5184141697277778 | 0.5593210565925165 | 0.4170482222548492 | T | T | T |
| 0.1968631718158812 | 0.0663458189287820 | 0.5834501246567615 | T | T | T |
| 0.0863204884799144 | 0.1299986250158521 | 0.5827969544663850 | T | T | T |
| 0.3701588275474347 | 0.1244419027882539 | 0.5831689491522269 | T | T | T |
| 0.0875332856463474 | 0.2836890444127503 | 0.5837766458140915 | T | T | T |
| 0.5238644614860294 | 0.2759171387170467 | 0.5830868587030505 | T | T | T |
| 0.1914399269370017 | 0.4591253894781713 | 0.5811857295907839 | T | T | T |
| 0.5823732916902774 | 0.4490763576394203 | 0.5834220519509273 | T | T | T |
| 0.3668558121766117 | 0.5620856899037738 | 0.5837053194687756 | T | T | T |
| 0.5187345078832625 | 0.5597189430947118 | 0.5828199811065859 | T | T | T |
| 0.1294546528922886 | 0.0833772524314929 | 0.6667974742171903 | T | T | T |
| 0.2804701216763170 | 0.0801921306577310 | 0.6670318003797848 | T | T | T |
| 0.4544497836710403 | 0.1923928096903572 | 0.6665258987881336 | T | T | T |
| 0.0734182786443242 | 0.2004295527600245 | 0.6663555844915158 | T | T | T |
| 0.5688933788271885 | 0.3655705115371616 | 0.6671471530636478 | T | T | T |
| 0.1266778372473432 | 0.3730813127014270 | 0.6678137780213869 | T | T | T |
| 0.5649291052441928 | 0.5162124571173852 | 0.6667549160985118 | T | T | T |
| 0.2774332514501589 | 0.5238536081491533 | 0.6679114734439749 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4493918443914223 | 0.5742122692242931 | 0.6662445497094347 | T | T | T |
| 0.1296728779093384 | 0.0837138877519665 | 0.8331844032854304 | T | T | T |
| 0.2805975651730740 | 0.0802914148673974 | 0.8330029600835001 | T | T | T |
| 0.4545148555078707 | 0.1923263764752053 | 0.8334052227507004 | T | T | T |
| 0.0744726249332468 | 0.2013181451598346 | 0.8332520909710911 | T | T | T |
| 0.5687811604897447 | 0.3654728751428879 | 0.8329680158053787 | T | T | T |
| 0.1293773366162629 | 0.3733244373592626 | 0.8326254546160677 | T | T | T |
| 0.5646723672934417 | 0.5160165249251033 | 0.8332355250448058 | T | T | T |
| 0.2772703851782525 | 0.5209983563890986 | 0.8325291040371021 | T | T | T |
| 0.4485807960534856 | 0.5732317134892811 | 0.8332499412779356 | T | T | T |
| 0.1971100757232233 | 0.0665289700939917 | 0.9166176495193351 | T | T | T |
| 0.0871221720438279 | 0.1306449799186554 | 0.9172511887105321 | T | T | T |
| 0.3703357858553645 | 0.1241871018938509 | 0.9169425285323063 | T | T | T |
| 0.0903824102449886 | 0.2850150142411556 | 0.9166299519718784 | T | T | T |
| 0.5240652375793567 | 0.2757240505217893 | 0.9170424033817997 | T | T | T |
| 0.5822426918134882 | 0.4488563497817799 | 0.9165999964781344 | T | T | T |
| 0.3655575470842324 | 0.5591112926351446 | 0.9166877929240627 | T | T | T |
| 0.5181841214493761 | 0.5590227613370587 | 0.9171418728542812 | T | T | T |
| 0.1911144821941706 | 0.4593942049261770 | 0.9126605703550847 | T | T | T |
| 0.1228037782284909 | 0.5173063122638459 | 0.1016484633770405 | T | T | T |
| 0.1643720444682276 | 0.5854487592886586 | 0.0796724291432860 | T | T | T |

OH\_N-CNT(10,0) ### KPOINTS: 2x2x2 ### E= -628.13623353 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C N O H

79 1 1 1

Selective dynamics

Direct

0.2405023839268081 0.0611337680563092 0.0837592844039556 T T T

0.1095448389170011 0.0837914381278973 0.0839321791475546 T T T

0.4065156208217649 0.1407358790935876 0.0838099738071935 T T T

0.5430612732360087 0.2907814189827858 0.0839579495144921 T T T

0.1152820083454203 0.3634517536318714 0.0818635334308750 T T T

0.2457394781552081 0.5159344618554255 0.0866132261731694 T T T

0.5426227077219499 0.5632150981661387 0.0842216507600353 T T T

0.4118012860944272 0.5872131309494675 0.0846692443282589 T T T

0.0653745821883589 0.2003381880469610 0.0839203134417197 T T T

0.5953216874804569 0.4532765494539046 0.0840578360183309 T T T

0.1667239028612309 0.0590701865742566 0.1671025666961726 T T T

0.4824223805071889 0.2101746660963993 0.1671481945089627 T T T

0.1724514666319522 0.4454235270029355 0.1674876787595734 T T T

0.4840884943829479 0.5866683409742540 0.1671948222128133 T T T

0.3232699412541579 0.0896684777790087 0.1670006369215500 T T T

0.0746446775343365 0.1325474700631371 0.1671214244481196 T T T

0.0789864648643050 0.2792654477084351 0.1656558860892675 T T T

0.5823082665927650 0.3747879988512616 0.1672942202540695 T T T

0.5810890961442524 0.5179005593355580 0.1672965018601043 T T T

0.3294556546159253 0.5630801544977503 0.1678641938043650 T T T

0.3232287898141515 0.0896508328518162 0.3339585343026780 T T T

0.0742064848924264 0.1323519459064076 0.3335973327902648 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0778176041643943 | 0.2786093098054069 | 0.3335343448707541 | T | T | T |
| 0.5824107514906017 | 0.3747341836908403 | 0.3339030934677386 | T | T | T |
| 0.5815038552106824 | 0.5181022056265575 | 0.3342479505627700 | T | T | T |
| 0.3299898304875802 | 0.5625934746496030 | 0.3350713262512814 | T | T | T |
| 0.1666660873952990 | 0.0590769183579817 | 0.3337758789414239 | T | T | T |
| 0.4824383109606045 | 0.2101206738254989 | 0.3339183737468532 | T | T | T |
| 0.1721468609201652 | 0.4439858712139765 | 0.3346684068965882 | T | T | T |
| 0.4848092302838045 | 0.5870738857943627 | 0.3345074803764432 | T | T | T |
| 0.0640863968004005 | 0.1997786055264231 | 0.4163609352947383 | T | T | T |
| 0.5954192296342949 | 0.4533922683611131 | 0.4172179211792001 | T | T | T |
| 0.2405663554215198 | 0.0611137152539605 | 0.4170969961833250 | T | T | T |
| 0.1095874504527281 | 0.0838800351767241 | 0.4168103172413938 | T | T | T |
| 0.4065703516026146 | 0.1407847087740176 | 0.4171313691741302 | T | T | T |
| 0.5431872080104819 | 0.2907899198641495 | 0.4170914128857701 | T | T | T |
| 0.1146163987469148 | 0.3623862610646978 | 0.4178123681549893 | T | T | T |
| 0.2466151189014077 | 0.5135466601693865 | 0.4193143350371981 | T | T | T |
| 0.5433223088732648 | 0.5639293330003912 | 0.4175437175577750 | T | T | T |
| 0.4119132444076942 | 0.5865490229450028 | 0.4177326630110415 | T | T | T |
| 0.2406062871193954 | 0.0609343952388174 | 0.5837260082409229 | T | T | T |
| 0.1096231613117768 | 0.0836757183593593 | 0.5838514939504202 | T | T | T |
| 0.4066296223739911 | 0.1404468366503006 | 0.5837882217495292 | T | T | T |
| 0.5430748320432423 | 0.2906301761537729 | 0.5839473569070543 | T | T | T |
| 0.1157712913892919 | 0.3621764148996612 | 0.5852324726200465 | T | T | T |
| 0.2466103349545561 | 0.5143486811191306 | 0.5859471038491662 | T | T | T |
| 0.5435235086964432 | 0.5638231636558466 | 0.5842053180277812 | T | T | T |
| 0.4121076604760041 | 0.5863615155620470 | 0.5848361442890685 | T | T | T |
| 0.0647702077224406 | 0.1996636547512809 | 0.5835711555688741 | T | T | T |
| 0.5953505072612091 | 0.4532293006116750 | 0.5840522741137462 | T | T | T |
| 0.1668101941517998 | 0.0588818481771016 | 0.6670316022276617 | T | T | T |
| 0.4825349556612465 | 0.2099481795528036 | 0.6670107599672065 | T | T | T |
| 0.1732074772367716 | 0.4433840217588467 | 0.6692919881688641 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4845676664462692 | 0.5862832482718301 | 0.6679110571162467 | T | T | T |
| 0.3233463284502494 | 0.0892417339026568 | 0.6669083265233672 | T | T | T |
| 0.0747615464726436 | 0.1323181304992076 | 0.6670233056821504 | T | T | T |
| 0.0807614928226346 | 0.2784213730503349 | 0.6671757142585042 | T | T | T |
| 0.5821701000028326 | 0.3746543535546497 | 0.6672691602617811 | T | T | T |
| 0.5815647577136493 | 0.5181002052267688 | 0.6673132327413461 | T | T | T |
| 0.3308699430561292 | 0.5635846612839377 | 0.6690870402861245 | T | T | T |
| 0.3232351797995068 | 0.0892792241692176 | 0.8338866241438065 | T | T | T |
| 0.0748430086185879 | 0.1323795016337415 | 0.8336805292875412 | T | T | T |
| 0.0833823085504824 | 0.2796681190520178 | 0.8338638836140915 | T | T | T |
| 0.5822863478505177 | 0.3746944837809847 | 0.8339374504535705 | T | T | T |
| 0.5814728423307817 | 0.5179473096319269 | 0.8342589757193460 | T | T | T |
| 0.3309157365533255 | 0.5650152510846986 | 0.8332723837099417 | T | T | T |
| 0.1666082710191444 | 0.0587360778255920 | 0.8337342263282175 | T | T | T |
| 0.4824782540430493 | 0.2099943373713055 | 0.8338364646907124 | T | T | T |
| 0.4836098949865335 | 0.5851562007337536 | 0.8345516881674891 | T | T | T |
| 0.0663364935641975 | 0.2003408389231931 | 0.9175772373870564 | T | T | T |
| 0.5954437711265060 | 0.4532910002921522 | 0.9173474396187504 | T | T | T |
| 0.2405528219554415 | 0.0609792769073341 | 0.9170531446809772 | T | T | T |
| 0.1095138262344924 | 0.0834885271564560 | 0.9169720557337993 | T | T | T |
| 0.4065763455479203 | 0.1406547583458904 | 0.9170870784322840 | T | T | T |
| 0.5430743748538571 | 0.2907905294291875 | 0.9170705398897190 | T | T | T |
| 0.1202745931733194 | 0.3631130742728227 | 0.9162947400609330 | T | T | T |
| 0.2404808701026872 | 0.5293800403939941 | 0.9136410843332223 | T | T | T |
| 0.5425391968944979 | 0.5629254213071206 | 0.9176820612433310 | T | T | T |
| 0.4102223022985936 | 0.5843686466067199 | 0.9174773458582891 | T | T | T |
| 0.1725258750781722 | 0.4434824885047096 | 0.8324647884762230 | T | T | T |
| 0.2020545349753483 | 0.5888418950354742 | 0.8914385662480752 | T | T | T |
| 0.2515631943329434 | 0.6509470381560276 | 0.9000558808658279 | T | T | T |

OH\_N-CNT(11,0) ### KPOINTS: 2x2x2 ### E= -692.07409870 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C N O H

87 1 1 1

Selective dynamics

Direct

0.1511827125626731 0.0533050221003165 0.0831375291047066 T T T

0.2961521204221077 0.0738379558094285 0.0831666425150108 T T T

0.0646235925921129 0.1235708136574734 0.0833230530547617 T T T

0.4505526480821983 0.1766845497049699 0.0834319389778093 T T T

0.0627023140127999 0.2588615245388503 0.0832096392352517 T T T

0.5670649121115197 0.3263911569327665 0.0832008171527742 T T T

0.1401737669523985 0.4159823175236160 0.0823446047579587 T T T

0.6077508097196732 0.4780258344088688 0.0831669790654993 T T T

0.2790321290970820 0.5454297116827389 0.0823304924346304 T T T

0.5578218160795685 0.5821078568665263 0.0833202616892260 T T T

0.4348485955621592 0.6054929810973018 0.0830921792072991 T T T

0.2192436860400893 0.0521789083061970 0.1666364956142885 T T T

0.0980521914703908 0.0780248186311838 0.1666296661649759 T T T

0.3755287097310553 0.1169549354340401 0.1667450088448021 T T T

0.0526152250755682 0.1854663406111858 0.1666820575288855 T T T

0.5161560458112591 0.2480567785974338 0.1667146392161147 T T T

0.0926806975697570 0.3372993213191517 0.1660999018131997 T T T

0.5983392439763356 0.4051491327074269 0.1666340124036622 T T T

0.2028639610894635 0.4890282159643652 0.1677292880336051 T T T

0.5936532326748123 0.5387662749176669 0.1666220477165850 T T T

0.3583624690609719 0.5849685419849061 0.1659584218326729 T T T

0.5034842998219815 0.6049840309211381 0.1666406079984041 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2191056383732209 | 0.0518437450168299 | 0.3333849372652656 | T | T | T |
| 0.0981241084091907 | 0.0779721478249612 | 0.3330761089719037 | T | T | T |
| 0.3755008332401850 | 0.1169818014020956 | 0.3332449832272893 | T | T | T |
| 0.0530853573855917 | 0.1857632600807163 | 0.3329597997011640 | T | T | T |
| 0.5162206994279924 | 0.2480897570172705 | 0.3332182255896735 | T | T | T |
| 0.0929437426545096 | 0.3378074920833116 | 0.3335651894311999 | T | T | T |
| 0.5986077173580789 | 0.4051997900211459 | 0.3333604930009123 | T | T | T |
| 0.2019349377070547 | 0.4901361149054775 | 0.3321696605706304 | T | T | T |
| 0.5936691971054683 | 0.5386841426989766 | 0.3330617775994802 | T | T | T |
| 0.3578626939054035 | 0.5847448908001918 | 0.3333706564628533 | T | T | T |
| 0.5031735323786222 | 0.6045624999801693 | 0.3328882059018251 | T | T | T |
| 0.1509704176512102 | 0.0529422685461681 | 0.4167316124947852 | T | T | T |
| 0.2961006533480910 | 0.0738938739455214 | 0.4167657237478286 | T | T | T |
| 0.0651830971938272 | 0.1239762002780285 | 0.4164708704492933 | T | T | T |
| 0.4505529209181596 | 0.1767389225462138 | 0.4165937381793819 | T | T | T |
| 0.0638498828904599 | 0.2594432385388293 | 0.4165976762638806 | T | T | T |
| 0.5671919250350730 | 0.3264279844670633 | 0.4167070637409621 | T | T | T |
| 0.1385664447774866 | 0.4167720159419439 | 0.4176027564979291 | T | T | T |
| 0.6078636815466913 | 0.4780323537636627 | 0.4166873636979464 | T | T | T |
| 0.2785837360178330 | 0.5472447774582703 | 0.4173369646562186 | T | T | T |
| 0.5574541078507904 | 0.5816470282964538 | 0.4163958348979733 | T | T | T |
| 0.4341414376107644 | 0.6043111821262883 | 0.4165232194068387 | T | T | T |
| 0.1509003465466175 | 0.0528129525248385 | 0.5831364710815906 | T | T | T |
| 0.2961240961289688 | 0.0738194631390975 | 0.5832379726954224 | T | T | T |
| 0.0653179684110593 | 0.1240163657206758 | 0.5833030534114713 | T | T | T |
| 0.4505699321564756 | 0.1767442637698924 | 0.5833988130528300 | T | T | T |
| 0.0652943611129148 | 0.2599729288747963 | 0.5827242087499482 | T | T | T |
| 0.5672752059513234 | 0.3264283928413295 | 0.5831796688740825 | T | T | T |
| 0.1378825557355881 | 0.4168261211598221 | 0.5830450482918192 | T | T | T |
| 0.6080200526788687 | 0.4781046583506725 | 0.5831139151262242 | T | T | T |
| 0.2787138318181071 | 0.5477066278463270 | 0.5829278014041044 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5574411223793031 | 0.5815343409378938 | 0.5832166940451848 | T | T | T |
| 0.4335450746915367 | 0.6029023006805178 | 0.5827032486795829 | T | T | T |
| 0.2190693365934508 | 0.0517429658993607 | 0.6666236222175889 | T | T | T |
| 0.0981053670837015 | 0.0778599835198908 | 0.6666975992907924 | T | T | T |
| 0.3755110421785436 | 0.1170473312354199 | 0.6667824729709940 | T | T | T |
| 0.0546191866243253 | 0.1866394446741249 | 0.6666257740389024 | T | T | T |
| 0.5161999615512779 | 0.2481291266034356 | 0.6667554773158654 | T | T | T |
| 0.0960507540125994 | 0.3389336510057478 | 0.6654163290162610 | T | T | T |
| 0.5986822481943777 | 0.4052315291788254 | 0.6666228769625752 | T | T | T |
| 0.1926556014252832 | 0.5018350393531010 | 0.6663630258018011 | T | T | T |
| 0.5938348394081754 | 0.5387152085760005 | 0.6666332103946344 | T | T | T |
| 0.3564665129023998 | 0.5813587185493766 | 0.6654545890155439 | T | T | T |
| 0.5022776785295324 | 0.6031255640387564 | 0.6666199193666468 | T | T | T |
| 0.2190945730017792 | 0.0518250594226215 | 0.8333465315440476 | T | T | T |
| 0.0980971225609470 | 0.0779594552410040 | 0.8330978226113710 | T | T | T |
| 0.3754982485168136 | 0.1169926568598039 | 0.8332528117855829 | T | T | T |
| 0.0537758840737775 | 0.1863017278281955 | 0.8330882781782444 | T | T | T |
| 0.5161841821219775 | 0.2481250009994001 | 0.8332708027711747 | T | T | T |
| 0.0945238908313369 | 0.3381534389112552 | 0.8330773390500286 | T | T | T |
| 0.5986200291181863 | 0.4052364039142298 | 0.8333874144621610 | T | T | T |
| 0.5937486933590174 | 0.5387526025127684 | 0.8330616389165207 | T | T | T |
| 0.3572827987209991 | 0.5828939079874410 | 0.8330600394272537 | T | T | T |
| 0.5026360494122548 | 0.6039101789935095 | 0.8330524777440576 | T | T | T |
| 0.1510928547637764 | 0.0531965655096715 | 0.9167418377228352 | T | T | T |
| 0.2961022444670485 | 0.0738730442913437 | 0.9167329381252590 | T | T | T |
| 0.0649798592871369 | 0.1239586666455944 | 0.9164551612488726 | T | T | T |
| 0.4505372763392176 | 0.1767312032317550 | 0.9166505724247005 | T | T | T |
| 0.0637642642064691 | 0.2596151246273556 | 0.9167630998474783 | T | T | T |
| 0.5670887899237893 | 0.3264461315605744 | 0.9167726269728542 | T | T | T |
| 0.1419541040001111 | 0.4158084086651330 | 0.9165265075498783 | T | T | T |
| 0.6078012662845528 | 0.4780625468643800 | 0.9167303481595411 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2789707573588018 | 0.5433285344906870 | 0.9164943531376315 | T | T | T |
| 0.5574425681918126 | 0.5817721886473385 | 0.9164959303463776 | T | T | T |
| 0.4340374985726996 | 0.6044791786603644 | 0.9167113449496456 | T | T | T |
| 0.2028533200403627 | 0.4890059481922762 | 0.8365100679272989 | T | T | T |
| 0.1484542370029635 | 0.5504091482312228 | 0.6546571598496576 | T | T | T |
| 0.1914204694280104 | 0.6108633877749978 | 0.6569219573263010 | T | T | T |

OH\_N-CNT(12,0) ### KPOINTS: 1x1x2 ### E= -755.43068872 eV

1.0000000000000000

15.588499999999998 -9.000000000000000 0.0000000000000000

0.0000000000000000 18.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.457919999999997

C N O H

95 1 1 1

Selective dynamics

Direct

0.6546568739223060 0.5363637329576447 0.4159019106715770 T T T

0.6545968661636338 0.5362912727605209 0.9159822591601687 T T T

0.4632457162256341 0.6465448429369913 0.4156927107987329 T T T

0.4629645420435346 0.6466654081460362 0.9159476695923137 T T T

0.3912115855457118 0.1088919075589459 0.4159135871634402 T T T

0.3911993659978541 0.1089984884725828 0.9158635962927208 T T T

0.1099882154587434 0.0678951046757405 0.4159740364639029 T T T

0.1098768744353104 0.0678038211309142 0.9159982679885352 T T T

0.6341757019949952 0.3908449993318531 0.4156435649721368 T T T

0.6343223377984069 0.3908354165978898 0.9156805381809626 T T T

0.5901644946005079 0.6285553453373904 0.4155868355447527 T T T

0.5899709535566909 0.6285056749230027 0.9156878246306223 T T T

0.1633535657063171 0.4710836601073143 0.4170767795333119 T T T

0.1664599178720042 0.4700439689937954 0.9160025616964321 T T T

0.0756366471463387 0.3135986050759573 0.4156193529219534 T T T

0.0755679878256108 0.3138560310985620 0.9159634819683816 T T T

0.2345274806743290 0.0466450778761556 0.4157089918838126 T T T

0.2345521653502475 0.0467118772148170 0.9157322122324371 T T T

0.5364949459915467 0.2346203310375501 0.4158816339621188 T T T

0.5365104636795652 0.2346251319348381 0.9158151705137243 T T T

0.3083238371157471 0.5952340191195051 0.4172509386667663 T T T

0.3081795817632391 0.5915019775887035 0.9159010025771323 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0538955950649930 | 0.1672658325942964 | 0.4156441001095648 | T | T | T |
| 0.0536464212035803 | 0.1672556556098234 | 0.9157538998469708 | T | T | T |
| 0.5904781853545432 | 0.6289231281086805 | 0.0827399399958899 | T | T | T |
| 0.5897473108914073 | 0.6281332992744807 | 0.5826657197453669 | T | T | T |
| 0.0531968598174671 | 0.1668657731829948 | 0.0827719288301875 | T | T | T |
| 0.0543015684023886 | 0.1675743629588407 | 0.5826850505183658 | T | T | T |
| 0.3085416304023686 | 0.5935392770362917 | 0.0816699250819878 | T | T | T |
| 0.3083697000645244 | 0.5961584899086528 | 0.5826460589034437 | T | T | T |
| 0.1096357320998456 | 0.0675837874157590 | 0.0824420700099215 | T | T | T |
| 0.1102341913470298 | 0.0680411252401949 | 0.5824429459295568 | T | T | T |
| 0.6547742548171765 | 0.5364353505360725 | 0.0823756367595235 | T | T | T |
| 0.6545056131169037 | 0.5361827347379917 | 0.5823946758108194 | T | T | T |
| 0.2344657123841387 | 0.0467089301525298 | 0.0827709955013821 | T | T | T |
| 0.2345241646240986 | 0.0463680215571261 | 0.5827738305606291 | T | T | T |
| 0.1645811932796778 | 0.4703284681891949 | 0.0816911449747589 | T | T | T |
| 0.1626983965940393 | 0.4712107118307537 | 0.5825814611442540 | T | T | T |
| 0.3911358903788944 | 0.1090309896691597 | 0.0825800831039758 | T | T | T |
| 0.3911942293503090 | 0.1088676855050569 | 0.5825936285212727 | T | T | T |
| 0.4638677300574675 | 0.6475406369108777 | 0.0829492076132026 | T | T | T |
| 0.4625627908667214 | 0.6453539044474759 | 0.5824198724291192 | T | T | T |
| 0.5365535722175848 | 0.2346528276378816 | 0.0825926670329577 | T | T | T |
| 0.5364741523468904 | 0.2346650380986471 | 0.5826147007909592 | T | T | T |
| 0.0746381226669082 | 0.3131931880423707 | 0.0829459016371096 | T | T | T |
| 0.0766883319085254 | 0.3139335716152088 | 0.5824486152417179 | T | T | T |
| 0.6343835303778597 | 0.3908710690655424 | 0.0827302103231346 | T | T | T |
| 0.6343586018636561 | 0.3907926356742950 | 0.5826977519302636 | T | T | T |
| 0.2309400867706257 | 0.5410086850733729 | 0.1674686103636165 | T | T | T |
| 0.2220946115158147 | 0.5550294782738462 | 0.6658978819482880 | T | T | T |
| 0.0542493672128836 | 0.2363211790193037 | 0.1660043767101188 | T | T | T |
| 0.0557772075101475 | 0.2370916753906889 | 0.6660468423274318 | T | T | T |
| 0.3115052152623057 | 0.0681367260157225 | 0.1659136662677996 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3115522420212591 | 0.0677712895359469 | 0.6659311488916013 | T | T | T |
| 0.3879017064176344 | 0.6290209534792655 | 0.1653387870708204 | T | T | T |
| 0.3860655732874441 | 0.6261919868515222 | 0.6648170071433231 | T | T | T |
| 0.6320767855415781 | 0.5912268160688740 | 0.1656347662863227 | T | T | T |
| 0.6315610628470976 | 0.5906899395656142 | 0.6658221404366815 | T | T | T |
| 0.4676341725363697 | 0.1659191761929255 | 0.1657667344990176 | T | T | T |
| 0.4675910388886487 | 0.1659532015062009 | 0.6656490325127430 | T | T | T |
| 0.0717984085114131 | 0.1093846217353856 | 0.1657117473787674 | T | T | T |
| 0.0726169015496204 | 0.1099272457418865 | 0.6658458614037940 | T | T | T |
| 0.1118964998828896 | 0.3923806889221744 | 0.1652915143866710 | T | T | T |
| 0.1148230876448705 | 0.3934504741278155 | 0.6649222970555881 | T | T | T |
| 0.5936271461083937 | 0.3113285068445635 | 0.1658667569095631 | T | T | T |
| 0.5936456508444810 | 0.3112821691907846 | 0.6658790324989363 | T | T | T |
| 0.5331686069389788 | 0.6481279349915964 | 0.1660120179622206 | T | T | T |
| 0.5319543101662464 | 0.6465041464917982 | 0.6659976019165129 | T | T | T |
| 0.1654960163861709 | 0.0463242178085308 | 0.1657664681716775 | T | T | T |
| 0.1657749518316090 | 0.0464059396426165 | 0.6658132015938991 | T | T | T |
| 0.6553861039468027 | 0.4677473388302230 | 0.1656915373684529 | T | T | T |
| 0.6552660218894928 | 0.4675836409271085 | 0.6657642360540317 | T | T | T |
| 0.0718947163658890 | 0.1093865516001246 | 0.3327447866573066 | T | T | T |
| 0.0722306836659228 | 0.1097161369753751 | 0.8327613739212772 | T | T | T |
| 0.5329635151090893 | 0.6478513658215500 | 0.3323319879919495 | T | T | T |
| 0.5323625116865546 | 0.6472057582189261 | 0.8324313457630259 | T | T | T |
| 0.6321878587545565 | 0.5912893271329052 | 0.3326676764677259 | T | T | T |
| 0.6316768599781137 | 0.5908476572249254 | 0.8327315198050571 | T | T | T |
| 0.4676973768677991 | 0.1657806605184985 | 0.3328887289819704 | T | T | T |
| 0.4676648790742249 | 0.1658689659536073 | 0.8327459417268693 | T | T | T |
| 0.0545768913764013 | 0.2364761124497365 | 0.3323379251879245 | T | T | T |
| 0.0550463577430602 | 0.2368276091075480 | 0.8324886435002700 | T | T | T |
| 0.1656057789137789 | 0.0463512990963687 | 0.3326151719671440 | T | T | T |
| 0.1656709629328871 | 0.0464362462106594 | 0.8325980198479835 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3874093361181452 | 0.6287098585937045 | 0.3331080270655133 | T | T | T |
| 0.3868255436471879 | 0.6273239166221239 | 0.8327152808368722 | T | T | T |
| 0.5935020212031415 | 0.3112834059255368 | 0.3324703321678525 | T | T | T |
| 0.5936470245663932 | 0.3112825722367960 | 0.8324977624446396 | T | T | T |
| 0.1122910054584044 | 0.3928383637730614 | 0.3329782876453274 | T | T | T |
| 0.1137062595633315 | 0.3929970083586661 | 0.8327462661311084 | T | T | T |
| 0.2302359346343688 | 0.5422138014825406 | 0.3317658229203738 | T | T | T |
| 0.3115695448662707 | 0.0680804941948279 | 0.3325017384384673 | T | T | T |
| 0.3115426955627156 | 0.0679177523822220 | 0.8325409059407219 | T | T | T |
| 0.6553375814517032 | 0.4677036771488678 | 0.3325463712098885 | T | T | T |
| 0.6553193313554716 | 0.4676623584849214 | 0.8325732217907463 | T | T | T |
| 0.2310278467475995 | 0.5407651975525778 | 0.8354428634808286 | T | T | T |
| 0.1901070942860770 | 0.6147120122087474 | 0.6528154519475046 | T | T | T |
| 0.1279040101909078 | 0.5818306686205461 | 0.6546643292414965 | T | T | T |

OH\_N-CNT(13,0) ### KPOINTS: 1x1x2 ### E= -1226.75569537 eV

1.0000000000000000

24.248699999999995 -14.000000000000000 0.0000000000000000

0.0000000000000000 28.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 12.838699999999993

C N O H

155 1 1 1

Selective dynamics

Direct

0.4406521145974194 0.4066845651583632 0.0277601984270550 T T T

0.4528679759128333 0.3698551220120320 0.1944131405835034 T T T

0.4527947846748359 0.3698020409983312 0.3055053130354084 T T T

0.3828159797356445 0.4496617706192148 0.0276988951941886 T T T

0.4407291847932223 0.4066733060571171 0.1388270302982573 T T T

0.4168472474480036 0.4337141339859826 0.1943608597102992 T T T

0.4163850570478563 0.4333517955962992 0.3055553467715302 T T T

0.2929360341519256 0.4449500818617811 0.0278689828431014 T T T

0.3828968529512196 0.4495785996457537 0.1387933086416045 T T T

0.3406040691030140 0.4530114646020865 0.1945766147623125 T T T

0.3398823577684553 0.4523807082633383 0.3054854432382169 T T T

0.1918802759609341 0.3947690190436282 0.0279022883343537 T T T

0.2930024043918750 0.4444975770252558 0.1391755892246150 T T T

0.2423627617422922 0.4240043825669810 0.1946601442983287 T T T

0.2420258231599908 0.4231718517549620 0.3053941325949119 T T T

0.1028854115346854 0.3087036601073299 0.0278524046754639 T T T

0.1920991461035852 0.3942265347052039 0.1382992617740750 T T T

0.1452841778061116 0.3542821649349597 0.1946238433174485 T T T

0.1461233609874579 0.3541209712161816 0.3053607019099123 T T T

0.0444436110324268 0.2078922754100352 0.0277516170752749 T T T

0.1031113194500106 0.3083908841137853 0.1391795543424657 T T T

0.0691193789373514 0.2587295431911738 0.1946043718995053 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0700545064458500 | 0.2591172623106461 | 0.3055039910489438 | T | T | T |
| 0.0318543803688323 | 0.1146941787849280 | 0.0278311820968224 | T | T | T |
| 0.0444757033860124 | 0.2077802476430618 | 0.1388632905805402 | T | T | T |
| 0.0318443756333339 | 0.1587498822328522 | 0.1944359133104340 | T | T | T |
| 0.0322841250528031 | 0.1589867214512324 | 0.3056118647026183 | T | T | T |
| 0.0687803031157437 | 0.0515437727971569 | 0.0278711221698629 | T | T | T |
| 0.0317548518270665 | 0.1145702131632599 | 0.1388601634745431 | T | T | T |
| 0.0442596614111947 | 0.0780148341195343 | 0.1944345073892196 | T | T | T |
| 0.0441175187872827 | 0.0778906312460997 | 0.3055094143256293 | T | T | T |
| 0.1445022896956307 | 0.0312779608188669 | 0.0279870129389686 | T | T | T |
| 0.0686225935514218 | 0.0514191664455678 | 0.1389833321099057 | T | T | T |
| 0.1025445303776759 | 0.0354585925416129 | 0.1946038510721269 | T | T | T |
| 0.1024600492653830 | 0.0354036126545467 | 0.3056343339163468 | T | T | T |
| 0.2427096660587907 | 0.0595142085109045 | 0.0279485252554489 | T | T | T |
| 0.1444770550222532 | 0.0313415164112609 | 0.1390580306668445 | T | T | T |
| 0.1920908062740330 | 0.0394975713842989 | 0.1946796911270776 | T | T | T |
| 0.1920932928454087 | 0.0395671860931622 | 0.3057513962701484 | T | T | T |
| 0.3409488400476348 | 0.1296753755276676 | 0.0279305842410626 | T | T | T |
| 0.2426944953608708 | 0.0595052784042789 | 0.1390459676570057 | T | T | T |
| 0.2933070522792252 | 0.0901620922889798 | 0.1945957547928581 | T | T | T |
| 0.2932927791231705 | 0.0901775322756972 | 0.3057206655183066 | T | T | T |
| 0.4165754404658886 | 0.2256459319645713 | 0.0279246904634788 | T | T | T |
| 0.3409697433816246 | 0.1296962363729235 | 0.1390257934923298 | T | T | T |
| 0.3828673592694686 | 0.1757652390101785 | 0.1946282804511720 | T | T | T |
| 0.3828287199465514 | 0.1757595711190565 | 0.3056918324936662 | T | T | T |
| 0.4524606680264636 | 0.3255227786391989 | 0.0278153302291314 | T | T | T |
| 0.4165511146870583 | 0.2256770643926552 | 0.1389825035447802 | T | T | T |
| 0.4401986544076646 | 0.2765718900231728 | 0.1945169343032501 | T | T | T |
| 0.4402466951356893 | 0.2765703975018296 | 0.3055484089952636 | T | T | T |
| 0.4525169151457525 | 0.3255595451952835 | 0.1389226527980788 | T | T | T |
| 0.4404221767365530 | 0.4064145145503318 | 0.3611465333958106 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4527511936119926 | 0.3696983607609753 | 0.5278507107194382 | T | T | T |
| 0.4526131259799036 | 0.3696327602871926 | 0.6389327235964389 | T | T | T |
| 0.3820482899076268 | 0.4486787074286152 | 0.3611537511145566 | T | T | T |
| 0.4402735403694162 | 0.4062053847489755 | 0.4721677831829370 | T | T | T |
| 0.4159670217474629 | 0.4327975107293806 | 0.5277992873473260 | T | T | T |
| 0.4159732110565731 | 0.4328964890998535 | 0.6389086199331783 | T | T | T |
| 0.2919340430436114 | 0.4435051705667493 | 0.3611041032609418 | T | T | T |
| 0.3815589575689848 | 0.4480149784317365 | 0.4722537491493626 | T | T | T |
| 0.3392452944957364 | 0.4512884437531295 | 0.5279158199748050 | T | T | T |
| 0.3397276537607203 | 0.4522476613300866 | 0.6386479929816412 | T | T | T |
| 0.2912080519541125 | 0.4428131593329119 | 0.4727282558643707 | T | T | T |
| 0.2422549109415781 | 0.4273190791726221 | 0.5274631673576641 | T | T | T |
| 0.2419744413845158 | 0.4266431909490824 | 0.6379558882609201 | T | T | T |
| 0.1046158837924954 | 0.3089088956111030 | 0.3611055815727721 | T | T | T |
| 0.1878939193950738 | 0.4069517489233260 | 0.4712053346320889 | T | T | T |
| 0.1439060536168208 | 0.3563736431497225 | 0.5274467110037371 | T | T | T |
| 0.1443410558396813 | 0.3563204528202589 | 0.6381067795164547 | T | T | T |
| 0.0457216953234694 | 0.2081926950803575 | 0.3612044880365538 | T | T | T |
| 0.1054669758222939 | 0.3092915598672450 | 0.4727243867715349 | T | T | T |
| 0.0711306376140315 | 0.2591770645168576 | 0.5279498005649322 | T | T | T |
| 0.0703288207272510 | 0.2592400001930207 | 0.6386822752458770 | T | T | T |
| 0.0317307007130273 | 0.1145057007433198 | 0.3611648147262935 | T | T | T |
| 0.0464059346356960 | 0.2083241054117640 | 0.4723011060310506 | T | T | T |
| 0.0328553170289261 | 0.1590902546912915 | 0.5277986246058582 | T | T | T |
| 0.0328123757276427 | 0.1591585756014890 | 0.6388992894503357 | T | T | T |
| 0.0682547147430148 | 0.0510763699745205 | 0.3611406641331109 | T | T | T |
| 0.0318516157842461 | 0.1144782168472824 | 0.4721751939408888 | T | T | T |
| 0.0439709526101252 | 0.0776945781860115 | 0.5278754915645502 | T | T | T |
| 0.0441574048039728 | 0.0778671186628025 | 0.6389779159679633 | T | T | T |
| 0.1444525316174146 | 0.0314281175023160 | 0.3612373478836006 | T | T | T |
| 0.0681539455982170 | 0.0509650778191164 | 0.4722664829138317 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1023819254096011 | 0.0353472494386246 | 0.5278864890523419 | T | T | T |
| 0.1024476029258601 | 0.0353649437461592 | 0.6389990556818389 | T | T | T |
| 0.2426955984524545 | 0.0595341746088448 | 0.3613277245310811 | T | T | T |
| 0.1444888119258791 | 0.0314868303054089 | 0.4723252214774893 | T | T | T |
| 0.1921411368920570 | 0.0396419823604648 | 0.5279456883047741 | T | T | T |
| 0.1921293743527825 | 0.0396348067533543 | 0.6389949249336396 | T | T | T |
| 0.3409243381496783 | 0.1296809392046399 | 0.3613052720842838 | T | T | T |
| 0.2427248798529811 | 0.0595712521328289 | 0.4723722339695842 | T | T | T |
| 0.2932812736735355 | 0.0901694325813522 | 0.5278945103754139 | T | T | T |
| 0.2932746240702119 | 0.0902009505031413 | 0.6389225316924759 | T | T | T |
| 0.4165646773348531 | 0.2256727404696768 | 0.3611663398879285 | T | T | T |
| 0.3408781941618627 | 0.1296584353390980 | 0.4723497497155995 | T | T | T |
| 0.3827638931738332 | 0.1757181437340322 | 0.5279230843576544 | T | T | T |
| 0.3827831390428684 | 0.1757434605836743 | 0.6389875476280900 | T | T | T |
| 0.4526489697145976 | 0.3255896233275227 | 0.3611257276684497 | T | T | T |
| 0.4165305508848639 | 0.2256510850615386 | 0.4722607498425306 | T | T | T |
| 0.4403353129558368 | 0.2765881371116687 | 0.5278674269949941 | T | T | T |
| 0.4403039702809328 | 0.2765458021942706 | 0.6389682215145963 | T | T | T |
| 0.4527059871954083 | 0.3255971698253754 | 0.4722410476090923 | T | T | T |
| 0.4401719342437330 | 0.4061879732913247 | 0.6945473437869555 | T | T | T |
| 0.4525312230549187 | 0.3696388759733976 | 0.8611904504592027 | T | T | T |
| 0.4526673414507691 | 0.3697577557130671 | 0.9722141795497329 | T | T | T |
| 0.3821450893697503 | 0.4488617655142359 | 0.6944330620618224 | T | T | T |
| 0.4402051050175199 | 0.4062750782219497 | 0.8055177507936734 | T | T | T |
| 0.4164843159792041 | 0.4335076202028130 | 0.8609942624655214 | T | T | T |
| 0.4167633141816603 | 0.4337538697010666 | 0.9721091712415716 | T | T | T |
| 0.2923274702384932 | 0.4447584132879051 | 0.6939130287000510 | T | T | T |
| 0.3824165956025649 | 0.4493053885190701 | 0.8053828597199343 | T | T | T |
| 0.3403976800464469 | 0.4533607615621466 | 0.8608991909056610 | T | T | T |
| 0.3405932665968094 | 0.4533672911629040 | 0.9720454768877024 | T | T | T |
| 0.1912863034555053 | 0.3969039794088854 | 0.6948418810113484 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2926828921622497 | 0.4452185368286761 | 0.8053417274055661 | T | T | T |
| 0.2423677110430409 | 0.4259424313009826 | 0.8612297463718314 | T | T | T |
| 0.2425042044261740 | 0.4254778404219781 | 0.9721322421520424 | T | T | T |
| 0.1036475189708972 | 0.3092955870303458 | 0.6939658906975532 | T | T | T |
| 0.1915498811304047 | 0.3959241047131487 | 0.8051922086516331 | T | T | T |
| 0.1442647724663351 | 0.3554488923543401 | 0.8612074857403912 | T | T | T |
| 0.1443513495268858 | 0.3549768664956221 | 0.9721472550188832 | T | T | T |
| 0.0456252561103073 | 0.2081967885653172 | 0.6944119666013595 | T | T | T |
| 0.1030692264441745 | 0.3091520109168774 | 0.8053871251664816 | T | T | T |
| 0.0691447924180156 | 0.2591268216832028 | 0.8609115613219069 | T | T | T |
| 0.0688667669397300 | 0.2589011747562001 | 0.9720731189853320 | T | T | T |
| 0.0319898399186421 | 0.1146447323739547 | 0.6945865983255242 | T | T | T |
| 0.0451491992088187 | 0.2081465818992692 | 0.8053758173492710 | T | T | T |
| 0.0321909024171964 | 0.1589899537844805 | 0.8610464848919462 | T | T | T |
| 0.0318820713803157 | 0.1588550630618004 | 0.9721543369049827 | T | T | T |
| 0.0683671551089869 | 0.0511464043577524 | 0.6945741517106105 | T | T | T |
| 0.0320651412901349 | 0.1147496039521083 | 0.8055711890565219 | T | T | T |
| 0.0445875809523172 | 0.0782582402553713 | 0.8612572014864286 | T | T | T |
| 0.0446334880591233 | 0.0783238138788566 | 0.9722804298333190 | T | T | T |
| 0.1444849171973843 | 0.0314224995670218 | 0.6945737306439521 | T | T | T |
| 0.0685751403312262 | 0.0513434032060824 | 0.8056946095434588 | T | T | T |
| 0.1025900218029156 | 0.0354706428993566 | 0.8612854885078125 | T | T | T |
| 0.1026907627563745 | 0.0355425761272022 | 0.9723580157001163 | T | T | T |
| 0.2427110782145498 | 0.0595756054910620 | 0.6945587122869555 | T | T | T |
| 0.1445133848310288 | 0.0314073774042873 | 0.8056518790869123 | T | T | T |
| 0.1921119439084572 | 0.0395108298948688 | 0.8612689892182532 | T | T | T |
| 0.1921082973687764 | 0.0394485694673732 | 0.9723632603101945 | T | T | T |
| 0.3408906442775309 | 0.1296875107804247 | 0.6945610247288719 | T | T | T |
| 0.2427108650994969 | 0.0595541327204530 | 0.8056390713193627 | T | T | T |
| 0.2933014369321589 | 0.0901962978406680 | 0.8612065129624462 | T | T | T |
| 0.2932853563803661 | 0.0902161902462299 | 0.9723301573794958 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4165703311211963 | 0.2256428377755214 | 0.6945809616474686 | T | T | T |
| 0.3409265687621597 | 0.1297113532406433 | 0.8056311179239471 | T | T | T |
| 0.3828502714001225 | 0.1757539769345474 | 0.8612561659294421 | T | T | T |
| 0.3828817776232029 | 0.1757406665829458 | 0.9723425667838407 | T | T | T |
| 0.4525790292394986 | 0.3255148966688922 | 0.6945498589533428 | T | T | T |
| 0.4165556064078687 | 0.2256608503149314 | 0.8056562060576309 | T | T | T |
| 0.4402257203045501 | 0.2765461439974769 | 0.8612823861709757 | T | T | T |
| 0.4401372011568956 | 0.2765264784530272 | 0.9723252099992126 | T | T | T |
| 0.4524907251497219 | 0.3255061630132397 | 0.8056532654208074 | T | T | T |
| 0.1920099345642589 | 0.3946962168083528 | 0.3586468853740072 | T | T | T |
| 0.1759554513401005 | 0.4518789911729955 | 0.4732485660914178 | T | T | T |
| 0.1365839205297984 | 0.4363258779838967 | 0.4627698762948234 | T | T | T |

### 1.1.3 OH adsorbate on B-doped CNT

OH\_B-CNT(5,5) ### KPOINTS: 2x2x3 ### E= -470.02996187 eV

1.000000000000000

13.8564000000000007 -8.000000000000000 0.000000000000000

0.000000000000000 16.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.394779999999999

C B O H

59 1 1 1

Selective dynamics

Direct

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5621953504874707 | 0.4239251745358858 | 0.0836226066227187 | T | T | T |
| 0.5621617353779075 | 0.4239364309796649 | 0.4167452908303052 | T | T | T |
| 0.5614373419904206 | 0.4235499969771576 | 0.7501517127479479 | T | T | T |
| 0.4832187529099097 | 0.5455573475341398 | 0.0838219147610063 | T | T | T |
| 0.4832710301549895 | 0.5455841960963610 | 0.4163295920784387 | T | T | T |
| 0.4798474145428528 | 0.5437997239771140 | 0.7501113095815102 | T | T | T |
| 0.3975948455092781 | 0.5515377931894064 | 0.0839092947173705 | T | T | T |
| 0.3975825027481811 | 0.5513886676059895 | 0.4160430931009229 | T | T | T |
| 0.3946527996610004 | 0.5508647192853666 | 0.7500679951379736 | T | T | T |
| 0.1206236943020330 | 0.3464241887517859 | 0.0837580250246434 | T | T | T |
| 0.1205755073556705 | 0.3464620261431176 | 0.4163799995603645 | T | T | T |
| 0.1131180526710032 | 0.3445766020570759 | 0.7500289137369031 | T | T | T |
| 0.0800579550966098 | 0.1539033522503683 | 0.0838658369468473 | T | T | T |
| 0.0800467674896672 | 0.1539211481365970 | 0.4163717164983641 | T | T | T |
| 0.0787051481627826 | 0.1531320338953109 | 0.7501263303588870 | T | T | T |
| 0.1178608104468521 | 0.0899525707770580 | 0.0838647363405268 | T | T | T |
| 0.1179153672732764 | 0.0900301251142459 | 0.4164612535310275 | T | T | T |
| 0.1175979864285395 | 0.0896809911009360 | 0.7501719180304225 | T | T | T |
| 0.2869987233784174 | 0.0792128313449540 | 0.0837070612489231 | T | T | T |
| 0.2870202988910743 | 0.0792013736591432 | 0.4167115343440125 | T | T | T |
| 0.2867410132927612 | 0.0788184249458698 | 0.7502230664910066 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3896766955214448 | 0.1357610856440291 | 0.0837954036829142 | T | T | T |
| 0.3897194350182593 | 0.1356939530599954 | 0.4166921474107389 | T | T | T |
| 0.3895430188248460 | 0.1359706883563256 | 0.7502783061300889 | T | T | T |
| 0.5414852611070438 | 0.3263345492049365 | 0.0837054682825005 | T | T | T |
| 0.5413811304647322 | 0.3263174504494165 | 0.4167219476134343 | T | T | T |
| 0.5414244692768698 | 0.3262369563791080 | 0.7501715381086385 | T | T | T |
| 0.1975756975516166 | 0.4448242959917076 | 0.0856285519783963 | T | T | T |
| 0.1974986429745417 | 0.4448476907647345 | 0.4144324659141284 | T | T | T |
| 0.2461241030001906 | 0.4837262164138382 | 0.2501025514165022 | T | T | T |
| 0.2438709049930897 | 0.4904592573045365 | 0.5771072879931365 | T | T | T |
| 0.2437145645491630 | 0.4903744385385269 | 0.9225692186296749 | T | T | T |
| 0.5575056482884044 | 0.4662715791713024 | 0.2501591662520349 | T | T | T |
| 0.5558181088543324 | 0.4656532860848089 | 0.5837582925728138 | T | T | T |
| 0.5557558758255399 | 0.4655663249351243 | 0.9165641461730826 | T | T | T |
| 0.1502603460085413 | 0.0710201042524533 | 0.2501870645637744 | T | T | T |
| 0.1505897138919612 | 0.0714070418592274 | 0.5836488497605358 | T | T | T |
| 0.1505050977999458 | 0.0712942804560127 | 0.9166828343302912 | T | T | T |
| 0.2368822837320995 | 0.0657654610266099 | 0.2502313100093677 | T | T | T |
| 0.2366567870367190 | 0.0656965995426208 | 0.5836326084761437 | T | T | T |
| 0.2366235834221834 | 0.0656497598652453 | 0.9167568887597587 | T | T | T |
| 0.5171837223362395 | 0.5282334712768563 | 0.2500967726711268 | T | T | T |
| 0.5146520399291986 | 0.5264418465685796 | 0.5837385613612367 | T | T | T |
| 0.5145567920160785 | 0.5263350948669400 | 0.9164956743899002 | T | T | T |
| 0.0955746871281167 | 0.2946863141692293 | 0.2501185996188224 | T | T | T |
| 0.0941569152856787 | 0.2934947658607414 | 0.5859474334064907 | T | T | T |
| 0.0941636222801985 | 0.2934852367347918 | 0.9141154094782126 | T | T | T |
| 0.4379419322356382 | 0.1766036412984002 | 0.2502453193272566 | T | T | T |
| 0.4378054472405618 | 0.1769533489448417 | 0.5836580979389139 | T | T | T |
| 0.4377624809516424 | 0.1770364713838876 | 0.9168532862498087 | T | T | T |
| 0.5154999631360407 | 0.2743384723578114 | 0.2502252288177505 | T | T | T |
| 0.5151446568148007 | 0.2741991297967024 | 0.5835674239903943 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5151836959702475 | 0.2742422774391918 | 0.9168480984074595 | T | T | T |
| 0.0750959449357032 | 0.1960611993343134 | 0.2501213983168910 | T | T | T |
| 0.0752296704687839 | 0.1963447064392825 | 0.5837609090835788 | T | T | T |
| 0.0751749715765711 | 0.1962863854023028 | 0.9164547741585797 | T | T | T |
| 0.3487983548049839 | 0.5401930364804958 | 0.2500418464504566 | T | T | T |
| 0.3452727213983311 | 0.5389283591598860 | 0.5806594453901313 | T | T | T |
| 0.3452947674624829 | 0.5391797464236902 | 0.9193310837959986 | T | T | T |
| 0.1766119322736021 | 0.4627518768400025 | 0.7492805485881171 | T | T | T |
| 0.1183222030805558 | 0.5118994253135347 | 0.7378986648512988 | T | T | T |
| 0.0718090123623040 | 0.4921644562504198 | 0.8346621739594945 | T | T | T |

OH\_B-CNT(6,6) #### KPOINTS: 2x2x3 #### E= -566.19177414 eV

1.0000000000000000

14.7224000000000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3992800000000001

C B O H

71 1 1 1

Selective dynamics

Direct

0.6142046618161552 0.4940728010924373 0.0835760990432113 T T T

0.6142993861282551 0.4941215163360187 0.4168281807717849 T T T

0.6145735729764158 0.4943787773144722 0.7502466292267410 T T T

0.5284656434388811 0.5989103725924205 0.0837391675899242 T T T

0.5283708690933263 0.5988004168480473 0.4165415710170742 T T T

0.5285867941055160 0.5991597106766142 0.7501194255277187 T T T

0.4480568867659229 0.6053706335823394 0.0837575512106806 T T T

0.4479906763936378 0.6053080792467592 0.4163983803570088 T T T

0.4484571368412433 0.6066833609699437 0.7499994695324884 T T T

0.1681770558965853 0.4519697426336331 0.0853348288772354 T T T

0.1679587740729371 0.4522426530908022 0.4148041424510204 T T T

0.0675009823258447 0.2626068021528119 0.0839426630352907 T T T

0.0675973822355522 0.2626798150493570 0.4162231171735118 T T T

0.0675015661517329 0.2649799654279820 0.7500972096697799 T T T

0.0625081070522319 0.1767237332671627 0.0837849762657128 T T T

0.0626249470420669 0.1768287177902286 0.4164455077893951 T T T

0.0640580380811969 0.1795819054266604 0.7501066233961804 T T T

0.1428970987605109 0.0669810105820678 0.0835548891471726 T T T

0.1430258977121259 0.0671035433865280 0.4168012528893297 T T T

0.1437043323915518 0.0678759304989323 0.7502046240821820 T T T

0.2214986062550832 0.0573500430138343 0.0835446211147008 T T T

0.2215423349835339 0.0573524332356673 0.4168745845797140 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2216877802668197 | 0.0574502686006334 | 0.7502315295277654 | T | T | T |
| 0.4117686408210958 | 0.1373357139383725 | 0.0836420888508401 | T | T | T |
| 0.4117515176456351 | 0.1372732314689868 | 0.4168126363610372 | T | T | T |
| 0.4116698326558987 | 0.1373750381788277 | 0.7502659837957586 | T | T | T |
| 0.4993910237353446 | 0.2167312221792872 | 0.0835984105539882 | T | T | T |
| 0.4993184630001873 | 0.2167478590033468 | 0.4168617535462315 | T | T | T |
| 0.4993102131253698 | 0.2168342128114891 | 0.7502391112025099 | T | T | T |
| 0.6075002132996516 | 0.4071145602682828 | 0.0837214554102494 | T | T | T |
| 0.6075972118492855 | 0.4071467117545670 | 0.4167018821193731 | T | T | T |
| 0.6076142626645021 | 0.4071588383023428 | 0.7502548398047754 | T | T | T |
| 0.2573331273189299 | 0.5306162626663071 | 0.0836043747316944 | T | T | T |
| 0.2571655289413364 | 0.5309390380889579 | 0.4164657255966936 | T | T | T |
| 0.2584908474284537 | 0.5374476179888095 | 0.7499402272056152 | T | T | T |
| 0.0711024064100903 | 0.1393706508299642 | 0.2501595449608836 | T | T | T |
| 0.0727974207571053 | 0.1414243147624984 | 0.5837530970275913 | T | T | T |
| 0.0726626121160951 | 0.1413061071051231 | 0.9164434438105401 | T | T | T |
| 0.1117858328726326 | 0.0836865301815106 | 0.2501909282315045 | T | T | T |
| 0.1127395735239635 | 0.0852135259984137 | 0.5837891338710025 | T | T | T |
| 0.1125701508397691 | 0.0850367972937085 | 0.9165369980128724 | T | T | T |
| 0.5611547190464734 | 0.5839825828439061 | 0.2501544772715523 | T | T | T |
| 0.5608362925844796 | 0.5835854795058720 | 0.5837585315187902 | T | T | T |
| 0.5609135975980745 | 0.5836856716926555 | 0.9165317991480302 | T | T | T |
| 0.1336843399834413 | 0.4056972062351021 | 0.2501412738289359 | T | T | T |
| 0.1260968599811768 | 0.4076896352929300 | 0.5770806035411497 | T | T | T |
| 0.1264074897818842 | 0.4076625899057155 | 0.9227515965071452 | T | T | T |
| 0.2671776013818319 | 0.0652955671096180 | 0.2501956655960311 | T | T | T |
| 0.2673713904087554 | 0.0654508662144856 | 0.5836614531913802 | T | T | T |
| 0.2673643512216688 | 0.0655147125781327 | 0.9168230934643433 | T | T | T |
| 0.3637615066605902 | 0.1058700939816679 | 0.2502201248334025 | T | T | T |
| 0.3636540686197476 | 0.1058715695975225 | 0.5836884272420321 | T | T | T |
| 0.3636440323603353 | 0.1059574188075382 | 0.9168150319107851 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0810045808892991 | 0.3092605220004492 | 0.2501095091883577 | T | T | T |
| 0.0811826157808250 | 0.3121169805816977 | 0.5807567102022064 | T | T | T |
| 0.0810594614832059 | 0.3120241216857575 | 0.9194020317960356 | T | T | T |
| 0.3054445881312997 | 0.5598979809372380 | 0.2500972102878370 | T | T | T |
| 0.3066102800642754 | 0.5619529742551693 | 0.5853783298532081 | T | T | T |
| 0.3066753300330859 | 0.5616500671595673 | 0.9144907058368795 | T | T | T |
| 0.5365666588344362 | 0.2626069341904015 | 0.2502581947284934 | T | T | T |
| 0.5365046114695228 | 0.2627551779988953 | 0.5837074552740641 | T | T | T |
| 0.5366163501569688 | 0.2627203362580520 | 0.9167422590137810 | T | T | T |
| 0.5916412341842341 | 0.3592709067130160 | 0.2502382464032722 | T | T | T |
| 0.5914717985962770 | 0.3591966973029379 | 0.5836186565397741 | T | T | T |
| 0.5914921168330194 | 0.3591880977551793 | 0.9168376079303379 | T | T | T |
| 0.6047567756106165 | 0.5306984051252649 | 0.2502079407435488 | T | T | T |
| 0.6045602391377388 | 0.5306903249066365 | 0.5838216562969709 | T | T | T |
| 0.6045527465888203 | 0.5307048851624208 | 0.9165911234658496 | T | T | T |
| 0.4025403616591330 | 0.5977192014364143 | 0.2500767833667978 | T | T | T |
| 0.4025206214741636 | 0.5978073841306779 | 0.5835557035403744 | T | T | T |
| 0.4026186816949950 | 0.5978105761283183 | 0.9164606599021616 | T | T | T |
| 0.1490655416472050 | 0.4700320112901899 | 0.7495114669266780 | T | T | T |
| 0.0982750681600930 | 0.5210065592500556 | 0.7404226554428458 | T | T | T |
| 0.1257366781498732 | 0.5735959963304073 | 0.8180443358381699 | T | T | T |

OH\_B-CNT(7,7) #### KPOINTS: 1x1x3 #### E= -661.95368023 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C N O H

83 1 1 1

Selective dynamics

Direct

0.1817078336674722 0.0469519889206350 0.0833097007038578 T T T

0.2642101997730927 0.0544227747938310 0.0833229863840515 T T T

0.0705658285424895 0.1149029067626622 0.0839213970489671 T T T

0.4449515929669262 0.1486487908118084 0.0832113066735122 T T T

0.0514617912503727 0.1825806629753139 0.0841396557112697 T T T

0.5258616462841409 0.2257689721744557 0.0830673255299776 T T T

0.0869159794801258 0.3550586547323071 0.0811367994835969 T T T

0.6366021612215780 0.4053855882272926 0.0831607344229116 T T T

0.1354605094771884 0.4452448784304374 0.0774556485546260 T T T

0.6576460179554032 0.4928311556485286 0.0832849161404158 T T T

0.3036781070077775 0.5972903657149329 0.0859408837324356 T T T

0.6179066034151938 0.6256394113549252 0.0834922102527507 T T T

0.3951275831681573 0.6407277967932025 0.0839260799533626 T T T

0.5597062484983544 0.6574771705615071 0.0837198140265540 T T T

0.0518002832162111 0.2235193295929500 0.2505830910343038 T T T

0.5610079753115744 0.2689619800190037 0.2497590990033648 T T T

0.0686307499331283 0.3095798263688119 0.2506068229307519 T T T

0.6169102203248044 0.3596042403920962 0.2497353005387722 T T T

0.1459696222722142 0.0540177614430108 0.2501290210413755 T T T

0.3091669775061684 0.0686554881676424 0.2500163642226791 T T T

0.0902958297484297 0.0886979967936971 0.2503618669487912 T T T

0.4005359216113792 0.1162327859605706 0.2499407786547730 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6581753401874244 | 0.5328824899028088 | 0.2498710513212372 | T | T | T |
| 0.2583794515734822 | 0.5712606127753178 | 0.2505393389388497 | T | T | T |
| 0.6384456695738250 | 0.6003757875647040 | 0.2499570099760516 | T | T | T |
| 0.4401314430776369 | 0.6554021004185410 | 0.2504609301226164 | T | T | T |
| 0.5233307902801995 | 0.6635519213615519 | 0.2502661495768811 | T | T | T |
| 0.1818052619159482 | 0.0471056642664263 | 0.4168457513513663 | T | T | T |
| 0.2642070853427581 | 0.0543329625340501 | 0.4167497478864961 | T | T | T |
| 0.0704319825985431 | 0.1148132989135103 | 0.4168382846693457 | T | T | T |
| 0.4449296247228964 | 0.1486373921131180 | 0.4166355573939454 | T | T | T |
| 0.0511738246998998 | 0.1824235847707386 | 0.4169288076360032 | T | T | T |
| 0.5258656100009053 | 0.2257612866789047 | 0.4164885134055413 | T | T | T |
| 0.0866687656526912 | 0.3549616382756631 | 0.4199889060234434 | T | T | T |
| 0.6365818423601485 | 0.4053941849426021 | 0.4163346779946023 | T | T | T |
| 0.1355465580433280 | 0.4452901880387054 | 0.4232477402923018 | T | T | T |
| 0.6576281520456697 | 0.4928335898395454 | 0.4164155420742557 | T | T | T |
| 0.3037437554139600 | 0.5971289785551327 | 0.4150936989433257 | T | T | T |
| 0.6178187173774490 | 0.6255389827896800 | 0.4165666602839683 | T | T | T |
| 0.3952258357914526 | 0.6409218507233833 | 0.4170776759723037 | T | T | T |
| 0.5596311515668591 | 0.6573949867133695 | 0.4167301025112179 | T | T | T |
| 0.1457411352207672 | 0.0539458226560478 | 0.5834812702022614 | T | T | T |
| 0.3091669453305129 | 0.0684767449187415 | 0.5835115017315367 | T | T | T |
| 0.0890606272555610 | 0.0876489612776123 | 0.5836351673861303 | T | T | T |
| 0.4004870156899514 | 0.1162550457322758 | 0.5834826978415266 | T | T | T |
| 0.0499319494763732 | 0.2208512986048504 | 0.5840896098935722 | T | T | T |
| 0.5610294733172748 | 0.2690676750365068 | 0.5832751379673032 | T | T | T |
| 0.0691442971728429 | 0.3075539855715614 | 0.5844227833243191 | T | T | T |
| 0.6167296648823978 | 0.3595687523273997 | 0.5832155244811856 | T | T | T |
| 0.1757976515343157 | 0.4866640587822492 | 0.5854280159442875 | T | T | T |
| 0.6582822863039379 | 0.5328963176977550 | 0.5834372098633324 | T | T | T |
| 0.2580912739808762 | 0.5638912812246448 | 0.5838599264562622 | T | T | T |
| 0.6380452459757922 | 0.5998606129314743 | 0.5834847790377793 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4399689274736954 | 0.6544412297911548 | 0.5842189467367986 | T | T | T |
| 0.5230642409464067 | 0.6631154631971993 | 0.5839082259526283 | T | T | T |
| 0.0690583890817524 | 0.1133030799499739 | 0.7504067374374185 | T | T | T |
| 0.0494200803841679 | 0.1807172953640661 | 0.7505487637507593 | T | T | T |
| 0.5260652441185240 | 0.2258238406772490 | 0.7497727342309024 | T | T | T |
| 0.0878571682285501 | 0.3527500222642147 | 0.7505733318756154 | T | T | T |
| 0.6367112747451422 | 0.4053430366670351 | 0.7497917698869675 | T | T | T |
| 0.1433859102458306 | 0.4430791685042965 | 0.7506245640419582 | T | T | T |
| 0.1815747480202378 | 0.0469719312899068 | 0.7500839247359479 | T | T | T |
| 0.2641330049366972 | 0.0541621304060423 | 0.7500648755536815 | T | T | T |
| 0.4450192564518053 | 0.1486332820724554 | 0.7499294562486517 | T | T | T |
| 0.6581216000156997 | 0.4930659591406255 | 0.7498769903757574 | T | T | T |
| 0.3027459346163520 | 0.5945465868122293 | 0.7506020680072260 | T | T | T |
| 0.6178770564323952 | 0.6254409466005164 | 0.7500038243454865 | T | T | T |
| 0.3951134597159419 | 0.6407150750914197 | 0.7505070351093429 | T | T | T |
| 0.5597272386087921 | 0.6575479248851538 | 0.7501941250024079 | T | T | T |
| 0.1456144452661707 | 0.0537372216231655 | 0.9167378585658106 | T | T | T |
| 0.3091885450959866 | 0.0685726877918198 | 0.9165695412322884 | T | T | T |
| 0.0890742156757019 | 0.0876227472339345 | 0.9170189289049605 | T | T | T |
| 0.4005166466401009 | 0.1162650065068183 | 0.9164457570498999 | T | T | T |
| 0.0502008719290561 | 0.2209832239098739 | 0.9170126293676674 | T | T | T |
| 0.5610080421067907 | 0.2690505405064206 | 0.9162309034918561 | T | T | T |
| 0.0693657822289697 | 0.3076440441186372 | 0.9166205205750304 | T | T | T |
| 0.6167070290441587 | 0.3595411857218663 | 0.9162766106561635 | T | T | T |
| 0.1757013211791805 | 0.4868293197173214 | 0.9156862376031066 | T | T | T |
| 0.6582224216417356 | 0.5328706281002298 | 0.9163734375333278 | T | T | T |
| 0.2579720982102355 | 0.5641366575062131 | 0.9172686827541194 | T | T | T |
| 0.6380156076459237 | 0.5998611728015257 | 0.9164796709116995 | T | T | T |
| 0.4398913840816315 | 0.6542031275187650 | 0.9167176409486156 | T | T | T |
| 0.5230425002641124 | 0.6630328936128214 | 0.9166434523070726 | T | T | T |
| 0.1566132608966605 | 0.5036791980767341 | 0.2498993801096685 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1037549041122355 | 0.5472847358102826 | 0.2399749906997218 | T | T | T |
| 0.1210992789614842 | 0.5905660521515010 | 0.3326748105010880 | T | T | T |

OH\_B-CNT(8,8) #### KPOINTS: 1x1x3 #### E= -757.50002451 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C B O H

95 1 1 1

Selective dynamics

Direct

0.2518745470522089 0.0425117923478017 0.0834059004860784 T T T

0.1150435685253648 0.0512496204112100 0.0834533939659245 T T T

0.3325616179339145 0.0692903093366593 0.0833868956471391 T T T

0.0691336074557628 0.0873697858651441 0.0833333832590412 T T T

0.4931018240647930 0.1754850517701173 0.0834204493375202 T T T

0.0398929213664153 0.2117408197007739 0.0835625398682224 T T T

0.5618176585661576 0.2489487278024548 0.0834479460458936 T T T

0.0572435189223664 0.2900569711008658 0.0836257693663326 T T T

0.6536064265830114 0.4118267473306274 0.0834126968577079 T T T

0.1459975011440691 0.4541845042935870 0.0832601428895268 T T T

0.6709866595131888 0.4901015912050194 0.0834681779228798 T T T

0.2157180742940427 0.5281040921296265 0.0848302199875510 T T T

0.6407615468115584 0.6138641624604718 0.0832415213721852 T T T

0.3764960181852590 0.6305490761093849 0.0838799215226426 T T T

0.5942165579075106 0.6492895849962025 0.0831236913332032 T T T

0.4568032621846845 0.6564335488147629 0.0835487424477435 T T T

0.2134622342831518 0.0364879363177812 0.2500015856240252 T T T

0.1444480561166735 0.0408949343635456 0.2499921729313850 T T T

0.3738392565053497 0.0895789563949223 0.2500185826463046 T T T

0.4547643580594680 0.1430041683640087 0.2500259525581855 T T T

0.0388314298727285 0.1755006816726959 0.2499736645550646 T T T

0.6715881204065605 0.5261663649121708 0.2500042003019011 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2548122773406629 | 0.5578286576810380 | 0.2499318301043335 | T | T | T |
| 0.6564022927011580 | 0.5885821570806571 | 0.2499983480738631 | T | T | T |
| 0.5647698319969870 | 0.6594000005741290 | 0.2499800515086801 | T | T | T |
| 0.0536122172817406 | 0.1126808328869335 | 0.2499818744196393 | T | T | T |
| 0.5912317222939194 | 0.2887769899504743 | 0.2500194966820455 | T | T | T |
| 0.0727371375895395 | 0.3309643280543499 | 0.2499487913275697 | T | T | T |
| 0.6373302778546523 | 0.3708188634462505 | 0.2500147228665948 | T | T | T |
| 0.1180419335921701 | 0.4140377776590251 | 0.2499316957344136 | T | T | T |
| 0.3356136057444010 | 0.6107929368647582 | 0.2499462761783237 | T | T | T |
| 0.4954548042535099 | 0.6628186396614060 | 0.2499666430944352 | T | T | T |
| 0.2518741458598901 | 0.0425118898630382 | 0.4166053881534673 | T | T | T |
| 0.1150435411882402 | 0.0512481448697834 | 0.4165266462205776 | T | T | T |
| 0.3325614569144837 | 0.0692908031568544 | 0.4166458079101742 | T | T | T |
| 0.0691347207339991 | 0.0873697342917960 | 0.4166341152644107 | T | T | T |
| 0.4931012702927430 | 0.1754861022971993 | 0.4166317384233287 | T | T | T |
| 0.0398956971152728 | 0.2117448780183251 | 0.4163740634871746 | T | T | T |
| 0.5618180402651530 | 0.2489501461158751 | 0.4165979841984772 | T | T | T |
| 0.0572357043830677 | 0.2900564840608644 | 0.4162854072894446 | T | T | T |
| 0.6536057809303110 | 0.4118278224328481 | 0.4166108457387676 | T | T | T |
| 0.1460003167549347 | 0.4541621360587975 | 0.4166166450056646 | T | T | T |
| 0.6709907597425607 | 0.4901035278412136 | 0.4165426656585944 | T | T | T |
| 0.2157448766974038 | 0.5280440290760885 | 0.4150113294079860 | T | T | T |
| 0.6407508938605205 | 0.6138560060083380 | 0.4167498345710109 | T | T | T |
| 0.3765108833545244 | 0.6305505262582970 | 0.4160180700641147 | T | T | T |
| 0.5942098521024989 | 0.6492832791763057 | 0.4168497933032423 | T | T | T |
| 0.4568179092888403 | 0.6564547226853200 | 0.4163794928312950 | T | T | T |
| 0.2135251720662838 | 0.0367101366945943 | 0.5834091112411232 | T | T | T |
| 0.1445055812592335 | 0.0408898509700641 | 0.5833790495274408 | T | T | T |
| 0.3738989880754201 | 0.0896932268037744 | 0.5834586222696884 | T | T | T |
| 0.0537234279656385 | 0.1128861006449411 | 0.5835476445693408 | T | T | T |
| 0.4547606299437421 | 0.1430349595694882 | 0.5834967907610117 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0390202905969637 | 0.1756271450250643 | 0.5834838819184996 | T | T | T |
| 0.5911767973106612 | 0.2888282690074403 | 0.5834406197436091 | T | T | T |
| 0.0724606230406466 | 0.3309247018552791 | 0.5833688297149636 | T | T | T |
| 0.6372755172928952 | 0.3708048903276270 | 0.5834302980193109 | T | T | T |
| 0.1150652899995590 | 0.4133117104340296 | 0.5852789292405621 | T | T | T |
| 0.6716397459123947 | 0.5262229889962825 | 0.5833230931033608 | T | T | T |
| 0.2526459161261677 | 0.5645379946523538 | 0.5770706441408853 | T | T | T |
| 0.6564545994425359 | 0.5885421163694030 | 0.5833285312066298 | T | T | T |
| 0.3336883029214137 | 0.6118799736974182 | 0.5805256145058298 | T | T | T |
| 0.5636594301449378 | 0.6583561153103524 | 0.5835715393199259 | T | T | T |
| 0.4941875660710029 | 0.6615392846727191 | 0.5835329687962877 | T | T | T |
| 0.2518174299002908 | 0.0425046737901854 | 0.7500052036790534 | T | T | T |
| 0.1148962817167889 | 0.0510154595911139 | 0.7499917436776282 | T | T | T |
| 0.3325949031130168 | 0.0692522130731853 | 0.7500156519167569 | T | T | T |
| 0.4931524944343495 | 0.1754384827757385 | 0.7500291849949560 | T | T | T |
| 0.0396193180822827 | 0.2116845988443390 | 0.7499694601130023 | T | T | T |
| 0.1385623667497471 | 0.4538323903976894 | 0.7499357742824054 | T | T | T |
| 0.6404312708668635 | 0.6135060864320490 | 0.7499967651260209 | T | T | T |
| 0.5934906459940176 | 0.6483491851979548 | 0.7499838665876909 | T | T | T |
| 0.0690356478524079 | 0.0873245068838949 | 0.7499864328632492 | T | T | T |
| 0.5618393166424179 | 0.2489620014882089 | 0.7500252063176459 | T | T | T |
| 0.0562388437067010 | 0.2900388442962126 | 0.7499583595514113 | T | T | T |
| 0.6535805061556970 | 0.4118185030152660 | 0.7500131385859373 | T | T | T |
| 0.6708799773685936 | 0.4900660044458465 | 0.7500062118698105 | T | T | T |
| 0.3748303381554366 | 0.6311186171805978 | 0.7499650809400596 | T | T | T |
| 0.4548374130145931 | 0.6552797997925306 | 0.7499750886869839 | T | T | T |
| 0.2135261669964124 | 0.0367110258563493 | 0.9165912904159119 | T | T | T |
| 0.1445068330959372 | 0.0408916069370931 | 0.9166071575154318 | T | T | T |
| 0.3738987130126491 | 0.0896928158551898 | 0.9165824616658657 | T | T | T |
| 0.0537179523970752 | 0.1128826431069042 | 0.9164176085862958 | T | T | T |
| 0.4547602998724850 | 0.1430345406690010 | 0.9165603537274341 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0390131392523160 | 0.1756218852031297 | 0.9164621192281387 | T | T | T |
| 0.5911765861082140 | 0.2888283176209058 | 0.9166037403534687 | T | T | T |
| 0.0724808453651736 | 0.3309298544811419 | 0.9165410161278317 | T | T | T |
| 0.6372759567171496 | 0.3708054518774762 | 0.9165958305314206 | T | T | T |
| 0.1150827928196070 | 0.4133177021431831 | 0.9146047729361373 | T | T | T |
| 0.6716335607309465 | 0.5262199612465680 | 0.9166830969349488 | T | T | T |
| 0.2525977164194889 | 0.5646461334909076 | 0.9227944597306441 | T | T | T |
| 0.6564594989117669 | 0.5885451079651716 | 0.9166719199519623 | T | T | T |
| 0.3336632317035170 | 0.6119146638424564 | 0.9193704006490746 | T | T | T |
| 0.5636630419584924 | 0.6583594983663283 | 0.9163992219113111 | T | T | T |
| 0.4941836187745430 | 0.6615285454915488 | 0.9164181765368339 | T | T | T |
| 0.1998600764797893 | 0.5446002400879292 | 0.7498367531787250 | T | T | T |
| 0.1561034461532046 | 0.5881639818719228 | 0.7491859473399375 | T | T | T |
| 0.1915911754211443 | 0.6431343478813072 | 0.7470432269634549 | T | T | T |

OH\_B-CNT(9,9) #### KPOINTS: 1x1x3 #### E= -852.87158199 eV

1.0000000000000000

18.1865334800000014 -10.5000000000000000 0.0000000000000000

0.0000000000000000 21.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4005503900000003

C B O H

107 1 1 1

Selective dynamics

Direct

0.1978461294743444 0.0287874871998867 0.0832091847360417 T T T

0.1344537710218008 0.0368875094431436 0.0832414075123157 T T T

0.3474018534190521 0.0654244308555947 0.0833043104536390 T T T

0.4255986724165874 0.1080747053527688 0.0833346330243496 T T T

0.0492831851404345 0.1071725719129566 0.0831503740404790 T T T

0.0328474925708893 0.1653179123383000 0.0831462570567255 T T T

0.5687478425338740 0.2328692459424064 0.0833106551527389 T T T

0.6258855530716383 0.3078261933515301 0.0833212186894690 T T T

0.0525818641855532 0.3092717097663967 0.0833574381482524 T T T

0.0841668738526514 0.3872983489937825 0.0814524968133777 T T T

0.6960886984084834 0.4633780361306577 0.0833743200279221 T T T

0.7054011545144423 0.5353627439449410 0.0833403437431672 T T T

0.1977518869140547 0.5411987719339436 0.0895455940767133 T T T

0.2714120775878250 0.5990035832153411 0.0861337261990214 T T T

0.6714904399222988 0.6501379971566833 0.0833756833206598 T T T

0.6293590560766799 0.6862298558111587 0.0834316631487710 T T T

0.4280243546550080 0.6829819730876716 0.0831970396174137 T T T

0.5035087291963110 0.7027782341648925 0.0831727208748560 T T T

0.2332027436898155 0.0314962586406487 0.2500356357714753 T T T

0.3083177839170014 0.0499517366763232 0.2500883281708873 T T T

0.4639255182784160 0.1349776968587033 0.2501613329344842 T T T

0.5358512936959041 0.1977415239518263 0.2501250514478745 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0419389721033330 | 0.2711388070810370 | 0.2504573641597196 | T | T | T |
| 0.1092161681595079 | 0.4274599451154632 | 0.2499574780930935 | T | T | T |
| 0.1672778963219106 | 0.5030532848951016 | 0.2514934028109950 | T | T | T |
| 0.3117003028816839 | 0.6248102547286153 | 0.2506995866624792 | T | T | T |
| 0.3896659341580946 | 0.6676621334486078 | 0.2503146288305318 | T | T | T |
| 0.1073410339868069 | 0.0480170490926865 | 0.2501622425078412 | T | T | T |
| 0.0643944262309621 | 0.0832500424093073 | 0.2501304051653594 | T | T | T |
| 0.0315195413067540 | 0.1986751283056033 | 0.2503136716263757 | T | T | T |
| 0.6494666308501261 | 0.3468780204903132 | 0.2500711165832496 | T | T | T |
| 0.6847578276174381 | 0.4250569407132192 | 0.2500738390601209 | T | T | T |
| 0.7034740022985669 | 0.5684178563929416 | 0.2500292166547347 | T | T | T |
| 0.6865126367583141 | 0.6261484417964537 | 0.2500481863694508 | T | T | T |
| 0.6024802966639572 | 0.6977179067032575 | 0.2499890881752464 | T | T | T |
| 0.5394139573260799 | 0.7063989074849966 | 0.2498629376775940 | T | T | T |
| 0.1977886453811986 | 0.0285265690683744 | 0.4166666784807275 | T | T | T |
| 0.1343238230067106 | 0.0367632366978993 | 0.4166666995894515 | T | T | T |
| 0.3473170528498823 | 0.0653125812444057 | 0.4166667763642828 | T | T | T |
| 0.4256198978663137 | 0.1080572002775825 | 0.4166668008430735 | T | T | T |
| 0.0491915043938605 | 0.1069989373550464 | 0.4166667074028286 | T | T | T |
| 0.0327396760103591 | 0.1652804541301201 | 0.4166666973458017 | T | T | T |
| 0.5687594130590659 | 0.2328133852553003 | 0.4166668379938836 | T | T | T |
| 0.6259108184311004 | 0.3078277955340911 | 0.4166667730286140 | T | T | T |
| 0.0528299696354595 | 0.3093638172446904 | 0.4166667899413375 | T | T | T |
| 0.0872832254635010 | 0.3883978677717756 | 0.4166668689089238 | T | T | T |
| 0.6961455021921907 | 0.4633597438128150 | 0.4166667326766137 | T | T | T |
| 0.7054501583476284 | 0.5353937673361053 | 0.4166666753950036 | T | T | T |
| 0.2016335861295412 | 0.5359595886971396 | 0.4166669994158679 | T | T | T |
| 0.2736300923724065 | 0.5982488303627712 | 0.4166668467208110 | T | T | T |
| 0.6715385713627131 | 0.6501954371821064 | 0.4166666925983211 | T | T | T |
| 0.6291965764770946 | 0.6861077924635233 | 0.4166667357035380 | T | T | T |
| 0.4288989411000998 | 0.6840831895461276 | 0.4166668455465252 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5042365877804079 | 0.7036762268472821 | 0.4166667732233543 | T | T | T |
| 0.2332027448350711 | 0.0314962800433623 | 0.5832978214860385 | T | T | T |
| 0.3083178325921837 | 0.0499518136917344 | 0.5832451602950733 | T | T | T |
| 0.1073410230720519 | 0.0480170246183533 | 0.5831711451301212 | T | T | T |
| 0.0643944130804621 | 0.0832500423578206 | 0.5832030268089522 | T | T | T |
| 0.4639255063335577 | 0.1349776233264683 | 0.5831721513588904 | T | T | T |
| 0.5358513258447545 | 0.1977415022043671 | 0.5832084154797423 | T | T | T |
| 0.0315195931071581 | 0.1986751363217281 | 0.5830198971418403 | T | T | T |
| 0.0419389729803383 | 0.2711388236563345 | 0.5828762133369776 | T | T | T |
| 0.6494666103648429 | 0.3468780097535351 | 0.5832623711588601 | T | T | T |
| 0.6847578386125095 | 0.4250569551343612 | 0.5832596118949880 | T | T | T |
| 0.1092158509704388 | 0.4274601568716465 | 0.5833763781643065 | T | T | T |
| 0.1672773232722782 | 0.5030536880176393 | 0.5818405917587177 | T | T | T |
| 0.7034740640569390 | 0.5684178777966177 | 0.5833041372088404 | T | T | T |
| 0.6865126705271660 | 0.6261484512153364 | 0.5832852631440102 | T | T | T |
| 0.3117001295549150 | 0.6248103778257934 | 0.5826343867782471 | T | T | T |
| 0.3896658633628438 | 0.6676621571213445 | 0.5830190568576482 | T | T | T |
| 0.6024802770642775 | 0.6977178727003036 | 0.5833444522258029 | T | T | T |
| 0.5394139045901346 | 0.7063987805341109 | 0.5834706248783330 | T | T | T |
| 0.1978461066643644 | 0.0287874919697366 | 0.7501243062718088 | T | T | T |
| 0.1344537786882060 | 0.0368875024442660 | 0.7500920349412676 | T | T | T |
| 0.3474018532809759 | 0.0654244123237297 | 0.7500291770007247 | T | T | T |
| 0.4255986664840000 | 0.1080746411033690 | 0.7499988704262628 | T | T | T |
| 0.5687478492609154 | 0.2328692118523317 | 0.7500227770679523 | T | T | T |
| 0.0525818280286638 | 0.3092717227771431 | 0.7499761794665167 | T | T | T |
| 0.0841667201942031 | 0.3872983839849775 | 0.7518812111257609 | T | T | T |
| 0.1977510801950013 | 0.5411995779230674 | 0.7437886035612657 | T | T | T |
| 0.2714116735562715 | 0.5990038825863789 | 0.7472000344249199 | T | T | T |
| 0.4280243654525523 | 0.6829821126678538 | 0.7501364905883848 | T | T | T |
| 0.0492832172970529 | 0.1071725979350132 | 0.7501830307400080 | T | T | T |
| 0.0328475548315307 | 0.1653179240972420 | 0.7501872945285145 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6258854743265481 | 0.3078261654659774 | 0.7500122546142929 | T | T | T |
| 0.6960886704397492 | 0.4633780343305238 | 0.7499591184179738 | T | T | T |
| 0.7054012133860275 | 0.5353627821981892 | 0.7499930933226485 | T | T | T |
| 0.6714905154609220 | 0.6501380513486582 | 0.7499577701744248 | T | T | T |
| 0.6293590407273313 | 0.6862298393271071 | 0.7499018519533077 | T | T | T |
| 0.5035086967188981 | 0.7027782286139638 | 0.7501608858889767 | T | T | T |
| 0.2331139897281477 | 0.0314215038387057 | 0.9166667518787712 | T | T | T |
| 0.3083577706266709 | 0.0498884403679964 | 0.9166667724992977 | T | T | T |
| 0.1070911671483210 | 0.0476592772874096 | 0.9166666965080505 | T | T | T |
| 0.0640846412221464 | 0.0830294385741890 | 0.9166666880722339 | T | T | T |
| 0.4638750260716630 | 0.1348662010662577 | 0.9166668297894084 | T | T | T |
| 0.5358635554928372 | 0.1977265966890435 | 0.9166668056564656 | T | T | T |
| 0.0312647593580120 | 0.1985409903911269 | 0.9166667304966731 | T | T | T |
| 0.0410141249197536 | 0.2710406914514410 | 0.9166668062781249 | T | T | T |
| 0.6495249601688333 | 0.3468959721887525 | 0.9166667542556955 | T | T | T |
| 0.6848004943935213 | 0.4251403882754616 | 0.9166667245667443 | T | T | T |
| 0.1014032232541953 | 0.4258794900954809 | 0.9166668762049495 | T | T | T |
| 0.7034784128534440 | 0.5684366457760270 | 0.9166667184746575 | T | T | T |
| 0.6864083023442772 | 0.6260821721277416 | 0.9166666924037259 | T | T | T |
| 0.3098280316128647 | 0.6251011717855168 | 0.9166666691150641 | T | T | T |
| 0.3879960944732003 | 0.6664491248574266 | 0.9166666915050690 | T | T | T |
| 0.6024384613659376 | 0.6976310211227362 | 0.9166667253499182 | T | T | T |
| 0.5390316895144245 | 0.7055870526275032 | 0.9166667325177065 | T | T | T |
| 0.1472844564856623 | 0.5138307395774573 | 0.9166677011308886 | T | T | T |
| 0.0935407235693394 | 0.5420231283089435 | 0.9166690715352496 | T | T | T |
| 0.1196852231154985 | 0.5951351512360817 | 0.9166683616225205 | T | T | T |

OH\_B-CNT(10,10) ### KPOINTS: 1x1x3 ### E= -948.12213040 eV

1.0000000000000000

19.0525588799999994 -11.0000000000000000 0.0000000000000000

0.0000000000000000 22.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4010841699999999

C B O H

119 1 1 1

Selective dynamics

Direct

0.1875147690464663 0.0234722826927099 0.0833352924274635 T T T

0.2545902114941978 0.0284356418206466 0.0833766424627104 T T T

0.0810155585314411 0.0602773445867260 0.0834375355348165 T T T

0.4018723857309681 0.0830698563045078 0.0833666697752847 T T T

0.0470934207877447 0.1010253061317555 0.0833836666962949 T T T

0.4755008683322728 0.1309473389812532 0.0833904263318175 T T T

0.0257388406538051 0.2179884460435760 0.0835739659247371 T T T

0.6069398054416072 0.2572318324365799 0.0834236137733036 T T T

0.0377806547510573 0.2879298406011729 0.0837273384508755 T T T

0.6589653239237058 0.3297201248879977 0.0833847434418702 T T T

0.1011046398491159 0.4372726803907833 0.0831452334311504 T T T

0.7250369758631801 0.4783087326164469 0.0833099649738540 T T T

0.1543267222934481 0.5104226659942354 0.0845954570533715 T T T

0.7360286066226629 0.5478557651449917 0.0833196674298289 T T T

0.2873635937511205 0.6341375439146777 0.0839768793853132 T T T

0.7125905040602876 0.6635843333191871 0.0833039430240488 T T T

0.3607331047062972 0.6820693045105958 0.0835554994148045 T T T

0.6795034997916568 0.7051128280111058 0.0833269806503795 T T T

0.5080882231709206 0.7398925753953435 0.0830848227954453 T T T

0.5751775298750064 0.7448546842803427 0.0832240777921060 T T T

0.0357569913057675 0.1262888628576689 0.2499286474128327 T T T

0.5769803346163945 0.2226777047684701 0.2499739908880555 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0486166200011375 | 0.3245040243789043 | 0.2499181206310291 | T | T | T |
| 0.0810185972012306 | 0.3999207305731510 | 0.2499106247538454 | T | T | T |
| 0.1859935161900750 | 0.5430146353828575 | 0.2499225355932089 | T | T | T |
| 0.7358191654699553 | 0.5802449558959045 | 0.2499684117049097 | T | T | T |
| 0.2520798787507941 | 0.6060425025091583 | 0.2499217508733544 | T | T | T |
| 0.3982886070768510 | 0.7020808862524761 | 0.2499392347551795 | T | T | T |
| 0.6578644901728983 | 0.7208663227784964 | 0.2499533738478824 | T | T | T |
| 0.6054090287962599 | 0.7407631993207221 | 0.2499439123760609 | T | T | T |
| 0.1567312335114176 | 0.0266105784254862 | 0.2499512443230541 | T | T | T |
| 0.2903239052931387 | 0.0364981251642721 | 0.2499552863534632 | T | T | T |
| 0.1031256706244174 | 0.0451205081331641 | 0.2499473522304957 | T | T | T |
| 0.3643626426211246 | 0.0639281605019233 | 0.2499591003230525 | T | T | T |
| 0.5109659282692002 | 0.1592106145875660 | 0.2499735883474692 | T | T | T |
| 0.0251097384717366 | 0.1852164634185655 | 0.2499238789491876 | T | T | T |
| 0.6806568811489461 | 0.3670785355371668 | 0.2499745216208483 | T | T | T |
| 0.7138520615317124 | 0.4417344576627914 | 0.2499723082288625 | T | T | T |
| 0.7239845567449226 | 0.6382988787597408 | 0.2499651575581552 | T | T | T |
| 0.4723216904056737 | 0.7312594909313286 | 0.2499362044060935 | T | T | T |
| 0.1875153958939497 | 0.0234707016210066 | 0.4165668430012159 | T | T | T |
| 0.2545906625198287 | 0.0284354333421883 | 0.4165272918402875 | T | T | T |
| 0.0810208748260752 | 0.0602843490335265 | 0.4164526962310176 | T | T | T |
| 0.4018704694680245 | 0.0830685443793360 | 0.4165557551140726 | T | T | T |
| 0.0470955774995038 | 0.1010285967988018 | 0.4164851398855052 | T | T | T |
| 0.4755009845925905 | 0.1309472561995083 | 0.4165480871261952 | T | T | T |
| 0.0257186835821297 | 0.2179790204636158 | 0.4162736451479350 | T | T | T |
| 0.6069393498787398 | 0.2572313653202618 | 0.4165268354977748 | T | T | T |
| 0.0377761555439656 | 0.2879259554230906 | 0.4161086014040959 | T | T | T |
| 0.6589651764574384 | 0.3297198786335448 | 0.4165607620601646 | T | T | T |
| 0.1011064713591319 | 0.4372673109307552 | 0.4166903722127395 | T | T | T |
| 0.7250379035152423 | 0.4783100002824753 | 0.4166279335274258 | T | T | T |
| 0.1543268480814496 | 0.5104123584643504 | 0.4152077006724732 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7360300592971598 | 0.5478567552570275 | 0.4166140587756786 | T | T | T |
| 0.2873630083675517 | 0.6341334538477866 | 0.4158843082815318 | T | T | T |
| 0.7125948738631006 | 0.6635865490466001 | 0.4166242700057921 | T | T | T |
| 0.3607342359737116 | 0.6820683704122299 | 0.4163028413045464 | T | T | T |
| 0.6794948227442112 | 0.7051039564256436 | 0.4165827819364566 | T | T | T |
| 0.5080968927625794 | 0.7399170881940159 | 0.4167980138754650 | T | T | T |
| 0.5751887690928096 | 0.7448823901716679 | 0.4166522930161409 | T | T | T |
| 0.1568266962256311 | 0.0268365483327212 | 0.5834526044086390 | T | T | T |
| 0.2903942455683037 | 0.0365841404720794 | 0.5833150957024772 | T | T | T |
| 0.1032024346931571 | 0.0451514741661688 | 0.5833970853618965 | T | T | T |
| 0.3643077203209691 | 0.0639273338227673 | 0.5833038295643619 | T | T | T |
| 0.0358080593608056 | 0.1264307043588266 | 0.5834492982099435 | T | T | T |
| 0.5110000843623841 | 0.1592826492895577 | 0.5833575742804359 | T | T | T |
| 0.0251500932218190 | 0.1852336908680572 | 0.5834509330572493 | T | T | T |
| 0.5769833425204636 | 0.2227089369337994 | 0.5833412473716617 | T | T | T |
| 0.0482193072712616 | 0.3243164902800066 | 0.5831966389608896 | T | T | T |
| 0.6806204825865459 | 0.3670784102000543 | 0.5832774068215366 | T | T | T |
| 0.0778501894891229 | 0.3987249807294707 | 0.5850546502039168 | T | T | T |
| 0.7138198753114430 | 0.4416904806609969 | 0.5833073631485310 | T | T | T |
| 0.1816478201706160 | 0.5476844566054255 | 0.5770225254551108 | T | T | T |
| 0.7357708033689525 | 0.5802615292677828 | 0.5832954374714063 | T | T | T |
| 0.2497696967906465 | 0.6068160484197009 | 0.5804325564797603 | T | T | T |
| 0.7239314802597560 | 0.6382841879216193 | 0.5832845593623354 | T | T | T |
| 0.3975623981850205 | 0.7011707510643810 | 0.5833639917507557 | T | T | T |
| 0.6578748656700163 | 0.7208552898064386 | 0.5832795266321075 | T | T | T |
| 0.4717272930991477 | 0.7304682967291773 | 0.5834301290984243 | T | T | T |
| 0.6055698746001640 | 0.7409753911887187 | 0.5832230337542200 | T | T | T |
| 0.0807397565481790 | 0.0599526593118197 | 0.7499391351552862 | T | T | T |
| 0.0468230857928320 | 0.1008725380965055 | 0.7499285033904947 | T | T | T |
| 0.6069393227887204 | 0.2571933544476873 | 0.7499817224076696 | T | T | T |
| 0.0933457908060411 | 0.4353965878358708 | 0.7499142678790263 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7360468622944049 | 0.5479149898579638 | 0.7499669734495661 | T | T | T |
| 0.2854307959948429 | 0.6345388414655087 | 0.7499305910927502 | T | T | T |
| 0.3592110705236157 | 0.6810346073855060 | 0.7499284772539191 | T | T | T |
| 0.6794312554787214 | 0.7050189979829998 | 0.7499499723477584 | T | T | T |
| 0.5751284959361490 | 0.7448117951045160 | 0.7499387419102869 | T | T | T |
| 0.1874530374785088 | 0.0234366456824811 | 0.7499471773127834 | T | T | T |
| 0.2546055263707407 | 0.0283763079159068 | 0.7499537387874409 | T | T | T |
| 0.4018103905886681 | 0.0829672298131729 | 0.7499608535922773 | T | T | T |
| 0.4755374866219595 | 0.1309408294822997 | 0.7499685133488346 | T | T | T |
| 0.0254649417174665 | 0.2178437643725295 | 0.7499226355561012 | T | T | T |
| 0.0368512531292016 | 0.2878086480062350 | 0.7499179117365798 | T | T | T |
| 0.6589799858739120 | 0.3297290908691283 | 0.7499761097154171 | T | T | T |
| 0.7250816831738585 | 0.4783485813712990 | 0.7499696072040211 | T | T | T |
| 0.7125614801515153 | 0.6635814121766633 | 0.7499591347319987 | T | T | T |
| 0.5078541240664749 | 0.7392304926778593 | 0.7499398416575686 | T | T | T |
| 0.1568276803038094 | 0.0268392302431895 | 0.9164433282205318 | T | T | T |
| 0.2903954029635391 | 0.0365839126740188 | 0.9165925490086760 | T | T | T |
| 0.1031995960718621 | 0.0451502386474917 | 0.9164910203832831 | T | T | T |
| 0.3643105900271773 | 0.0639280488058189 | 0.9166140393383643 | T | T | T |
| 0.0358207345754937 | 0.1264368621985712 | 0.9164112140729216 | T | T | T |
| 0.5109988633597539 | 0.1592816895485628 | 0.9165862408004848 | T | T | T |
| 0.0251792192415612 | 0.1852469398206986 | 0.9164014091347764 | T | T | T |
| 0.5769825308156622 | 0.2227077149160454 | 0.9166088628766326 | T | T | T |
| 0.0482172602547157 | 0.3243178209083764 | 0.9166384144022688 | T | T | T |
| 0.6806211389867184 | 0.3670789471510724 | 0.9166716487180061 | T | T | T |
| 0.0778499880864226 | 0.3987264299570978 | 0.9147700097065153 | T | T | T |
| 0.7138209077098803 | 0.4416917793228770 | 0.9166327488146845 | T | T | T |
| 0.1816324402533347 | 0.5477080037119322 | 0.9228057079051400 | T | T | T |
| 0.7357718776075460 | 0.5802618073060996 | 0.9166318905345181 | T | T | T |
| 0.2497652127542623 | 0.6068210633947434 | 0.9194173228292962 | T | T | T |
| 0.7239304801564603 | 0.6382840049719254 | 0.9166436552088513 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3975602175121242 | 0.7011688873818972 | 0.9165046102672846 | T | T | T |
| 0.6578899249053155 | 0.7208719251633842 | 0.9166168073665911 | T | T | T |
| 0.4717201708322962 | 0.7304477065319872 | 0.9164494242307223 | T | T | T |
| 0.6055663863409043 | 0.7409636627841417 | 0.9166570469623332 | T | T | T |
| 0.1338359049415634 | 0.5192144961688345 | 0.7498682254121336 | T | T | T |
| 0.0793449051533976 | 0.5422005338232888 | 0.7495879983599856 | T | T | T |
| 0.1019314665343902 | 0.5927710294423250 | 0.7466045329575344 | T | T | T |

OH\_B-CNT(8,0) #### KPOINTS: 2x2x2 #### E= -499.03183838 eV

1.0000000000000000

12.9903810600000007 -7.5000000000000000 0.0000000000000000

0.0000000000000000 15.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5305455000000006

C B O H

63 1 1 1

Selective dynamics

Direct

0.0765273249248548 0.1923646031114101 0.0824243169779450 T T T

0.4982768580257019 0.2614308124015445 0.0838980661301876 T T T

0.1351696361630182 0.3762171318741988 0.0821956657312077 T T T

0.5610983389220983 0.4458089739295843 0.0841711855788811 T T T

0.1530932429681597 0.0823018558129111 0.0841747975852120 T T T

0.3272537531985297 0.1092470465666096 0.0839145795698735 T T T

0.3093790023733753 0.5316715784629734 0.0822673659468071 T T T

0.4820692847655823 0.5537392801649678 0.0824807886165221 T T T

0.2330540444198361 0.0771667794557103 0.1676856153178051 T T T

0.0976709898270937 0.1220192806599579 0.1671289747874479 T T T

0.4200838495903799 0.1748611652542936 0.1674435568222763 T T T

0.2136670071055067 0.4660218482125294 0.1648668520119224 T T T

0.5387441375603447 0.5151431403505251 0.1671368428249378 T T T

0.4020253980351103 0.5578338898821936 0.1657132679929588 T T T

0.0912179171184320 0.2808839115303210 0.1657105597600430 T T T

0.5475626119603280 0.3571872759091222 0.1677054872201879 T T T

0.0910175698693476 0.2810518393158676 0.3318332393185146 T T T

0.5476189402965991 0.3569611681876457 0.3339823897712940 T T T

0.2332222358794156 0.0771387308751374 0.3339697904377780 T T T

0.0979641074367551 0.1226044628635214 0.3334318780733666 T T T

0.4203725678139090 0.1744391833037994 0.3344757252198802 T T T

0.2143304357728482 0.4650085845181522 0.3283507679423254 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5382277627584251 | 0.5149056393599647 | 0.3334636281628663 | T | T | T |
| 0.4019000125815770 | 0.5578865106864135 | 0.3318565468692197 | T | T | T |
| 0.1542210275078197 | 0.0838561305675015 | 0.4172171498727207 | T | T | T |
| 0.3275089169484578 | 0.1090940497020342 | 0.4177783821725719 | T | T | T |
| 0.3082536033476315 | 0.5285515580367561 | 0.4125382085136978 | T | T | T |
| 0.4805739527208808 | 0.5524207427371899 | 0.4169804321893629 | T | T | T |
| 0.0779017750871001 | 0.1937690850801046 | 0.4169800250845809 | T | T | T |
| 0.4984279640476647 | 0.2610252540487525 | 0.4177878236715116 | T | T | T |
| 0.1377562107179017 | 0.3767787553396460 | 0.4125781742120815 | T | T | T |
| 0.5595995821522309 | 0.4448804129888492 | 0.4172501930445141 | T | T | T |
| 0.0793150085449687 | 0.1958999051909528 | 0.5840921086830575 | T | T | T |
| 0.4986301915030808 | 0.2609515050615376 | 0.5839181373620559 | T | T | T |
| 0.1371768469511051 | 0.3796153993477583 | 0.5776413383961341 | T | T | T |
| 0.5591913003144390 | 0.4447738585017949 | 0.5843417201541428 | T | T | T |
| 0.1544310123946995 | 0.0842457107177314 | 0.5843149015670840 | T | T | T |
| 0.3276104044618386 | 0.1089109934666704 | 0.5839331132494012 | T | T | T |
| 0.3058275125888167 | 0.5297429341475761 | 0.5776453847631283 | T | T | T |
| 0.4783037119529506 | 0.5513241748267476 | 0.5841609658801270 | T | T | T |
| 0.2335668701816162 | 0.0774408687238999 | 0.6676247524617147 | T | T | T |
| 0.1003933790740354 | 0.1250291086784607 | 0.6676616425456710 | T | T | T |
| 0.4206685652718516 | 0.1741212752195825 | 0.6674872609570680 | T | T | T |
| 0.2106249378888694 | 0.4700561323440766 | 0.6566752458148021 | T | T | T |
| 0.5354680376872866 | 0.5127711177914458 | 0.6676861995726405 | T | T | T |
| 0.3983560264308788 | 0.5564340726658128 | 0.6660516138438755 | T | T | T |
| 0.0929747054280550 | 0.2844829020204847 | 0.6660006779625871 | T | T | T |
| 0.5473161098092818 | 0.3567234957409847 | 0.6676480743039749 | T | T | T |
| 0.0926493307019285 | 0.2840340246169639 | 0.8352992096789033 | T | T | T |
| 0.5475957994270851 | 0.3567562904895920 | 0.8338198812517149 | T | T | T |
| 0.2334978050885806 | 0.0770600430403289 | 0.8337947964503616 | T | T | T |
| 0.0999644089616329 | 0.1242229635236712 | 0.8334050167760956 | T | T | T |
| 0.4206776103055625 | 0.1741614680321048 | 0.8345226731223518 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5361584682414593 | 0.5130758010135121 | 0.8334145801149460 | T | T | T |
| 0.3987086327107190 | 0.5568955513654161 | 0.8353592079887159 | T | T | T |
| 0.1539958813857416 | 0.0830675640837791 | 0.9171209951286952 | T | T | T |
| 0.3276288019544411 | 0.1091618101285531 | 0.9177841151570765 | T | T | T |
| 0.3092031243138921 | 0.5360536843493530 | 0.9186032544821017 | T | T | T |
| 0.4800691362056808 | 0.5519628423372719 | 0.9165345880721095 | T | T | T |
| 0.0784720369011562 | 0.1939895044592183 | 0.9165549846138670 | T | T | T |
| 0.4983061775335843 | 0.2610553538754563 | 0.9178147389727919 | T | T | T |
| 0.1312493459726325 | 0.3769744213136886 | 0.9186550282353519 | T | T | T |
| 0.5601856408152538 | 0.4450204926241115 | 0.9171565858369538 | T | T | T |
| 0.1973893908135894 | 0.4875786572712488 | 0.8354680054777935 | T | T | T |
| 0.1433771191682722 | 0.5478358745091162 | 0.8547927944163158 | T | T | T |
| 0.1851266071181356 | 0.6173795173309249 | 0.8171141292758938 | T | T | T |

OH\_B-CNT(9,0) #### KPOINTS: 2x2x2 #### E= -563.21368871 eV

1.0000000000000000

13.8564064600000005 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5367054200000005

C B O H

71 1 1 1

Selective dynamics

Direct

0.1993203855641937 0.0678552823265293 0.0827032635307895 T T T

0.0891220197713444 0.1319329895664219 0.0823190057612355 T T T

0.3717694716278487 0.1230423572264414 0.0825331255536542 T T T

0.0846655158895436 0.2833277960154164 0.0834801486685198 T T T

0.5245161630436029 0.2751691377668824 0.0824891632906391 T T T

0.1874316738943323 0.4601308113888654 0.0918519851162387 T T T

0.5802294627736759 0.4476680609072333 0.0826557514190302 T T T

0.3644097957290994 0.5623271572380212 0.0833550808850821 T T T

0.5156245730450139 0.5574413964459863 0.0822496787975559 T T T

0.1325101935941476 0.0859091703045103 0.1660537149030460 T T T

0.2821048703057809 0.0799666099106214 0.1663758891213556 T T T

0.4560595745584783 0.1910970665960360 0.1660735880348219 T T T

0.0730805702319696 0.2007073823173413 0.1654957055200668 T T T

0.5680023082771415 0.3648535769510871 0.1663367943718430 T T T

0.1245684223421406 0.3727987677592613 0.1711646114740448 T T T

0.5619596580208449 0.5143668548100220 0.1660055310155970 T T T

0.2748946773747478 0.5227361492237751 0.1710574618569894 T T T

0.4468538942838650 0.5734730493213716 0.1653882970200702 T T T

0.1320241269917420 0.0849741090378603 0.3327381050520329 T T T

0.2819879701620076 0.0798721160177090 0.3323918134460605 T T T

0.4558828199316201 0.1912793226572145 0.3327994004525324 T T T

0.0720658527822930 0.1986580635945515 0.3328286848351964 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5680640163585907 | 0.3649898913446781 | 0.3323670638670079 | T | T | T |
| 0.1256654766694476 | 0.3701598695727183 | 0.3361535283123142 | T | T | T |
| 0.5628729688989115 | 0.5148707620281688 | 0.3326544991908454 | T | T | T |
| 0.2776110371278557 | 0.5217923366797800 | 0.3361505188412856 | T | T | T |
| 0.4489514120308876 | 0.5745705090584975 | 0.3327797094652497 | T | T | T |
| 0.1987147268904889 | 0.0669367660104849 | 0.4158967172507957 | T | T | T |
| 0.0873153894377678 | 0.1299084337084960 | 0.4164241756262824 | T | T | T |
| 0.3715840862467292 | 0.1231329217212603 | 0.4162551675843881 | T | T | T |
| 0.0847817097708630 | 0.2806759076954623 | 0.4176430324754717 | T | T | T |
| 0.5243987660441808 | 0.2753944903198212 | 0.4162640159638925 | T | T | T |
| 0.1926624614148666 | 0.4550298083343735 | 0.4208188867893132 | T | T | T |
| 0.5811035277453859 | 0.4483147749855182 | 0.4158522656719443 | T | T | T |
| 0.3671078689414189 | 0.5624079940743947 | 0.4175702297395445 | T | T | T |
| 0.5176753184591206 | 0.5593321648008803 | 0.4163376114071566 | T | T | T |
| 0.1987619822437808 | 0.0670172564191256 | 0.5827400390879454 | T | T | T |
| 0.0870792754245924 | 0.1295890123458551 | 0.5828003768509560 | T | T | T |
| 0.3715413054011961 | 0.1232228027124040 | 0.5824833430008048 | T | T | T |
| 0.0849649117689015 | 0.2808165420948197 | 0.5835447347713342 | T | T | T |
| 0.5242428011335362 | 0.2754011504398892 | 0.5824536348534618 | T | T | T |
| 0.1917244597635826 | 0.4560623302679923 | 0.5842859138215546 | T | T | T |
| 0.5809989698925534 | 0.4482480993167612 | 0.5827019158180632 | T | T | T |
| 0.3670230925143252 | 0.5623877692195363 | 0.5834752868357274 | T | T | T |
| 0.5180345047520140 | 0.5596199767148473 | 0.5827863743161497 | T | T | T |
| 0.1315707008278716 | 0.0844343854306564 | 0.6661797634459207 | T | T | T |
| 0.2818557301659444 | 0.0798238823359663 | 0.6663135756694256 | T | T | T |
| 0.4557351459543583 | 0.1913803319719602 | 0.6658798346746025 | T | T | T |
| 0.0714681441990659 | 0.1980378815927373 | 0.6671031145821388 | T | T | T |
| 0.5680001749904444 | 0.3650913104714568 | 0.6662704649204820 | T | T | T |
| 0.1228289688258287 | 0.3697473649633949 | 0.6674950623825053 | T | T | T |
| 0.5634463573026101 | 0.5153716270539501 | 0.6661724110743528 | T | T | T |
| 0.2780975888181397 | 0.5248941764936217 | 0.6674014460381139 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4496545857816688 | 0.5753568296049959 | 0.6669905068236215 | T | T | T |
| 0.1322248360265411 | 0.0851310731895104 | 0.8327259295348943 | T | T | T |
| 0.2819850326980258 | 0.0799048354953311 | 0.8324264992621866 | T | T | T |
| 0.4557542767005383 | 0.1913503992171580 | 0.8327143733857895 | T | T | T |
| 0.0731842263145722 | 0.1997407534642512 | 0.8333935409127208 | T | T | T |
| 0.5679342582067739 | 0.3649343205068230 | 0.8323943940859547 | T | T | T |
| 0.1177423476215561 | 0.3706848865093548 | 0.8309017149939930 | T | T | T |
| 0.5627243152101441 | 0.5146671558234399 | 0.8326660590479402 | T | T | T |
| 0.2768910141619817 | 0.5298108792057745 | 0.8309727248833395 | T | T | T |
| 0.4478896374628839 | 0.5735913276375142 | 0.8333502202575803 | T | T | T |
| 0.1991193006144034 | 0.0674591643442417 | 0.9160850927722234 | T | T | T |
| 0.0891320532844750 | 0.1315626223938603 | 0.9165172859357340 | T | T | T |
| 0.3716459904983466 | 0.1230701898644442 | 0.9162390428504750 | T | T | T |
| 0.0848863596209084 | 0.2834365088908581 | 0.9147583660428650 | T | T | T |
| 0.5244342731672780 | 0.2752786129213353 | 0.9162357317205908 | T | T | T |
| 0.5805803711671145 | 0.4478696851601340 | 0.9160449761868601 | T | T | T |
| 0.3642953765466179 | 0.5623167708815328 | 0.9146813140934554 | T | T | T |
| 0.5159884822406677 | 0.5574768409676368 | 0.9164203483198500 | T | T | T |
| 0.1718052542593939 | 0.4750130300550866 | 0.9140025265605779 | T | T | T |
| 0.1126166589604459 | 0.5228228233499155 | 0.8932673286160953 | T | T | T |
| 0.1446944692450322 | 0.5871615329541966 | 0.9364505092578549 | T | T | T |

OH\_B-CNT(10,0) #### KPOINTS: 2x2x2 #### E= -627.53257032 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C B O H

79 1 1 1

Selective dynamics

Direct

0.2413868559087680 0.0615775053332005 0.0841264973986973 T T T

0.1100924565626912 0.0839896736386203 0.0841456344689505 T T T

0.4073201217572945 0.1414116899632515 0.0843163889612588 T T T

0.5440652539418654 0.2916403639364255 0.0842953154791577 T T T

0.1091968564246217 0.3588056914673474 0.0824590671718942 T T T

0.2489912038717113 0.5126058130430133 0.0825556263071665 T T T

0.5475329814978924 0.5659075106496764 0.0841823434773372 T T T

0.4145691219255468 0.5861474385432929 0.0828750385338867 T T T

0.0613244843016897 0.1973405721080450 0.0828300588348011 T T T

0.5986521109386984 0.4546213469657780 0.0841465068162238 T T T

0.1676705652225652 0.0598111983617556 0.1674092500456919 T T T

0.4830793671557877 0.2109762356919538 0.1677650132855816 T T T

0.1711680419399537 0.4416112951465726 0.1647862470494812 T T T

0.4886159813194180 0.5884009022926588 0.1671029824459536 T T T

0.3242507950014444 0.0899437469778926 0.1675007900092480 T T T

0.0735566197885154 0.1312966443752995 0.1670895747594109 T T T

0.0747859698283421 0.2754482446640315 0.1660766046630914 T T T

0.5840114587125659 0.3754548516553667 0.1674938020638993 T T T

0.5857226260661846 0.5201835655561542 0.1674482325810217 T T T

0.3325951847823411 0.5592243702814725 0.1660914995112343 T T T

0.3243808280485632 0.0898901308462575 0.3342845616791638 T T T

0.0737834612025850 0.1317015377489086 0.3337936457125649 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0749005696254963 | 0.2755404651590482 | 0.3321038150336291 | T | T | T |
| 0.5841607103163768 | 0.3753972397658208 | 0.3342840030203884 | T | T | T |
| 0.5855279635840892 | 0.5201131892221221 | 0.3342259967217997 | T | T | T |
| 0.3324951699311723 | 0.5590374364700683 | 0.3321300559765686 | T | T | T |
| 0.1677344574194293 | 0.0599789935475742 | 0.3341940567340810 | T | T | T |
| 0.4833229808678776 | 0.2108380064054485 | 0.3341617723990942 | T | T | T |
| 0.1722569983448428 | 0.4407705981028681 | 0.3286904243895704 | T | T | T |
| 0.4882044242385119 | 0.5881097020987686 | 0.3338370820885636 | T | T | T |
| 0.0623577810620636 | 0.1982209387565767 | 0.4169879498303425 | T | T | T |
| 0.5982891039699878 | 0.4543040341489752 | 0.4176892100854685 | T | T | T |
| 0.2416928815243969 | 0.0619660866279155 | 0.4176629037390412 | T | T | T |
| 0.1108449620692170 | 0.0848715683494325 | 0.4173079718736281 | T | T | T |
| 0.4075792163512692 | 0.1412735101638787 | 0.4174476680286541 | T | T | T |
| 0.5443901456761707 | 0.2914677937628952 | 0.4174793184974462 | T | T | T |
| 0.1124186442005206 | 0.3594920763045884 | 0.4129074288017219 | T | T | T |
| 0.2487892243710642 | 0.5095599161751192 | 0.4128447800190542 | T | T | T |
| 0.5467273712486562 | 0.5650863145426293 | 0.4173328799757905 | T | T | T |
| 0.4137770143374553 | 0.5849655562286645 | 0.4169945098474855 | T | T | T |
| 0.2416848232247269 | 0.0619376086739179 | 0.5840573685449193 | T | T | T |
| 0.1112211648554255 | 0.0855224167114410 | 0.5843165999609369 | T | T | T |
| 0.4075933267950519 | 0.1412116995732183 | 0.5841976522997478 | T | T | T |
| 0.5444499009792062 | 0.2914393471780788 | 0.5842244041137817 | T | T | T |
| 0.1110216695871877 | 0.3617705495723819 | 0.5782881535169634 | T | T | T |
| 0.2460514804496921 | 0.5102560672591931 | 0.5783163205298055 | T | T | T |
| 0.5461103711774753 | 0.5645879686621050 | 0.5843414628894328 | T | T | T |
| 0.4119261418343238 | 0.5836443340331717 | 0.5843661109389774 | T | T | T |
| 0.0633220458465684 | 0.2000835090382853 | 0.5843268978473013 | T | T | T |
| 0.5983361502806247 | 0.4542685716803110 | 0.5840921952684814 | T | T | T |
| 0.1681020661251542 | 0.0604572432244055 | 0.6674659267876616 | T | T | T |
| 0.4833579816804265 | 0.2107749728102188 | 0.6676180957992439 | T | T | T |
| 0.1668216650045319 | 0.4447540878862358 | 0.6570549331538791 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4865180884607139 | 0.5859231941181208 | 0.6677424470336044 | T | T | T |
| 0.3243893599255525 | 0.0900379121315180 | 0.6674181522093142 | T | T | T |
| 0.0757363196214592 | 0.1336237353693801 | 0.6677208112552019 | T | T | T |
| 0.0748496642103601 | 0.2779984635815059 | 0.6659693681371515 | T | T | T |
| 0.5840051057125261 | 0.3753026789829152 | 0.6674657505907219 | T | T | T |
| 0.5851122339393878 | 0.5196334532140929 | 0.6674955143794957 | T | T | T |
| 0.3298367599005184 | 0.5584126344875567 | 0.6659867298525244 | T | T | T |
| 0.3242529811935945 | 0.0899622176106469 | 0.8342950863092762 | T | T | T |
| 0.0753816592516780 | 0.1329373905649697 | 0.8338176212618615 | T | T | T |
| 0.0741109401029550 | 0.2774147255481308 | 0.8352551254149283 | T | T | T |
| 0.5840108302149903 | 0.3754085683371772 | 0.8343071704421876 | T | T | T |
| 0.5854556734035948 | 0.5199320575400180 | 0.8340867740409438 | T | T | T |
| 0.3303379934244984 | 0.5593207538901916 | 0.8352716914228323 | T | T | T |
| 0.1678048041065622 | 0.0600621675640051 | 0.8340680811641703 | T | T | T |
| 0.4832352532295824 | 0.2108484247010116 | 0.8341733898557931 | T | T | T |
| 0.4871789379328698 | 0.5863851850259455 | 0.8338655113000127 | T | T | T |
| 0.0627488719703297 | 0.1985938736017660 | 0.9166092759345986 | T | T | T |
| 0.5984848104385236 | 0.4544211406829952 | 0.9176455761091428 | T | T | T |
| 0.2415000307334932 | 0.0617400299656529 | 0.9176229268047945 | T | T | T |
| 0.1106599067401073 | 0.0845420121257586 | 0.9171890701041349 | T | T | T |
| 0.4073677978915016 | 0.1414555408661234 | 0.9175441638653153 | T | T | T |
| 0.5440254747280159 | 0.2915581975429550 | 0.9175535953383839 | T | T | T |
| 0.1042668868555026 | 0.3589557071652427 | 0.9188261709903447 | T | T | T |
| 0.2477551587047142 | 0.5166696442562860 | 0.9187398831323859 | T | T | T |
| 0.5470374969734768 | 0.5652307286186852 | 0.9172189964624463 | T | T | T |
| 0.4135025639802847 | 0.5846553801572992 | 0.9166356290241459 | T | T | T |
| 0.1504520976511939 | 0.4565361390616350 | 0.8348641903801535 | T | T | T |
| 0.0886097050310126 | 0.4952126638998033 | 0.8513415506287135 | T | T | T |
| 0.1165718404929406 | 0.5562332480062876 | 0.8104071165862387 | T | T | T |



OH\_B-CNT(11,0) #### KPOINTS: 2x2x2 #### E= -691.43942243 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C B O H

87 1 1 1

Selective dynamics

Direct

0.150885647211690 0.0534420080905162 0.0842653491656585 T T T

0.2960633741271661 0.0741561552532271 0.0847048077495265 T T T

0.0641288855773159 0.1234234103113465 0.0840663140396103 T T T

0.4506753818529350 0.1759867651310056 0.0850915860981234 T T T

0.0614858113310411 0.2582497210252209 0.0823293290003510 T T T

0.5668284813587198 0.3258189925074980 0.0847063174396823 T T T

0.1378096068093860 0.4153699574972682 0.0815310334854624 T T T

0.6090402735586429 0.4779956379701000 0.0842213163408805 T T T

0.2824847289416850 0.5487752080529471 0.0815574887663068 T T T

0.5605899586728497 0.5830976287509487 0.0839525713785610 T T T

0.4380092485998283 0.6069848548945943 0.0822681686687260 T T T

0.2191813713297304 0.0525416548019318 0.1679124992775604 T T T

0.0977552924285965 0.0780106845355974 0.1675433226980891 T T T

0.3754522480318467 0.1166715502058760 0.1683565332623561 T T T

0.0517457191020210 0.1851270097853747 0.1669197518434019 T T T

0.5160825853805958 0.2475057959078738 0.1683347251324906 T T T

0.0920630775420592 0.3364645103038096 0.1653978011390564 T T T

0.5985390605674625 0.4046270619167553 0.1678678540838745 T T T

0.2049527351784802 0.4887059183385541 0.1638309762516474 T T T

0.5960376843692149 0.5393596131775520 0.1674557957037694 T T T

0.3616499158009603 0.5859108076727186 0.1653267903869099 T T T

0.5063933927790504 0.6062213419808794 0.1668503883427477 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2190633340950956 | 0.0522956737286246 | 0.3348149525632345 | T | T | T |
| 0.0977604515024388 | 0.0779992403975395 | 0.3341314446797364 | T | T | T |
| 0.3753926091185967 | 0.1166780634534464 | 0.3347595340249358 | T | T | T |
| 0.0520331587534130 | 0.1854340678250298 | 0.3334308900279200 | T | T | T |
| 0.5160995874790442 | 0.2476083960279190 | 0.3347483784861729 | T | T | T |
| 0.0923097938450567 | 0.3365609593087231 | 0.3314089139748359 | T | T | T |
| 0.5987667662811450 | 0.4047488121236793 | 0.3347967604408051 | T | T | T |
| 0.2058530010781122 | 0.4876014109495889 | 0.3279735009570114 | T | T | T |
| 0.5960666445500423 | 0.5394195569315162 | 0.3340590282994728 | T | T | T |
| 0.3614957644651504 | 0.5857085786260150 | 0.3313483410515713 | T | T | T |
| 0.5060543331204700 | 0.6060025091080331 | 0.3333290156936606 | T | T | T |
| 0.1508533756932799 | 0.0532325595000203 | 0.4179770859775298 | T | T | T |
| 0.2959892907971843 | 0.0741469036739314 | 0.4181756666592508 | T | T | T |
| 0.0649768142385723 | 0.1240857943209518 | 0.4172268444710835 | T | T | T |
| 0.4505393123028493 | 0.1761711901541816 | 0.4181129151856523 | T | T | T |
| 0.0627491360208613 | 0.2589976854441472 | 0.4165895591506604 | T | T | T |
| 0.5668316486470084 | 0.3259414239503434 | 0.4181290633731147 | T | T | T |
| 0.1409078536656413 | 0.4154002267137387 | 0.4121735635226390 | T | T | T |
| 0.6092360104338669 | 0.4780564560025460 | 0.4179127217042642 | T | T | T |
| 0.2819300011118053 | 0.5457839740685481 | 0.4120336953314866 | T | T | T |
| 0.5598965250604945 | 0.5823927325250308 | 0.4171503294227421 | T | T | T |
| 0.4370825895828062 | 0.6057161175061895 | 0.4164659297349027 | T | T | T |
| 0.1509045660342474 | 0.0534728369214821 | 0.5842526988345376 | T | T | T |
| 0.2960513524697442 | 0.0741184623782640 | 0.5846879562039580 | T | T | T |
| 0.0653288363031928 | 0.1246539040312255 | 0.5843042895030812 | T | T | T |
| 0.4506748750503870 | 0.1759891857580714 | 0.5848810734528554 | T | T | T |
| 0.0636717158459931 | 0.2604353103825094 | 0.5838709739374104 | T | T | T |
| 0.5668330206420344 | 0.3258253849710992 | 0.5846541267581550 | T | T | T |
| 0.1400966565021608 | 0.4177453760715899 | 0.5774456781201810 | T | T | T |
| 0.6089665172051154 | 0.4779754410174809 | 0.5842129494019317 | T | T | T |
| 0.2799555870508170 | 0.5470116569147767 | 0.5773988342759170 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5593429949875324 | 0.5820980562000868 | 0.5842229852248126 | T | T | T |
| 0.4356975983711199 | 0.6049958386614424 | 0.5837576599377853 | T | T | T |
| 0.2192260934170807 | 0.0526696859479648 | 0.6678867000216310 | T | T | T |
| 0.0980920964805691 | 0.0784405834070974 | 0.6677572924476054 | T | T | T |
| 0.3754987296041254 | 0.1165263007538739 | 0.6682024655242975 | T | T | T |
| 0.0539031705809206 | 0.1867952367722351 | 0.6674204486164931 | T | T | T |
| 0.5161962751960365 | 0.2474110063359595 | 0.6681812127376410 | T | T | T |
| 0.0925198310503028 | 0.3389172367389018 | 0.6654719371995790 | T | T | T |
| 0.5983488730662151 | 0.4045593841915422 | 0.6678302896807735 | T | T | T |
| 0.2021767337510533 | 0.4923067106035010 | 0.6562213834892821 | T | T | T |
| 0.5955517578685523 | 0.5390380996631852 | 0.6676940858467053 | T | T | T |
| 0.3594166234117129 | 0.5858448730358742 | 0.6653399797244329 | T | T | T |
| 0.5046433302201316 | 0.6043072191212956 | 0.6673302453572877 | T | T | T |
| 0.2192398655903761 | 0.0526723014473865 | 0.8347192361253039 | T | T | T |
| 0.0978561591831794 | 0.0780725705359439 | 0.8341140958479212 | T | T | T |
| 0.3755161370995395 | 0.1164221709377108 | 0.8347234497164422 | T | T | T |
| 0.0536154482424414 | 0.1863460518639949 | 0.8334812842159284 | T | T | T |
| 0.5162675208393543 | 0.2473458771226353 | 0.8347124796367883 | T | T | T |
| 0.0915972545595816 | 0.3385594526443792 | 0.8347105547676660 | T | T | T |
| 0.5983547586613894 | 0.4045083036588112 | 0.8346763982540134 | T | T | T |
| 0.5958865702509684 | 0.5391660129171431 | 0.8340582608753352 | T | T | T |
| 0.3599369186984833 | 0.5867681812255712 | 0.8345925911577528 | T | T | T |
| 0.5051334686080138 | 0.6045834483077308 | 0.8333802698918392 | T | T | T |
| 0.1509777139537397 | 0.0534762721147709 | 0.9179028901793681 | T | T | T |
| 0.2960629177581193 | 0.0742596168650916 | 0.9181429127381583 | T | T | T |
| 0.0648373668376520 | 0.1238835575617199 | 0.9170966001030012 | T | T | T |
| 0.4507169179408408 | 0.1758736544407373 | 0.9181883529704157 | T | T | T |
| 0.0626816450852680 | 0.2590790180821425 | 0.9161739040572827 | T | T | T |
| 0.5667081189578781 | 0.3257824774179957 | 0.9181042117221727 | T | T | T |
| 0.1333970360583838 | 0.4163933495598529 | 0.9180303231285583 | T | T | T |
| 0.6089585556995668 | 0.4778473992032835 | 0.9178334538323289 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2821988846579068 | 0.5532441630025086 | 0.9178757200278448 | T | T | T |
| 0.5600749791907935 | 0.5823937051200011 | 0.9170394035120646 | T | T | T |
| 0.4372122603171313 | 0.6060226073319560 | 0.9161093160528297 | T | T | T |
| 0.1900551109943417 | 0.5072394165422238 | 0.8336585104106539 | T | T | T |
| 0.1446064675632171 | 0.5581047162204757 | 0.8462775273980951 | T | T | T |
| 0.1817752882390534 | 0.6168592655451038 | 0.8145841320944077 | T | T | T |

OH\_B-CNT(12,0) ### KPOINTS: 1x1x2 ### E= -754.74638928 eV

1.0000000000000000

15.588499999999998 -9.000000000000000 0.0000000000000000

0.0000000000000000 18.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.457919999999997

C B O H

95 1 1 1

Selective dynamics

Direct

0.6558116147327506 0.5368136552986746 0.4172902916276136 T T T

0.6560272780329843 0.5369657486177174 0.9173473113395226 T T T

0.4672673767606502 0.6494428407240295 0.4159050079685932 T T T

0.4668297277930217 0.6491898214731526 0.9154988766397403 T T T

0.3910639787265109 0.1096777065445352 0.4177407209330271 T T T

0.3912193120649324 0.1094306553723605 0.9177266390600280 T T T

0.1084842636546668 0.0665546904262936 0.4173645830440855 T T T

0.1083993389950443 0.0665264143171272 0.9174167852073314 T T T

0.6338451596986568 0.3907382525928797 0.4174203545421044 T T T

0.6334370186636394 0.3906217025322142 0.9173930092231396 T T T

0.5934551961747685 0.6307129323884412 0.4166133761014163 T T T

0.5933558730462247 0.6305509796260007 0.9165279383085064 T T T

0.1671347837562508 0.4665579643149861 0.4123336759553134 T T T

0.1591591718420788 0.4695186766473133 0.9172410926948199 T T T

0.0735413418147118 0.3107441490142457 0.4159803937948293 T T T

0.0735438275106909 0.3111780863599948 0.9155749938966589 T T T

0.2345671721123075 0.0478614980870774 0.4174547587379360 T T T

0.2347794878920418 0.0482558459745736 0.9174203514303164 T T T

0.5365083242933490 0.2346101748683189 0.4177066317410027 T T T

0.5366277782668738 0.2343696069375445 0.9177003802483985 T T T

0.3121108256339316 0.5915284310786286 0.4123364363388724 T T T

0.3122865521659630 0.6013223222487243 0.9173482032199898 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0505981544412534 | 0.1642445632754423 | 0.4167107323221428 | T | T | T |
| 0.0506258284384520 | 0.1643180680771876 | 0.9166269573351574 | T | T | T |
| 0.5939499679923900 | 0.6312333845747543 | 0.0836061297962633 | T | T | T |
| 0.5927723562702545 | 0.6302707803633411 | 0.5836786674022324 | T | T | T |
| 0.0499150838059020 | 0.1638547581741849 | 0.0836910479783385 | T | T | T |
| 0.0511193009335290 | 0.1648771531809423 | 0.5837535387221363 | T | T | T |
| 0.3124747126154018 | 0.5951256329879531 | 0.0811701210998083 | T | T | T |
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| 0.1085009919919841 | 0.0665946306044551 | 0.5839326031117767 | T | T | T |
| 0.6560438966481390 | 0.5370232143154451 | 0.0839816416746033 | T | T | T |
| 0.6557914198386624 | 0.5367922089429276 | 0.5838559959586896 | T | T | T |
| 0.2346386843639189 | 0.0480725166300769 | 0.0846156395591073 | T | T | T |
| 0.2346706941114450 | 0.0480004540148445 | 0.5845879100544015 | T | T | T |
| 0.1639072057555141 | 0.4672405550498754 | 0.0812591773160895 | T | T | T |
| 0.1664004460897773 | 0.4694353932783003 | 0.5781660590763669 | T | T | T |
| 0.3911051872380955 | 0.1094487750162970 | 0.0844996360297104 | T | T | T |
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| 0.4678431056468266 | 0.6501253521389401 | 0.0822382454689254 | T | T | T |
| 0.4658230671544389 | 0.6489217267238998 | 0.5836614446967446 | T | T | T |
| 0.5366574775016738 | 0.2344989238807742 | 0.0845021172976094 | T | T | T |
| 0.5365574686149966 | 0.2345132181122373 | 0.5845263003533828 | T | T | T |
| 0.0725285823921812 | 0.3103000037038443 | 0.0823341623473200 | T | T | T |
| 0.0743769954995277 | 0.3122233692082209 | 0.5837713325281004 | T | T | T |
| 0.6336186956192932 | 0.3907059551081870 | 0.0845913201241438 | T | T | T |
| 0.6337021989529861 | 0.3906488351759814 | 0.5845449621800947 | T | T | T |
| 0.2340619634119929 | 0.5376840363229446 | 0.1634857571958179 | T | T | T |
| 0.2312106101688526 | 0.5424346666155744 | 0.6569622292306154 | T | T | T |
| 0.0510124334373751 | 0.2333084287927780 | 0.1663502331192396 | T | T | T |
| 0.0529032145388230 | 0.2346178046915123 | 0.6667736387752464 | T | T | T |
| 0.3115429149968697 | 0.0693042888633353 | 0.1676833808838303 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.3115977826455989 | 0.0694639734496704 | 0.6677117880966644 | T | T | T |
| 0.3915718388144395 | 0.6297468256319820 | 0.1650479930688308 | T | T | T |
| 0.3898648312182097 | 0.6312410687416854 | 0.6650246186039047 | T | T | T |
| 0.6347712012561800 | 0.5927024512689915 | 0.1669033975048919 | T | T | T |
| 0.6341471776773999 | 0.5921873183870334 | 0.6668310066440242 | T | T | T |
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| 0.4678072612095027 | 0.1657402429981294 | 0.6676347591181142 | T | T | T |
| 0.0691637236168562 | 0.1067764620401369 | 0.1669743495030844 | T | T | T |
| 0.0697360331458097 | 0.1072798111409680 | 0.6669252837347905 | T | T | T |
| 0.1121078361769834 | 0.3893357908982994 | 0.1650942851083381 | T | T | T |
| 0.1116129968356712 | 0.3916592040575643 | 0.6651365953659639 | T | T | T |
| 0.5932788902832359 | 0.3112544045673843 | 0.1676621468679339 | T | T | T |
| 0.5931383688414488 | 0.3112477948091122 | 0.6676968972088408 | T | T | T |
| 0.5370666869275198 | 0.6510005448418836 | 0.1662742657688394 | T | T | T |
| 0.5354334895454033 | 0.6493173192811411 | 0.6666690124413732 | T | T | T |
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| 0.0692538918761418 | 0.1068559746195139 | 0.3341591367408799 | T | T | T |
| 0.0695467730882745 | 0.1070906737047975 | 0.8338991457814477 | T | T | T |
| 0.5367408291563257 | 0.6506800929815317 | 0.3331086383548073 | T | T | T |
| 0.5356918673339799 | 0.6492515134745698 | 0.8330498070121971 | T | T | T |
| 0.6346478048770740 | 0.5926316312708734 | 0.3340682093520013 | T | T | T |
| 0.6344309346308713 | 0.5923611569990768 | 0.8338043119631052 | T | T | T |
| 0.4676663701321478 | 0.1659533419613826 | 0.3347052083377925 | T | T | T |
| 0.4678902501439909 | 0.1655737904846169 | 0.8347052896790187 | T | T | T |
| 0.0514647273074522 | 0.2335787674201946 | 0.3331974630231424 | T | T | T |
| 0.0527553205228892 | 0.2343256004135735 | 0.8331522176592927 | T | T | T |
| 0.1651524075380517 | 0.0465561182449544 | 0.3342834485902936 | T | T | T |
| 0.1653233090391710 | 0.0468084873309065 | 0.8343393040390937 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.3915968338180735 | 0.6295039860558489 | 0.3312933061220835 | T | T | T |
| 0.3901152309625860 | 0.6319708477916919 | 0.8342198756589232 | T | T | T |
| 0.5932692408164815 | 0.3112999012664817 | 0.3344181376748096 | T | T | T |
| 0.5930641857032314 | 0.3112092488257419 | 0.8344683811764377 | T | T | T |
| 0.1124736449214099 | 0.3892147655989178 | 0.3313721996168423 | T | T | T |
| 0.1107830181155053 | 0.3916779600414052 | 0.8343325007888632 | T | T | T |
| 0.2351267306601867 | 0.5360701048830551 | 0.3280094541506627 | T | T | T |
| 0.3115037419933304 | 0.0693512575836623 | 0.3344337193315318 | T | T | T |
| 0.3116315673412379 | 0.0694969613010981 | 0.8344859415679506 | T | T | T |
| 0.6554455254824761 | 0.4677376338018690 | 0.3342526766977884 | T | T | T |
| 0.6552719955216747 | 0.4676417585723132 | 0.8342943551997651 | T | T | T |
| 0.2204881478338556 | 0.5601264376584708 | 0.8335816028564502 | T | T | T |
| 0.1882692950334973 | 0.6228408996733229 | 0.8461401646610811 | T | T | T |
| 0.1342608423096701 | 0.6012626135573770 | 0.7915594598296403 | T | T | T |

OH\_B-CNT(13,0) #### KPOINTS: 1x1x2 #### E= -1226.17822840 eV

1.0000000000000000

24.248699999999995 -14.000000000000000 0.0000000000000000

0.0000000000000000 28.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 12.838699999999993

C B O H

155 1 1 1

Selective dynamics

Direct

0.4412239717567988 0.4066839710034792 0.0281145216282437 T T T

0.4527669056151492 0.3694235574608043 0.1949796544524392 T T T

0.4524292067895644 0.3691966419083212 0.3058741151207827 T T T

0.3834378281716887 0.4495909593286218 0.0278921680524838 T T T

0.4406615809772205 0.4063138475938933 0.1392922400255056 T T T

0.4162532951047055 0.4327582164584055 0.1948696373172301 T T T

0.4153814829960135 0.4321346405480871 0.3059985203833999 T T T

0.2936147704254777 0.4445214335063608 0.0262842529905168 T T T

0.3826594964848670 0.4490684748763005 0.1389858907126980 T T T

0.3402178589334447 0.4525605893600735 0.1940406343700055 T T T

0.3391186134422420 0.4522289726430006 0.3057474524357982 T T T

0.1924812103448404 0.3933430392790550 0.0255731744642026 T T T

0.2932244637966633 0.4445726892093089 0.1369901595254093 T T T

0.2426485505315663 0.4249826548352563 0.1913995049108338 T T T

0.2415448055166953 0.4267471887812267 0.3018925344226412 T T T

0.1029928142542584 0.3077066180632095 0.0262112235244988 T T T

0.1922420416641711 0.3939199209887720 0.1357471683326852 T T T

0.1446471489028888 0.3545453313465499 0.1913347839633710 T T T

0.1443815669140806 0.3568370656719180 0.3018870676071032 T T T

0.0444764858818336 0.2071764697423465 0.0278360282240420 T T T

0.1031123815804412 0.3081597186953701 0.1369290653099932 T T T

0.0697222834040546 0.2588566822482241 0.1939402157307571 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0705458287375691 | 0.2598448506646874 | 0.3056621598873686 | T | T | T |
| 0.0312942087508344 | 0.1138144602493647 | 0.0280980467471740 | T | T | T |
| 0.0451742921324710 | 0.2077275979813956 | 0.1389135715064835 | T | T | T |
| 0.0328454557749482 | 0.1587912383651902 | 0.1947974469637099 | T | T | T |
| 0.0336752873167846 | 0.1593622681187700 | 0.3059254671252268 | T | T | T |
| 0.0681284138681123 | 0.0506193847810811 | 0.0281745453158786 | T | T | T |
| 0.0318578848700711 | 0.1142474511608152 | 0.1392480063604362 | T | T | T |
| 0.0443560616217620 | 0.0776281317985287 | 0.1949447888950227 | T | T | T |
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| 0.1446327633020176 | 0.0315196123800287 | 0.0282856092844551 | T | T | T |
| 0.0682622901057593 | 0.0506688912644471 | 0.1392569084476172 | T | T | T |
| 0.1024635488665588 | 0.0350758490155264 | 0.1948450170839017 | T | T | T |
| 0.1023394444075299 | 0.0348579730910700 | 0.3058508482908588 | T | T | T |
| 0.2427547275387389 | 0.0593760625715355 | 0.0283276994603843 | T | T | T |
| 0.1446136725169165 | 0.0314011854304332 | 0.1391910480465056 | T | T | T |
| 0.1922183322181333 | 0.0395377496942642 | 0.1949404127597507 | T | T | T |
| 0.1922048212959246 | 0.0395297686319649 | 0.3059903019969947 | T | T | T |
| 0.3409516229750414 | 0.1295984177052444 | 0.0283240150713335 | T | T | T |
| 0.2427447756012984 | 0.0593594784525051 | 0.1393622506515520 | T | T | T |
| 0.2933344334756993 | 0.0900450174759893 | 0.1950614947912962 | T | T | T |
| 0.2933036967340613 | 0.0900952148554191 | 0.3060006118655198 | T | T | T |
| 0.4165064665129055 | 0.2255971489419983 | 0.0283042340634160 | T | T | T |
| 0.3409600988331681 | 0.1295769593066734 | 0.1393553793153886 | T | T | T |
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| 0.4165615594771160 | 0.2255309948051417 | 0.1392012687657970 | T | T | T |
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| 0.4525547495288421 | 0.3692014530229843 | 0.5281474556232412 | T | T | T |
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| 0.4165815876628273 | 0.4329755473658950 | 0.6386754489557316 | T | T | T |
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| 0.2438859263366171 | 0.4321373130762722 | 0.5297942090930795 | T | T | T |
| 0.2434244318760336 | 0.4278846573797489 | 0.6389667069752228 | T | T | T |
| 0.1031176916950466 | 0.3101207410203293 | 0.3603541775932284 | T | T | T |
| 0.1406954159712802 | 0.3570291255814227 | 0.5297104881188768 | T | T | T |
| 0.1429376335081340 | 0.3551789346470927 | 0.6390391674866460 | T | T | T |
| 0.0467948327610894 | 0.2085149001293489 | 0.3614569108038679 | T | T | T |
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| 0.0328040476891690 | 0.1147081645606430 | 0.4722910500493124 | T | T | T |
| 0.0444252106441620 | 0.0775667505302896 | 0.5281373627923459 | T | T | T |
| 0.0441852464013861 | 0.0774406503577222 | 0.6390790414417917 | T | T | T |
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| 0.1022390445391535 | 0.0347392369328431 | 0.5283269609751315 | T | T | T |
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| 0.1444264670016259 | 0.0311177022134898 | 0.4726700865929550 | T | T | T |
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| 0.4413361438135051 | 0.4067290704489282 | 0.8055529014061076 | T | T | T |
| 0.4176906377790990 | 0.4339297473584126 | 0.8610391261190625 | T | T | T |
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| 0.2937246201583208 | 0.4445388862664336 | 0.8053068703766275 | T | T | T |
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| 0.0687206830924316 | 0.2578363810995997 | 0.8607864998652431 | T | T | T |
| 0.0686950942612392 | 0.2579034035557896 | 0.9715212411975989 | T | T | T |
| 0.0317610377913429 | 0.1140435337032960 | 0.6945503885761981 | T | T | T |
| 0.0443060198045414 | 0.2069629968422704 | 0.8050955217316198 | T | T | T |
| 0.0313970016992495 | 0.1578728926153270 | 0.8610454429610727 | T | T | T |
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| 0.0680359153511459 | 0.0504052122737857 | 0.6948971371260276 | T | T | T |
| 0.0312239211918982 | 0.1136950845053328 | 0.8055728437527340 | T | T | T |
| 0.0436295034995273 | 0.0770718878936897 | 0.8614646024713145 | T | T | T |
| 0.0435866914911070 | 0.0770999338794311 | 0.9724985391806373 | T | T | T |
| 0.1445008081786284 | 0.0313022268817571 | 0.6951139184376610 | T | T | T |
| 0.0679752429198336 | 0.0504174381885028 | 0.8059719121901919 | T | T | T |
| 0.1023565434982551 | 0.0350817761749027 | 0.8616374597733757 | T | T | T |
| 0.1023977665776965 | 0.0351563059931422 | 0.9726294354998394 | T | T | T |
| 0.2427110322559145 | 0.0595800884665400 | 0.6950255692121726 | T | T | T |
| 0.1445373662238149 | 0.0314018952883046 | 0.8060895888812860 | T | T | T |
| 0.1922316570375811 | 0.0396658584946345 | 0.8616872237096239 | T | T | T |
| 0.1922503138036098 | 0.0396528266787134 | 0.9726833734503907 | T | T | T |
| 0.3409212692885721 | 0.1296726537765503 | 0.6950479048284998 | T | T | T |
| 0.2427099867079055 | 0.0594837050534823 | 0.8060500997261130 | T | T | T |
| 0.2933306722932253 | 0.0900808780266624 | 0.8617529388393778 | T | T | T |
| 0.2933603531532389 | 0.0899781667344981 | 0.9726975417133531 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4166629128608861 | 0.2255311070876281 | 0.6951269781970728 | T | T | T |
| 0.3409541795157816 | 0.1296644292060444 | 0.8060749111275137 | T | T | T |
| 0.3827263356688019 | 0.1756967069294574 | 0.8617092707089471 | T | T | T |
| 0.3827064362657612 | 0.1756919383172725 | 0.9727029737005374 | T | T | T |
| 0.4529328017812784 | 0.3253986436039966 | 0.6948834765717956 | T | T | T |
| 0.4166091927112444 | 0.2256009116556481 | 0.8060955762222342 | T | T | T |
| 0.4405305167777281 | 0.2765446123423573 | 0.8616429752129247 | T | T | T |
| 0.4405159444524394 | 0.2765644368897882 | 0.9726354936286087 | T | T | T |
| 0.4530836399458507 | 0.3255407207898428 | 0.8059516078358745 | T | T | T |
| 0.1861474016354230 | 0.4121235900951850 | 0.4728189209185573 | T | T | T |
| 0.1719574177082241 | 0.4574423608645564 | 0.4808203876939224 | T | T | T |
| 0.1352959334997897 | 0.4449113891795280 | 0.4544527277411857 | T | T | T |

## 1.2 OOH adsorbate

### 1.2.1 OOH adsorbate on undoped CNT

OOH\_CNT(5,5) ### KPOINTS: 2x2x3 ### E= -473.88563998 eV

1.0000000000000000  
13.8564000000000007 -8.0000000000000000 0.0000000000000000  
0.0000000000000000 16.0000000000000000 0.0000000000000000  
0.0000000000000000 0.0000000000000000 7.3947799999999999

C O H

60 2 1

Selective dynamics

Direct

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5645801935994990 | 0.4267400683450591 | 0.0836742685085667 | T | T | T |
| 0.5646136503840344 | 0.4267686306271684 | 0.4167804678249960 | T | T | T |
| 0.5644559480819995 | 0.4266126459092378 | 0.7502274799328233 | T | T | T |
| 0.4870914433466707 | 0.5492306245102525 | 0.0838599736141920 | T | T | T |
| 0.4871345232279158 | 0.5492308170961763 | 0.4172436047584404 | T | T | T |
| 0.4858337195723621 | 0.5484976841522680 | 0.7505684451019301 | T | T | T |
| 0.3994201141460032 | 0.5518925527252125 | 0.0840346442114544 | T | T | T |
| 0.3994549051243989 | 0.5518750408238887 | 0.4173762139202322 | T | T | T |
| 0.3988870658182492 | 0.5520810298764065 | 0.7507368665035341 | T | T | T |
| 0.1206229855349166 | 0.3434785591895691 | 0.0846461758173379 | T | T | T |
| 0.1207374524290542 | 0.3434197567444870 | 0.4169494973041687 | T | T | T |
| 0.1216409390349907 | 0.3433078575404810 | 0.7507281408682613 | T | T | T |
| 0.0782347133424142 | 0.1507499476185798 | 0.0840973596498141 | T | T | T |
| 0.0781571584120936 | 0.1506766275245834 | 0.4169474847781649 | T | T | T |
| 0.0779935962187786 | 0.1505959341218060 | 0.7505526519931067 | T | T | T |
| 0.1159187097690422 | 0.0865477275229101 | 0.0838496585579859 | T | T | T |
| 0.1158875227737543 | 0.0865045732552018 | 0.4167923570549222 | T | T | T |
| 0.1159165473943082 | 0.0862693320620957 | 0.7503295024179426 | T | T | T |
| 0.2863909491620829 | 0.0785372969878808 | 0.0835992606317703 | T | T | T |
| 0.2863928397935458 | 0.0785404830645473 | 0.4165436481627997 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2862603795830980 | 0.0782464797017323 | 0.7500808820119107 | T | T | T |
| 0.3889927766010347 | 0.1370739848153469 | 0.0835149161977593 | T | T | T |
| 0.3890117311026801 | 0.1370556124669573 | 0.4164706783822550 | T | T | T |
| 0.3890565533796192 | 0.1369836178841278 | 0.7500136593209210 | T | T | T |
| 0.5410255383216269 | 0.3281755904254339 | 0.0834400595170849 | T | T | T |
| 0.5410149021028213 | 0.3281845408781247 | 0.4166703476899092 | T | T | T |
| 0.5409396588344598 | 0.3281280618889802 | 0.7500467691872031 | T | T | T |
| 0.1987535965995233 | 0.4411009425828561 | 0.0845976177380259 | T | T | T |
| 0.1988035945785310 | 0.4410065529899798 | 0.4170002326127520 | T | T | T |
| 0.1869204341291192 | 0.4513615306428718 | 0.7507226688126888 | T | T | T |
| 0.2471577384078254 | 0.4808829720841173 | 0.2508382772467976 | T | T | T |
| 0.2459807974735898 | 0.4837109998830036 | 0.5820842888943174 | T | T | T |
| 0.2458957027102816 | 0.4838972058836231 | 0.9193787518962085 | T | T | T |
| 0.5607055831946037 | 0.4696603343899218 | 0.2502877709904968 | T | T | T |
| 0.5600822556671518 | 0.4693750762866463 | 0.5837488515286349 | T | T | T |
| 0.5600446012624246 | 0.4693522711847228 | 0.9168217714588318 | T | T | T |
| 0.1484542221056575 | 0.0678259175376025 | 0.2502719025298733 | T | T | T |
| 0.1490140800173020 | 0.0682343112206596 | 0.5837968368282596 | T | T | T |
| 0.1490033618118835 | 0.0682261632598166 | 0.9167415040197460 | T | T | T |
| 0.2359287624042583 | 0.0640113968050736 | 0.2501199419078471 | T | T | T |
| 0.2359401582547508 | 0.0640814435485697 | 0.5835594146470365 | T | T | T |
| 0.2359273028812700 | 0.0640281138615873 | 0.9166337295053359 | T | T | T |
| 0.5211106443029611 | 0.5323111404460878 | 0.2504907547567215 | T | T | T |
| 0.5206398913979524 | 0.5317727131917401 | 0.5840264316526632 | T | T | T |
| 0.5206219863884913 | 0.5317812773623065 | 0.9169885310584804 | T | T | T |
| 0.0948249114907066 | 0.2918838251507727 | 0.2508310872346485 | T | T | T |
| 0.0979000359416855 | 0.2922895359455341 | 0.5853330947876251 | T | T | T |
| 0.0978100969789646 | 0.2923292932030548 | 0.9160403611123371 | T | T | T |
| 0.4368092981049852 | 0.1784953639199803 | 0.2500027640852840 | T | T | T |
| 0.4368824386123536 | 0.1786258099912182 | 0.5833870486055778 | T | T | T |
| 0.4368813380154615 | 0.1786076680416102 | 0.9166063185128706 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5143533741113521 | 0.2762160453311777 | 0.2500432528536789 | T | T | T |
| 0.5142442269749581 | 0.2760812418025847 | 0.5833723930837548 | T | T | T |
| 0.5142818266852502 | 0.2760757203030640 | 0.9166594973909431 | T | T | T |
| 0.0735217902658953 | 0.1931779253120101 | 0.2506120025613377 | T | T | T |
| 0.0750697656206157 | 0.1939015561286682 | 0.5844318146168400 | T | T | T |
| 0.0750087545264797 | 0.1938808237760930 | 0.9167085824880875 | T | T | T |
| 0.3498764676022613 | 0.5385076685940859 | 0.2507676125379288 | T | T | T |
| 0.3476583843167451 | 0.5364086408857660 | 0.5838672337061070 | T | T | T |
| 0.3476628837202854 | 0.5365384643072026 | 0.9175879774705723 | T | T | T |
| 0.1290178566356551 | 0.5060925968976672 | 0.7514700085763956 | T | T | T |
| 0.0244704506828714 | 0.4384442890029074 | 0.7338245872437497 | T | T | T |
| 0.0042248690344268 | 0.4365780904869082 | 0.8584900711280559 | T | T | T |

-0.0123931732243125 0.4582716624955215 0.6901461488601455 T T T

OOH\_CNT(6,6) ### KPOINTS: 2x2x3 ### E= -570.26973306 eV

1.000000000000000

14.722400000000000 -8.500000000000000 0.000000000000000

0.000000000000000 17.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.399280000000001

C O H

72 2 1

Selective dynamics

Direct

0.6150085361439113 0.4963886398105058 0.0831911773004645 T T T

0.6149891758253243 0.4963898109011936 0.4165410684245628 T T T

0.6149971299821094 0.4963415249473541 0.7498717027226597 T T T

0.5306808234048386 0.6024309702517108 0.0830835222742437 T T T

0.5307932095318262 0.6025129280662509 0.4166159097198229 T T T

0.5297063878663655 0.6020675284245695 0.7498993966551013 T T T

0.4506818970757417 0.6093634427983405 0.0830682330920539 T T T

0.4507764539795199 0.6094000600281011 0.4166274609839686 T T T

0.4505170302179859 0.6100646143584827 0.7499316050351502 T T T

0.1733523443512321 0.4531416441339495 0.0837293107869350 T T T

0.1733103223458820 0.4531409040612412 0.4160148947178975 T T T

0.1733494810819413 0.4530173627867435 0.7498716652993400 T T T

0.0679482929515077 0.2620579844025010 0.0834211144474199 T T T

0.0679197072718646 0.2620519245494501 0.4163224612518046 T T T

0.0680971111845882 0.2621494833538766 0.7498697355807549 T T T

0.0586022891160672 0.1738767890316687 0.0834141301269769 T T T

0.0586113950599677 0.1738838061342188 0.4163131866539596 T T T

0.0584101934911704 0.1735299216053931 0.7498633467465300 T T T

0.1381601511366255 0.0633108458555543 0.0832845498385043 T T T

0.1381546345908624 0.0633030352475993 0.4164236417753588 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1380365928258943 | 0.0631971029622082 | 0.7498570803397860 | T | T | T |
| 0.2181640239280041 | 0.0560419515833275 | 0.0833837903336279 | T | T | T |
| 0.2181611138566153 | 0.0560368551643040 | 0.4162888004804347 | T | T | T |
| 0.2182071286928976 | 0.0559939363180745 | 0.7498508141971137 | T | T | T |
| 0.4087757707295879 | 0.1389646601460709 | 0.0833063558567392 | T | T | T |
| 0.4087747896080063 | 0.1389600691417354 | 0.4163621675579462 | T | T | T |
| 0.4087133188040233 | 0.1387760899551612 | 0.7498414710267337 | T | T | T |
| 0.4963016551490818 | 0.2184533837667621 | 0.0833358389893687 | T | T | T |
| 0.4963074969175378 | 0.2184530050687918 | 0.4163539978342690 | T | T | T |
| 0.4963328200006241 | 0.2184348970561804 | 0.7498489285799806 | T | T | T |
| 0.6068448014905321 | 0.4087591844507594 | 0.0832249449489546 | T | T | T |
| 0.6068186208872206 | 0.4087517672867801 | 0.4165083708487933 | T | T | T |
| 0.6066556817333579 | 0.4087539817519898 | 0.7498624798022530 | T | T | T |
| 0.2614813328147739 | 0.5328224320098170 | 0.0833584624252213 | T | T | T |
| 0.2615048163554384 | 0.5327001857329786 | 0.4161543560348455 | T | T | T |
| 0.2545883995515326 | 0.5483071280752070 | 0.7497083197192499 | T | T | T |
| 0.0662271672564124 | 0.1360478670944570 | 0.2498684360672945 | T | T | T |
| 0.0664016218073601 | 0.1359750924388667 | 0.5833089045694195 | T | T | T |
| 0.0663618454890212 | 0.1359511326183841 | 0.9164135717611392 | T | T | T |
| 0.1066866875512642 | 0.0798294441495942 | 0.2498558222427700 | T | T | T |
| 0.1067113878759633 | 0.0798755534032630 | 0.5834048579735933 | T | T | T |
| 0.1066994381518851 | 0.0798711242789411 | 0.9163042276323694 | T | T | T |
| 0.5631369581196700 | 0.5872082413624570 | 0.2498492018568624 | T | T | T |
| 0.5627797994564793 | 0.5868074628812806 | 0.5833310152022796 | T | T | T |
| 0.5627470595815570 | 0.5867728564562997 | 0.9164341209539263 | T | T | T |
| 0.1371088525870910 | 0.4072723707186494 | 0.2498512453174001 | T | T | T |
| 0.1389820296376170 | 0.4068794022721888 | 0.5843192700641743 | T | T | T |
| 0.1389895877937163 | 0.4068792877788504 | 0.9154436118028451 | T | T | T |
| 0.2641452669055763 | 0.0650463650948634 | 0.2498421885864360 | T | T | T |
| 0.2642492990829851 | 0.0652074672940409 | 0.5832054178336691 | T | T | T |
| 0.2642536157257781 | 0.0652141900320053 | 0.9164810384081493 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3608631903806779 | 0.1072582112822506 | 0.2498304465809946 | T | T | T |
| 0.3607859410021688 | 0.1072161525871584 | 0.5831634808857992 | T | T | T |
| 0.3607859816240030 | 0.1072255872095214 | 0.9165092461108370 | T | T | T |
| 0.0835932470875056 | 0.3097740186456103 | 0.2498736205580624 | T | T | T |
| 0.0851129830252137 | 0.3100801504099560 | 0.5836421808419877 | T | T | T |
| 0.0851195124625570 | 0.3100805927529693 | 0.9160986681017095 | T | T | T |
| 0.3096596242945580 | 0.5619365774748024 | 0.2497500526672556 | T | T | T |
| 0.3093484148519696 | 0.5658292812309473 | 0.5809630948390010 | T | T | T |
| 0.3092674102147939 | 0.5660746301397631 | 0.9186765474848456 | T | T | T |
| 0.5337504937842770 | 0.2641834340123571 | 0.2498474576658780 | T | T | T |
| 0.5337799848421965 | 0.2643130911471240 | 0.5832146341089356 | T | T | T |
| 0.5337654071103196 | 0.2643199953910322 | 0.9164877988491921 | T | T | T |
| 0.5898573964520395 | 0.3606377230266104 | 0.2498699328915294 | T | T | T |
| 0.5897949055672861 | 0.3606061650351593 | 0.5832448678066792 | T | T | T |
| 0.5897888508233006 | 0.3606096553633720 | 0.9164797666925265 | T | T | T |
| 0.6058592879100946 | 0.5332609847987669 | 0.2498492962740130 | T | T | T |
| 0.6056642357684544 | 0.5332867637854342 | 0.5833050155157941 | T | T | T |
| 0.6056503808151519 | 0.5332680820453405 | 0.9164395620240822 | T | T | T |
| 0.4058764803659400 | 0.6018711069304935 | 0.2498500253275958 | T | T | T |
| 0.4039352934846639 | 0.6007041254366698 | 0.5829896833676805 | T | T | T |
| 0.4037836501021371 | 0.6007407673150567 | 0.9167346510315404 | T | T | T |
| 0.2822497966706946 | 0.7040184304243498 | 0.7497756056353653 | T | T | T |
| 0.2103191404393686 | 0.6068858218655320 | 0.7488022477156098 | T | T | T |
| 0.2865728439437542 | 0.7174009425966922 | 0.6210748943419371 | T | T | T |

OOH\_CNT(7,7) #### KPOINTS: 1x1x3 #### E= -666.11175789 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C O H

84 2 1

Selective dynamics

Direct

0.1818076970948527 0.0483554402819141 0.0841947990103877 T T T

0.2641762683788751 0.0552099351492024 0.0842006975921713 T T T

0.0707915809188799 0.1168871835110337 0.0840562643184297 T T T

0.4451218918782174 0.1491914364905584 0.0842788326390148 T T T

0.0509283238153468 0.1842864490961748 0.0841193171748246 T T T

0.5262641598854556 0.2261695649104107 0.0842579920271045 T T T

0.0850219949761137 0.3554861822689337 0.0845720867687558 T T T

0.6380711071152588 0.4057099890527572 0.0842285257631072 T T T

0.1411779382849626 0.4463147656724166 0.0842230128628526 T T T

0.6590782296696661 0.4932203089174816 0.0841916477233006 T T T

0.3041806436704169 0.5940477550960117 0.0838731434960876 T T T

0.6182044974223652 0.6253787473248902 0.0841207987115050 T T T

0.3953326946629352 0.6401543101752970 0.0838522618856842 T T T

0.5597293188466435 0.6569584341090072 0.0840593676817295 T T T

0.0496746442190105 0.2232968048565596 0.2506637458779222 T T T

0.5615184640503110 0.2693247077979635 0.2508352153752125 T T T

0.0668432767690760 0.3102521886093617 0.2507371184302298 T T T

0.6179693989471866 0.3598844067121489 0.2508224810505559 T T T

0.1778950127729337 0.4882651039696741 0.2506997305308628 T T T

0.1462157901625943 0.0558228233028422 0.2506560974486807 T T T

0.3090658622246216 0.0692797131817154 0.2507592666497967 T T T

0.0899221075785246 0.0903530234092543 0.2506185928353910 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4006104152155689 | 0.1168278438355671 | 0.2508013240518613 | T | T | T |
| 0.6592409733425580 | 0.5330578240433740 | 0.2508309614782142 | T | T | T |
| 0.2598772311787347 | 0.5637858409877045 | 0.2507517241254267 | T | T | T |
| 0.6386095102118616 | 0.5998808869419465 | 0.2507927601744797 | T | T | T |
| 0.4402376296602745 | 0.6544604535527120 | 0.2506950858403004 | T | T | T |
| 0.5232416546206839 | 0.6628704466642675 | 0.2506795530560254 | T | T | T |
| 0.1817962573053221 | 0.0483657842382358 | 0.4171642395453710 | T | T | T |
| 0.2641791624110275 | 0.0552510095853873 | 0.4172732459295861 | T | T | T |
| 0.0707145638820489 | 0.1168194061173767 | 0.4171525545785796 | T | T | T |
| 0.4451453072450090 | 0.1491706892485996 | 0.4173415971387884 | T | T | T |
| 0.0508528068056728 | 0.1842470087559344 | 0.4171384868128151 | T | T | T |
| 0.5262463219240555 | 0.2261948854127739 | 0.4174185036936852 | T | T | T |
| 0.0848280230228948 | 0.3555837450246943 | 0.4168461421053420 | T | T | T |
| 0.6381201754673580 | 0.4056856564991095 | 0.4174190374972340 | T | T | T |
| 0.1408786889690716 | 0.4465017118361168 | 0.4172554184616572 | T | T | T |
| 0.6590676154674526 | 0.4931826740736300 | 0.4174332200460192 | T | T | T |
| 0.3041255349936935 | 0.5943796299564913 | 0.4176255288154779 | T | T | T |
| 0.6181276462597053 | 0.6253238118359922 | 0.4173655532324334 | T | T | T |
| 0.3953510696704424 | 0.6403420873786080 | 0.4175360672277967 | T | T | T |
| 0.5597744502174805 | 0.6570676550330667 | 0.4173152708262368 | T | T | T |
| 0.1460333069821768 | 0.0555150925277143 | 0.5840766560103097 | T | T | T |
| 0.3091993324959181 | 0.0694269437627093 | 0.5841528420272464 | T | T | T |
| 0.0902158711412687 | 0.0903491474301176 | 0.5840713132067271 | T | T | T |
| 0.4005677778632543 | 0.1170689201378205 | 0.5841890945105843 | T | T | T |
| 0.0511937556407715 | 0.2242239247089047 | 0.5843404776512705 | T | T | T |
| 0.5616664491745882 | 0.2693288734953362 | 0.5842161391799027 | T | T | T |
| 0.0685203998722636 | 0.3108084593855665 | 0.5850340308735033 | T | T | T |
| 0.6179870181122550 | 0.3597678601376918 | 0.5841701042935453 | T | T | T |
| 0.1746227654386618 | 0.4907670618900378 | 0.5820117849087961 | T | T | T |
| 0.6592417893068958 | 0.5331585162056048 | 0.5841574904723116 | T | T | T |
| 0.2580988886451158 | 0.5627529833463863 | 0.5838899582652728 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6386561842200283 | 0.5999449250383477 | 0.5840862803662861 | T | T | T |
| 0.4401166774861910 | 0.6543045055992505 | 0.5842060383514757 | T | T | T |
| 0.5230740343915415 | 0.6628789118787231 | 0.5841341249718184 | T | T | T |
| 0.0708700835977950 | 0.1167233858253547 | 0.7505980834522786 | T | T | T |
| 0.0512461477648128 | 0.1845875689512805 | 0.7505697768509055 | T | T | T |
| 0.5264515994201368 | 0.2261520355232192 | 0.7508326591054045 | T | T | T |
| 0.0843665708001149 | 0.3553006804278995 | 0.7506976291438154 | T | T | T |
| 0.6379297940459379 | 0.4055848271569125 | 0.7508487185924738 | T | T | T |
| 0.1247232753823568 | 0.4517519991459297 | 0.7512114323804052 | T | T | T |
| 0.1815111111656970 | 0.0480041828113590 | 0.7506990147317012 | T | T | T |
| 0.2641902019374680 | 0.0551658307386985 | 0.7507195411383282 | T | T | T |
| 0.4450589692336265 | 0.1492450868907605 | 0.7508147338911385 | T | T | T |
| 0.6588819165637230 | 0.4931222639964364 | 0.7508268693090985 | T | T | T |
| 0.3034470559821922 | 0.5947107567943989 | 0.7507569739714516 | T | T | T |
| 0.6181490629607407 | 0.6254467560290088 | 0.7507461575972686 | T | T | T |
| 0.3944036180387273 | 0.6395611264594718 | 0.7506740126456153 | T | T | T |
| 0.5599258119964897 | 0.6572026259029110 | 0.7506846356804801 | T | T | T |
| 0.1460254659517536 | 0.0555014901225177 | 0.9172741394434194 | T | T | T |
| 0.3091850239168216 | 0.0694033566337102 | 0.9173270183290740 | T | T | T |
| 0.0902127109262928 | 0.0903509448062920 | 0.9171299877538390 | T | T | T |
| 0.4005445149168399 | 0.1171049964261087 | 0.9174071074504179 | T | T | T |
| 0.0511852994406743 | 0.2241857060177007 | 0.9168723235542011 | T | T | T |
| 0.5616866169510181 | 0.2693001665370703 | 0.9174612388616397 | T | T | T |
| 0.0685815564331575 | 0.3107408929896187 | 0.9163284354009225 | T | T | T |
| 0.6179347201948582 | 0.3597578884840538 | 0.9175190240821031 | T | T | T |
| 0.1751174538142404 | 0.4903605630215327 | 0.9197216669186292 | T | T | T |
| 0.6592623529165690 | 0.5331866907791611 | 0.9174176449490024 | T | T | T |
| 0.2582516341793301 | 0.5623117696715071 | 0.9176664487980657 | T | T | T |
| 0.6387261817806476 | 0.6000186293520622 | 0.9174063564142901 | T | T | T |
| 0.4400952392053534 | 0.6541931209426591 | 0.9171537469574702 | T | T | T |
| 0.5230166590904014 | 0.6627461020996686 | 0.9172352626079296 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0727634140858379 | 0.5545366185967588 | 0.7717187352938820 | T | T | T |
| 0.0453563577681323 | 0.4621782585371448 | 0.7549555366840422 | T | T | T |
| 0.0700370292161527 | 0.5685619511983785 | 0.6457814824327054 | T | T | T |

OOH\_CNT(8,8) #### KPOINTS: 1x1x3 #### E= -761.66510163 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C O H

96 2 1

Selective dynamics

Direct

0.2521540368545095 0.0430442175191573 0.0834305223111454 T T T

0.1149190589315005 0.0512472146769181 0.0834415964638616 T T T

0.3327679864683555 0.0692773243509139 0.0835114818415666 T T T

0.0685581386524702 0.0869235402711111 0.0833906144016405 T T T

0.4932372277429113 0.1758556974414004 0.0834607980808186 T T T

0.0384769198202184 0.2107864933437016 0.0833195391874895 T T T

0.5619174917505839 0.2493550387279523 0.0834303382535771 T T T

0.0561676576271138 0.2892776772890751 0.0831865170456036 T T T

0.6535004965921565 0.4122796794187040 0.0833111083201758 T T T

0.1448594028685969 0.4525771661201936 0.0834286615089848 T T T

0.6699480463944458 0.4902990544823231 0.0833117910181956 T T T

0.2137669719912560 0.5263025769786490 0.0829470288425490 T T T

0.6378898524202593 0.6128632457655731 0.0832480221899538 T T T

0.3739942255157765 0.6303408576008361 0.0827580868302820 T T T

0.5915271681060675 0.6485191641353411 0.0831107807578188 T T T

0.4545025925539005 0.6567474771130520 0.0827844159270263 T T T

0.2138654261639057 0.0373346806074701 0.2500498541738203 T T T

0.1445342612368209 0.0411715852342931 0.2499770660870616 T T T

0.3740606283704126 0.0895643562960771 0.2501393780639524 T T T

0.4549496389044673 0.1432804007700684 0.2501476101616904 T T T

0.0373284971196480 0.1745210230937558 0.2498283233327134 T T T

0.6701585190179807 0.5262032135569369 0.2498976892463362 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2525934355187041 | 0.5573428109610857 | 0.2495649946103831 | T | T | T |
| 0.6540056162815012 | 0.5879841026599226 | 0.2498356187712003 | T | T | T |
| 0.5620001471202398 | 0.6587635367360735 | 0.2497610963788971 | T | T | T |
| 0.0527700054562351 | 0.1120670810601758 | 0.2498750498814178 | T | T | T |
| 0.5913433934660072 | 0.2891728152972609 | 0.2500886213531915 | T | T | T |
| 0.0714556236558162 | 0.3300622337870517 | 0.2496878171903653 | T | T | T |
| 0.6374887320143232 | 0.3712935082212540 | 0.2500258397884523 | T | T | T |
| 0.1164183327029445 | 0.4128493328247334 | 0.2496301315672088 | T | T | T |
| 0.3332032298251116 | 0.6105759645162362 | 0.2495769385476718 | T | T | T |
| 0.4928970374100343 | 0.6627752754815439 | 0.2496310376283630 | T | T | T |
| 0.2521622990684975 | 0.0430533071863387 | 0.4167311251762744 | T | T | T |
| 0.1149088360709361 | 0.0512418331161210 | 0.4164580844385737 | T | T | T |
| 0.3327725236905921 | 0.0692841431953468 | 0.4167492750373535 | T | T | T |
| 0.0685406968004850 | 0.0869096771218196 | 0.4163889208361021 | T | T | T |
| 0.4932320717302980 | 0.1758524201165159 | 0.4167993243287316 | T | T | T |
| 0.0385884430063637 | 0.2108515192540266 | 0.4163043956918391 | T | T | T |
| 0.5619110692917791 | 0.2493503820387276 | 0.4168022395234178 | T | T | T |
| 0.0561526198010359 | 0.2892913570644235 | 0.4162270758577699 | T | T | T |
| 0.6534875147792907 | 0.4122771853105373 | 0.4166931308969655 | T | T | T |
| 0.1448073240634610 | 0.4525269737593359 | 0.4158105100389871 | T | T | T |
| 0.6699357747355710 | 0.4902867667055112 | 0.4165378757580785 | T | T | T |
| 0.2138795080507036 | 0.5261226397292028 | 0.4160723773254726 | T | T | T |
| 0.6378707282981338 | 0.6128300917728877 | 0.4164530458769618 | T | T | T |
| 0.3740000097025851 | 0.6302568165072817 | 0.4163259173928357 | T | T | T |
| 0.5914443692324671 | 0.6484005876579761 | 0.4164576397093266 | T | T | T |
| 0.4545131452085941 | 0.6567647548477769 | 0.4164527689536492 | T | T | T |
| 0.2138489932394021 | 0.0373283848495900 | 0.5835234672062943 | T | T | T |
| 0.1447514073925467 | 0.0414104723765597 | 0.5834001269484530 | T | T | T |
| 0.3741081418405812 | 0.0896627685382468 | 0.5835468644189691 | T | T | T |
| 0.0524953087382347 | 0.1118775816841914 | 0.5832891354913349 | T | T | T |
| 0.4548924179914491 | 0.1432662917558132 | 0.5835881289257450 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0375895030214006 | 0.1744913696071100 | 0.5832936698849304 | T | T | T |
| 0.5913276579548369 | 0.2892443037393823 | 0.5834579774009888 | T | T | T |
| 0.0729021668514340 | 0.3303235765352764 | 0.5834477170639378 | T | T | T |
| 0.6374135334346930 | 0.3712217102073628 | 0.5833796688885996 | T | T | T |
| 0.1175715591160010 | 0.4126374190667170 | 0.5839821487969971 | T | T | T |
| 0.6700636887240751 | 0.5261417434181325 | 0.5832602784316571 | T | T | T |
| 0.2513985604314415 | 0.5602652750802399 | 0.5805111417401487 | T | T | T |
| 0.6540076972424641 | 0.5879385572563184 | 0.5831385637536833 | T | T | T |
| 0.3318583679749686 | 0.6100371215065598 | 0.5826196362932071 | T | T | T |
| 0.5616076579017980 | 0.6583125589750072 | 0.5832430779719958 | T | T | T |
| 0.4927425701327122 | 0.6625175827448974 | 0.5831506106605130 | T | T | T |
| 0.2520779882357368 | 0.0429179164717329 | 0.7500516256190395 | T | T | T |
| 0.1150035754146255 | 0.0513620705590360 | 0.7499424926201558 | T | T | T |
| 0.3328082498352224 | 0.0692718421123368 | 0.7501258787943930 | T | T | T |
| 0.4932262448083066 | 0.1757860278578983 | 0.7501372121068191 | T | T | T |
| 0.0384212313593941 | 0.2105312895631693 | 0.7497983243382310 | T | T | T |
| 0.1442086793428703 | 0.4524527723220603 | 0.7496152979491839 | T | T | T |
| 0.2041808753025283 | 0.5370151206715835 | 0.7491730958335950 | T | T | T |
| 0.6379918303533940 | 0.6129869825556037 | 0.7498204644801516 | T | T | T |
| 0.5915580655185957 | 0.6484125858712779 | 0.7497521809952330 | T | T | T |
| 0.0681102732951060 | 0.0866319736907694 | 0.7498990457936994 | T | T | T |
| 0.5619592230450668 | 0.2493784978757115 | 0.7501027121742311 | T | T | T |
| 0.0566039257150104 | 0.2893984948429785 | 0.7497299495493031 | T | T | T |
| 0.6535168847068383 | 0.4122585518455663 | 0.7500180501408911 | T | T | T |
| 0.6699681053653168 | 0.4902965399796412 | 0.7499449956983082 | T | T | T |
| 0.3737853570477180 | 0.6312906269835535 | 0.7495673021766736 | T | T | T |
| 0.4538169558384509 | 0.6564837540215768 | 0.7496310263246265 | T | T | T |
| 0.2138450286041148 | 0.0373232211872936 | 0.9165727221410832 | T | T | T |
| 0.1447510689708381 | 0.0414162729302411 | 0.9165312980812947 | T | T | T |
| 0.3741124442815212 | 0.0896635674161132 | 0.9167062566922485 | T | T | T |
| 0.0525096375637851 | 0.1118807139907756 | 0.9164669109424362 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4548919624525794 | 0.1432659374978201 | 0.9167032508741377 | T | T | T |
| 0.0375150855607568 | 0.1744431735929487 | 0.9163726546751080 | T | T | T |
| 0.5913280723540310 | 0.2892443860577523 | 0.9167263607763537 | T | T | T |
| 0.0729864435712407 | 0.3303293016628161 | 0.9159394124800312 | T | T | T |
| 0.6374147233400824 | 0.3712197045964396 | 0.9166880243310022 | T | T | T |
| 0.1176729469161586 | 0.4126527574142961 | 0.9153070660816319 | T | T | T |
| 0.6700312978428613 | 0.5261348132867864 | 0.9165640581255798 | T | T | T |
| 0.2511668935196799 | 0.5606902501433582 | 0.9182630381342507 | T | T | T |
| 0.6539562907549373 | 0.5879124994947765 | 0.9165995551060485 | T | T | T |
| 0.3318261096605036 | 0.6103260139912774 | 0.9164245059234652 | T | T | T |
| 0.5616706183858939 | 0.6583991067884712 | 0.9162622057720633 | T | T | T |
| 0.4927631833982234 | 0.6625336712923395 | 0.9161548285295844 | T | T | T |
| 0.2018119548937713 | 0.6589220326677201 | 0.7277810834657092 | T | T | T |
| 0.1526386720375751 | 0.5738544291266605 | 0.7459917823127435 | T | T | T |
| 0.1988608230431585 | 0.6747702885675082 | 0.8503110404755015 | T | T | T |

OOH\_CNT(9,9) ### KPOINTS: 1x1x3 ### E= -857.02168197 eV

1.000000000000000

18.1865334800000014 -10.500000000000000 0.000000000000000

0.000000000000000 21.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.4005503900000003

C O H

108 2 1

Selective dynamics

Direct

0.1976623073359779 0.0293567119871181 0.0836850821661691 T T T

0.1346521406430446 0.0380867808829516 0.0838130970988587 T T T

0.3469669314263152 0.0656322948593129 0.0835171015894119 T T T

0.4251451053915978 0.1082118451470201 0.0835732793699053 T T T

0.0497989942575116 0.1086434580940172 0.0837583200798070 T T T

0.0332519194217134 0.1666383296233164 0.0837603611178785 T T T

0.5684069727716782 0.2325724448855804 0.0836153426166286 T T T

0.6251235987259577 0.3076497575046437 0.0835235473611194 T T T

0.0538171741944931 0.3105750494179835 0.0836212860248518 T T T

0.0886118372685167 0.3886309944101184 0.0835698727802618 T T T

0.6961565411023415 0.4632997413039427 0.0834568211533694 T T T

0.7068421613173564 0.5357883732795951 0.0835627391515300 T T T

0.1993062594170753 0.5378675661909966 0.0836946874661648 T T T

0.2719290668310687 0.6000245529567338 0.0840779202446667 T T T

0.6731767154764684 0.6505108357536317 0.0836879724923111 T T T

0.6296260773827661 0.6850871159169861 0.0837542449996437 T T T

0.4274954600044159 0.6812009507108985 0.0837654091168446 T T T

0.5027113706170446 0.6998565075509793 0.0838576350236276 T T T

0.2328299589459025 0.0317479413706256 0.2502590993528396 T T T

0.3079333256730107 0.0500477085685448 0.2501667251644436 T T T

0.4634797721289100 0.1348930272762412 0.2501255247046130 T T T

0.5356053491043651 0.1974273372957756 0.2501620964836820 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0422086029861750 | 0.2722127907410720 | 0.2504445892778196 | T | T | T |
| 0.1116545730506588 | 0.4271341442677179 | 0.2505453223685412 | T | T | T |
| 0.1679308069240249 | 0.5020275067644130 | 0.2504896774298310 | T | T | T |
| 0.3100027771744083 | 0.6256570661539409 | 0.2502758323818902 | T | T | T |
| 0.3887894005879741 | 0.6667410423039662 | 0.2503074306043170 | T | T | T |
| 0.1075511377841619 | 0.0491955578757559 | 0.2504078368792097 | T | T | T |
| 0.0648069266574720 | 0.0846660960097053 | 0.2504598600701594 | T | T | T |
| 0.0316886644358138 | 0.1998074753388277 | 0.2505036646043943 | T | T | T |
| 0.6485872457086062 | 0.3466749933185724 | 0.2501088527810824 | T | T | T |
| 0.6843575811202983 | 0.4249511859999379 | 0.2500723688495529 | T | T | T |
| 0.7054323137345235 | 0.5691029705612995 | 0.2501797376639058 | T | T | T |
| 0.6887666260335865 | 0.6270945047073918 | 0.2502536032787214 | T | T | T |
| 0.6022207121306020 | 0.6957539711131064 | 0.2503003312679655 | T | T | T |
| 0.5382212736748481 | 0.7031271052483345 | 0.2503862001302348 | T | T | T |
| 0.1976300464064698 | 0.0292993978149587 | 0.4169081193315995 | T | T | T |
| 0.1346587506238206 | 0.0380875613537097 | 0.4169436027038549 | T | T | T |
| 0.3469712032434136 | 0.0656323215921389 | 0.4167708234472075 | T | T | T |
| 0.4251479614014164 | 0.1082112187047184 | 0.4167517593557737 | T | T | T |
| 0.0497966236547514 | 0.1086613839344820 | 0.4171503082863931 | T | T | T |
| 0.0331145378019827 | 0.1665802106438282 | 0.4172852603304656 | T | T | T |
| 0.5684073931143862 | 0.2325764711326038 | 0.4166821235647292 | T | T | T |
| 0.6251284270595985 | 0.3076503819983925 | 0.4167171595218001 | T | T | T |
| 0.0538780494546770 | 0.3104916593442169 | 0.4173689978145615 | T | T | T |
| 0.0889394171384550 | 0.3884658035274248 | 0.4174025555705150 | T | T | T |
| 0.6961111413629846 | 0.4632737856471343 | 0.4166958533447684 | T | T | T |
| 0.7068071065920272 | 0.5357957262820565 | 0.4166879675173554 | T | T | T |
| 0.1995958977500961 | 0.5376967631193625 | 0.4171038263255495 | T | T | T |
| 0.2718516735336948 | 0.6002602318222630 | 0.4167363639910711 | T | T | T |
| 0.6732376755697997 | 0.6505628084749229 | 0.4167739212799610 | T | T | T |
| 0.6296103160217662 | 0.6850856251854200 | 0.4168906764953685 | T | T | T |
| 0.4274959737505498 | 0.6813105360663346 | 0.4169286265987167 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5027426218827593 | 0.6999279981499156 | 0.4168661345703920 | T | T | T |
| 0.2328541971161707 | 0.0317891596722683 | 0.5836784300879171 | T | T | T |
| 0.3079161247572599 | 0.0501124689272459 | 0.5835888179173629 | T | T | T |
| 0.1077054739673576 | 0.0493842500596148 | 0.5837569942760454 | T | T | T |
| 0.0651159254279027 | 0.0849083425339969 | 0.5837683232606428 | T | T | T |
| 0.4634780365272654 | 0.1349193419939681 | 0.5834995794881878 | T | T | T |
| 0.5355681647453061 | 0.1974309675479872 | 0.5835160721052960 | T | T | T |
| 0.0318417168923747 | 0.2000487838475278 | 0.5840079724212194 | T | T | T |
| 0.0420528008853940 | 0.2722549496889985 | 0.5840318952480635 | T | T | T |
| 0.6486015172356375 | 0.3467304337083298 | 0.5834889209754385 | T | T | T |
| 0.6842234224753549 | 0.4248956956332305 | 0.5834740332205927 | T | T | T |
| 0.1115180867416358 | 0.4284181871212923 | 0.5837506377679363 | T | T | T |
| 0.1649125473529308 | 0.5036969772901816 | 0.5815066986822994 | T | T | T |
| 0.7055533674872737 | 0.5691766344962472 | 0.5835357741243828 | T | T | T |
| 0.6885751103692133 | 0.6268660895427073 | 0.5836098242183358 | T | T | T |
| 0.3101172036240551 | 0.6250371631811730 | 0.5849416595041648 | T | T | T |
| 0.3885541365216986 | 0.6657923563610643 | 0.5841711646765952 | T | T | T |
| 0.6019947743080517 | 0.6954857085947173 | 0.5837871320936666 | T | T | T |
| 0.5381997700413119 | 0.7029210813751624 | 0.5837908489264116 | T | T | T |
| 0.1976003591238735 | 0.0292093130228954 | 0.7502730495401803 | T | T | T |
| 0.1346196207568427 | 0.0379730288495628 | 0.7503730667858899 | T | T | T |
| 0.3469369752150945 | 0.0656053711974386 | 0.7501360754026056 | T | T | T |
| 0.4251511062412888 | 0.1081949330380679 | 0.7501319503129563 | T | T | T |
| 0.5684091209792427 | 0.2325511394346547 | 0.7501286237802129 | T | T | T |
| 0.0536739212468959 | 0.3111725238748060 | 0.7505755404564722 | T | T | T |
| 0.0872740292705389 | 0.3889182102824265 | 0.7506060558629031 | T | T | T |
| 0.1906733308944139 | 0.5485240248597588 | 0.7498605984319434 | T | T | T |
| 0.2718507719930605 | 0.6009269698111511 | 0.7503565717402872 | T | T | T |
| 0.4274561183718024 | 0.6812069790809320 | 0.7503627983422445 | T | T | T |
| 0.0500827566562745 | 0.1088754856252904 | 0.7504779094810079 | T | T | T |
| 0.0334743930440472 | 0.1667007333125164 | 0.7505438147450658 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6252002900043964 | 0.3076866232580356 | 0.7501251119001671 | T | T | T |
| 0.6961283893533426 | 0.4632744979424940 | 0.7500940355327185 | T | T | T |
| 0.7070931772202707 | 0.5359576051038909 | 0.7501364744819681 | T | T | T |
| 0.6731036483622406 | 0.6503722116976233 | 0.7502641421992382 | T | T | T |
| 0.6295176111802853 | 0.6850088608651286 | 0.7502629146102155 | T | T | T |
| 0.5029072575917668 | 0.6999605188403031 | 0.7503856781836903 | T | T | T |
| 0.2328636158197360 | 0.0317981696413580 | 0.9168431160282237 | T | T | T |
| 0.3079151632508989 | 0.0500954054002542 | 0.9167662210416813 | T | T | T |
| 0.1076288403661302 | 0.0492966735462380 | 0.9170350999150239 | T | T | T |
| 0.0650483236674027 | 0.0848419761544658 | 0.9171142429599156 | T | T | T |
| 0.4634673317496020 | 0.1349056439992758 | 0.9167561258141101 | T | T | T |
| 0.5355644492848682 | 0.1974250966131416 | 0.9168037721001162 | T | T | T |
| 0.0319991790848182 | 0.2001247161281864 | 0.9170877201396184 | T | T | T |
| 0.0420760466318869 | 0.2723053988564941 | 0.9170550370342500 | T | T | T |
| 0.6485739939573988 | 0.3467218968767488 | 0.9167284239116846 | T | T | T |
| 0.6842189880050379 | 0.4249000636698825 | 0.9166842017728919 | T | T | T |
| 0.1110498945935809 | 0.4286829242372588 | 0.9172817151745374 | T | T | T |
| 0.1644425319971921 | 0.5042506403700070 | 0.9189475363880549 | T | T | T |
| 0.7055400893784300 | 0.5691487374704508 | 0.9167281581612705 | T | T | T |
| 0.6885037306967712 | 0.6268273087530214 | 0.9168109599227137 | T | T | T |
| 0.3101433113896636 | 0.6246333357827488 | 0.9157679300004244 | T | T | T |
| 0.3885047722455725 | 0.6655557442110416 | 0.9165411639755968 | T | T | T |
| 0.6019909312268037 | 0.6954664204015006 | 0.9168321795425067 | T | T | T |
| 0.5381678893089097 | 0.7028092499406581 | 0.9169126431130040 | T | T | T |
| 0.1831936750128929 | 0.6597031592574116 | 0.8431803975876114 | T | T | T |
| 0.1494510149086903 | 0.5933141021497570 | 0.7279612676523126 | T | T | T |
| 0.1482745104844561 | 0.6433002069604561 | 0.9425953437847758 | T | T | T |

OOH\_CNT(10,10) ### KPOINTS: 1x1x3 ### E= -952.21537823 eV

1.0000000000000000

19.0525588799999994 -11.0000000000000000 0.0000000000000000

0.0000000000000000 22.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4010841699999999

C O H

120 2 1

Selective dynamics

Direct

0.1876040968235444 0.0242255696268157 0.0831304917470153 T T T

0.2543514103171182 0.0284598933696690 0.0831778968215423 T T T

0.0814164494513699 0.0615267118434417 0.0830674433457639 T T T

0.4015514340675959 0.0831621555010662 0.0832370297055520 T T T

0.0471017196906810 0.1018715397439118 0.0830557715012501 T T T

0.4752319790999087 0.1310857298707417 0.0832642185956746 T T T

0.0240475759163223 0.2176899735556596 0.0830608255606982 T T T

0.6067022461038637 0.2571881618400674 0.0832765794248331 T T T

0.0364071357472177 0.2876961636883504 0.0831128250546625 T T T

0.6587808837347352 0.3297372660347151 0.0832648857907466 T T T

0.1028039827099527 0.4359554211706492 0.0831965860093739 T T T

0.7246944240753257 0.4782147400028127 0.0832110645381080 T T T

0.1545429825357495 0.5083647511089466 0.0833272769403746 T T T

0.7357255317594261 0.5478324335177394 0.0831593598164809 T T T

0.2850433805967306 0.6344210110120251 0.0832116353323878 T T T

0.7126623002214766 0.6637062264834913 0.0830571854047051 T T T

0.3593931810082631 0.6816480922521928 0.0830713533285647 T T T

0.6795931677848259 0.7053403226308907 0.0830095539546077 T T T

0.5069646910974153 0.7384083907300062 0.0829953584722588 T T T

0.5743411551551539 0.7436579742018108 0.0829842060489606 T T T

0.0354960888079139 0.1269745306657573 0.2496907265893637 T T T

0.5767297833635822 0.2226985082806205 0.2499103746195046 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0481339369783618 | 0.3244082953892237 | 0.2498859341219239 | T | T | T |
| 0.0815815839283684 | 0.3989798934036988 | 0.2499614039331334 | T | T | T |
| 0.1832917448448884 | 0.5434163843204961 | 0.2499314612449408 | T | T | T |
| 0.7354624021021668 | 0.5801440663694301 | 0.2497454100838843 | T | T | T |
| 0.2495608000695644 | 0.6068818744715702 | 0.2495020059087724 | T | T | T |
| 0.3967701949597713 | 0.7004937651409392 | 0.2495298696374965 | T | T | T |
| 0.6577189869041620 | 0.7207344368698437 | 0.2494652239736329 | T | T | T |
| 0.6048354342228898 | 0.7400360750869147 | 0.2494925979323243 | T | T | T |
| 0.1571609080634901 | 0.0279461148000910 | 0.2497538075474887 | T | T | T |
| 0.2901095833702725 | 0.0365021627239990 | 0.2498495435862052 | T | T | T |
| 0.1038234361532813 | 0.0466812813444676 | 0.2496760369788995 | T | T | T |
| 0.3640547144269498 | 0.0639798234878806 | 0.2498991094157791 | T | T | T |
| 0.5106878292603537 | 0.1593658203637579 | 0.2499143978157289 | T | T | T |
| 0.0239064287597093 | 0.1851460119943879 | 0.2497016154827207 | T | T | T |
| 0.6803724869822534 | 0.3670689971894156 | 0.2498692228563355 | T | T | T |
| 0.7135059914833873 | 0.4416530465416462 | 0.2498934166129813 | T | T | T |
| 0.7238595174509860 | 0.6383059513986798 | 0.2496493478027362 | T | T | T |
| 0.4709615733092823 | 0.7292752184196216 | 0.2494969339876161 | T | T | T |
| 0.1876387479751505 | 0.0242517504220405 | 0.4164667925300577 | T | T | T |
| 0.2543762429694773 | 0.0284880834690022 | 0.4165415486667742 | T | T | T |
| 0.0814717113293068 | 0.0616206286134843 | 0.4163585784312102 | T | T | T |
| 0.4015564854258367 | 0.0831819258805698 | 0.4166134552840114 | T | T | T |
| 0.0470493306390654 | 0.1018590584773568 | 0.4163228910653448 | T | T | T |
| 0.4751940162149766 | 0.1310836921809599 | 0.4166335601017335 | T | T | T |
| 0.0242217399163942 | 0.2178241104073382 | 0.4164045946140624 | T | T | T |
| 0.6067061772401408 | 0.2572239382365490 | 0.4166282202315529 | T | T | T |
| 0.0364254510669139 | 0.2877248524641938 | 0.4163828378590404 | T | T | T |
| 0.6587175409688529 | 0.3297083726105122 | 0.4166239957208244 | T | T | T |
| 0.1027726224324978 | 0.4370473907416674 | 0.4162887343943872 | T | T | T |
| 0.7246899978579633 | 0.4782543053051462 | 0.4166681884825129 | T | T | T |
| 0.1518440797570793 | 0.5097699976249825 | 0.4149387085315095 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7356672052355419 | 0.5477669984027828 | 0.4165856319152269 | T | T | T |
| 0.2854032471137564 | 0.6333930742724603 | 0.4173816668488843 | T | T | T |
| 0.7125898561360923 | 0.6636561016234054 | 0.4165024786978141 | T | T | T |
| 0.3593403897780370 | 0.6805234465371073 | 0.4167124408551973 | T | T | T |
| 0.6794381492122776 | 0.7051251369699120 | 0.4164119346520519 | T | T | T |
| 0.5070639090922847 | 0.7381977508674501 | 0.4163775161719817 | T | T | T |
| 0.5744465422849500 | 0.7438568948205599 | 0.4164022082145125 | T | T | T |
| 0.1571513071009930 | 0.0279435050084645 | 0.5831212645174539 | T | T | T |
| 0.2901128760710256 | 0.0364948059326805 | 0.5831876495721660 | T | T | T |
| 0.1038351713014681 | 0.0466598577730504 | 0.5830800704577501 | T | T | T |
| 0.3640486396640804 | 0.0639649879469830 | 0.5832262428838192 | T | T | T |
| 0.0352267509810502 | 0.1268370233825526 | 0.5830351082890276 | T | T | T |
| 0.5106803763269930 | 0.1593411619613554 | 0.5832677664369706 | T | T | T |
| 0.0238182757323384 | 0.1850062099061399 | 0.5830250788510125 | T | T | T |
| 0.5767704474859776 | 0.2227091263203548 | 0.5832768851115046 | T | T | T |
| 0.0484152416415926 | 0.3249050387218310 | 0.5830392998371239 | T | T | T |
| 0.6803697551703969 | 0.3670395356520567 | 0.5832586171869032 | T | T | T |
| 0.0808997880719378 | 0.3991243612492851 | 0.5830777770776758 | T | T | T |
| 0.7135624234368491 | 0.4416903703509677 | 0.5832256932002885 | T | T | T |
| 0.1755437323168699 | 0.5508238751344297 | 0.5835673491255587 | T | T | T |
| 0.7354894287634419 | 0.5801280614867798 | 0.5831394265884561 | T | T | T |
| 0.2499578562932727 | 0.6069456266697451 | 0.5830725282781415 | T | T | T |
| 0.7239225358525332 | 0.6383753376759828 | 0.5830777220165909 | T | T | T |
| 0.3967568889775935 | 0.7000222835792944 | 0.5829680711365745 | T | T | T |
| 0.6577893119072159 | 0.7208076821460301 | 0.5829987804482144 | T | T | T |
| 0.4711926379462809 | 0.7292880854942537 | 0.5829562091180240 | T | T | T |
| 0.6051041738927775 | 0.7405747653530027 | 0.5829747779085566 | T | T | T |
| 0.0814657966256134 | 0.0616129268137451 | 0.7497652342297147 | T | T | T |
| 0.0470369918217366 | 0.1018546724250093 | 0.7497510450507504 | T | T | T |
| 0.6067060836894109 | 0.2572225739533635 | 0.7499066565969166 | T | T | T |
| 0.1030770617798071 | 0.4368684212538576 | 0.7500336873693301 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7356699910187020 | 0.5477691477035135 | 0.7497254167709437 | T | T | T |
| 0.2855399133912584 | 0.6331741574258153 | 0.7486589975494047 | T | T | T |
| 0.3594266483290341 | 0.6804338706796235 | 0.7492946838974944 | T | T | T |
| 0.6794327627716943 | 0.7051256144032521 | 0.7496054427645574 | T | T | T |
| 0.5744570419170407 | 0.7438747290717236 | 0.7495190625326175 | T | T | T |
| 0.1876364008229263 | 0.0242513171028384 | 0.7497822809866735 | T | T | T |
| 0.2543770389745739 | 0.0284835548812725 | 0.7497992211482859 | T | T | T |
| 0.4015556235310150 | 0.0831799209728116 | 0.7498496209310389 | T | T | T |
| 0.4751988702861118 | 0.1310841085604118 | 0.7498844410674047 | T | T | T |
| 0.0242631314208159 | 0.2178290187005402 | 0.7496443680150398 | T | T | T |
| 0.0365447533926389 | 0.2877538199063062 | 0.7496987918822131 | T | T | T |
| 0.6587206949903160 | 0.3297085655307764 | 0.7498958269143668 | T | T | T |
| 0.7246918313009614 | 0.4782521134487728 | 0.7497468826173739 | T | T | T |
| 0.1523675419025070 | 0.5094291176263686 | 0.7515361848332237 | T | T | T |
| 0.7125843818382036 | 0.6636505285279399 | 0.7496088950441581 | T | T | T |
| 0.5070582757335418 | 0.7381936428386454 | 0.7495303331172974 | T | T | T |
| 0.1571636673432411 | 0.0279556860355616 | 0.9164774209595306 | T | T | T |
| 0.2901099323632080 | 0.0365028508322610 | 0.9165146921343975 | T | T | T |
| 0.1038283668747741 | 0.0466857386219027 | 0.9164641554018943 | T | T | T |
| 0.3640517046005395 | 0.0639808217586406 | 0.9165492131786424 | T | T | T |
| 0.0354949168682996 | 0.1269792976162368 | 0.9163920023006095 | T | T | T |
| 0.5106883775160937 | 0.1593682050703048 | 0.9166127252226073 | T | T | T |
| 0.0239308184574464 | 0.1851586615970496 | 0.9163650467970672 | T | T | T |
| 0.5767263764841658 | 0.2226992886946774 | 0.9166309645503339 | T | T | T |
| 0.0482459732784329 | 0.3243867869929954 | 0.9163161809507430 | T | T | T |
| 0.6803728873324524 | 0.3670715028484792 | 0.9166308697365394 | T | T | T |
| 0.0817879800831536 | 0.3989217656726800 | 0.9163952296042885 | T | T | T |
| 0.7135034844962365 | 0.4416517181149087 | 0.9165527228399817 | T | T | T |
| 0.1836111507354339 | 0.5431242430418185 | 0.9166500926002064 | T | T | T |
| 0.7354604421773056 | 0.5801434018343455 | 0.9165253132730483 | T | T | T |
| 0.2497426391092853 | 0.6066901046679322 | 0.9168096922974956 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7238547078728063 | 0.6382986441453909 | 0.9164971923135281 | T | T | T |
| 0.3967922814877460 | 0.7004089278709061 | 0.9165318944273699 | T | T | T |
| 0.6577135489590256 | 0.7207387768230756 | 0.9165236040292084 | T | T | T |
| 0.4709667688916692 | 0.7292543394375768 | 0.9164672351976474 | T | T | T |
| 0.6048386564397314 | 0.7400470484699041 | 0.9164536842209529 | T | T | T |
| 0.1678390844011684 | 0.6665870827235134 | 0.5962505289059281 | T | T | T |
| 0.1256194703363229 | 0.5902979358898791 | 0.5865268395868825 | T | T | T |
| 0.1680137816178327 | 0.6746693912992614 | 0.7257033373197579 | T | T | T |

OOH\_CNT(8,0) ### KPOINTS: 2x2x2 ### E= -502.88917101 eV

1.0000000000000000

12.9903810600000007 -7.5000000000000000 0.0000000000000000

0.0000000000000000 15.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5305455000000006

C O H

64 2 1

Selective dynamics

Direct

0.0786065247636644 0.1930171223148550 0.0833901104185363 T T T

0.4984877354726761 0.2609229080321222 0.0834075248796040 T T T

0.1362432488024509 0.3768843933518862 0.0826934259451218 T T T

0.5591172249515016 0.4448092562975903 0.0840347067986043 T T T

0.1540206478628810 0.0821081530050351 0.0839302891961664 T T T

0.3279277178382291 0.1084430798278068 0.0833262681784152 T T T

0.3058323787984017 0.5287838194054588 0.0827592120769300 T T T

0.4787430578098609 0.5512513775087121 0.0834833341077807 T T T

0.2337045013051490 0.0765331432393875 0.1671315901139627 T T T

0.0990292054306154 0.1222612342547759 0.1674403687911598 T T T

0.4208118748495798 0.1740375658768644 0.1669162960468880 T T T

0.2114239657328841 0.4661810376983330 0.1675689323255440 T T T

0.5358878899416034 0.5133796717262519 0.1675203887045137 T T T

0.3989208451603477 0.5562019192935679 0.1666005962112023 T T T

0.0921235154820181 0.2813450708603814 0.1664730612434692 T T T

0.5468758039512543 0.3567854827380968 0.1672248129939143 T T T

0.0916922181412045 0.2813645199611070 0.3336238417109579 T T T

0.5468596172208284 0.3567958299092728 0.3336325635684202 T T T

0.2336653676880663 0.0764721188527053 0.3336259806671119 T T T

0.0989883522819692 0.1225797267688072 0.3334773789132517 T T T

0.4208587028636629 0.1739267583099428 0.3339074082681470 T T T

0.2121384984777227 0.4653798790521151 0.3319242269272580 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5356375568763826 | 0.5135735773766452 | 0.3336331652192267 | T | T | T |
| 0.3990078092999389 | 0.5568799062642137 | 0.3337036348911114 | T | T | T |
| 0.1544894375509047 | 0.0827128035551220 | 0.4169422959414088 | T | T | T |
| 0.3280435030345367 | 0.1083896051927323 | 0.4172634190909097 | T | T | T |
| 0.3058193129412760 | 0.5286340884239750 | 0.4165628837481112 | T | T | T |
| 0.4787291506684350 | 0.5518299316618933 | 0.4172368352866084 | T | T | T |
| 0.0782983829038951 | 0.1931667118461287 | 0.4171117355671418 | T | T | T |
| 0.4984155138224423 | 0.2607787215991388 | 0.4173200671421498 | T | T | T |
| 0.1367129345398655 | 0.3768485538618378 | 0.4166449371779560 | T | T | T |
| 0.5583810365695163 | 0.4444053462550649 | 0.4170613175238052 | T | T | T |
| 0.0789353369681235 | 0.1940696530820184 | 0.5841952108847270 | T | T | T |
| 0.4985427077033176 | 0.2607860605475470 | 0.5834439390171684 | T | T | T |
| 0.1368408718224774 | 0.3781964706679630 | 0.5828481131468068 | T | T | T |
| 0.5583173394464653 | 0.4444631594810264 | 0.5840989143282330 | T | T | T |
| 0.1544148377320845 | 0.0827596415406233 | 0.5839833736353379 | T | T | T |
| 0.3280184939089199 | 0.1082810381119693 | 0.5833644028086273 | T | T | T |
| 0.3045781996332358 | 0.5287358648711815 | 0.5827767561308678 | T | T | T |
| 0.4776831763091422 | 0.5511581496947271 | 0.5843535427183915 | T | T | T |
| 0.2338399742975672 | 0.0765509026533332 | 0.6671970305083926 | T | T | T |
| 0.0997886485944159 | 0.1230848315200489 | 0.6674091545211531 | T | T | T |
| 0.4209373391153375 | 0.1737951386042886 | 0.6669280895941025 | T | T | T |
| 0.2108007916037531 | 0.4672995203628753 | 0.6640508931819058 | T | T | T |
| 0.5348637838264545 | 0.5126231211795330 | 0.6675455380091514 | T | T | T |
| 0.3981761204247689 | 0.5561873653039644 | 0.6671997392496299 | T | T | T |
| 0.0920151180068182 | 0.2819329976894847 | 0.6670323537213905 | T | T | T |
| 0.5468678116302051 | 0.3566287744096056 | 0.6672780899078377 | T | T | T |
| 0.0946467060388743 | 0.2830189628434991 | 0.8345595320556481 | T | T | T |
| 0.5472550854415762 | 0.3567038846280917 | 0.8335256180942376 | T | T | T |
| 0.2336922369886973 | 0.0762348612323385 | 0.8335095613688744 | T | T | T |
| 0.0997564304469129 | 0.1228861689926573 | 0.8332712018225469 | T | T | T |
| 0.4209091365264701 | 0.1737557801139271 | 0.8338413089936019 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2026913414680541 | 0.4783256096765543 | 0.8362090124092173 | T | T | T |
| 0.5351288475133366 | 0.5126157991527278 | 0.8334401884020622 | T | T | T |
| 0.3964896821001919 | 0.5531808331025130 | 0.8347985510841932 | T | T | T |
| 0.1542682657552419 | 0.0821810260826772 | 0.9169102471500952 | T | T | T |
| 0.3279627506850544 | 0.1084170246381368 | 0.9172206584772008 | T | T | T |
| 0.3057891173283127 | 0.5294295580775741 | 0.9182499151867732 | T | T | T |
| 0.4778486814060008 | 0.5500673766292126 | 0.9172089263550474 | T | T | T |
| 0.0796561378086539 | 0.1936528915135372 | 0.9171046185331081 | T | T | T |
| 0.4985002826623615 | 0.2607660523420393 | 0.9172491156744995 | T | T | T |
| 0.1352120937695756 | 0.3768151169213647 | 0.9180814317499753 | T | T | T |
| 0.5589752513882642 | 0.4445041151287695 | 0.9170345797733760 | T | T | T |
| 0.2148182424351363 | 0.6468871644059314 | 0.8311557938549984 | T | T | T |
| 0.1456506790539354 | 0.5361678431556963 | 0.8637767877362870 | T | T | T |
| 0.2356829609945109 | 0.6720678558587119 | 0.9377052002391596 | T | T | T |

OOH\_CNT(9,0) #### KPOINTS: 2x2x2 #### E= -567.13053961 eV

1.0000000000000000

13.8564064600000005 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5367054200000005

C O H

72 2 1

Selective dynamics

Direct

0.1978584319157420 0.0679521274443864 0.0819730326160994 T T T

0.0865842971881638 0.1308829308997977 0.0816917810975339 T T T

0.3705817397707665 0.1233925133805835 0.0814704923448492 T T T

0.0839597286488633 0.2826891760027522 0.0824302873873731 T T T

0.5240540497122579 0.2749642726277647 0.0814524714178382 T T T

0.1921172009755054 0.4580703174511100 0.0854842288131273 T T T

0.5821284997139888 0.4480865664874249 0.0819300953653345 T T T

0.3680689682331971 0.5623900806672106 0.0823225320277092 T T T

0.5199349821562047 0.5598472398379417 0.0816230874268465 T T T

0.1305845884454301 0.0853343926290741 0.1654400739515486 T T T

0.2808274732457798 0.0802790685981135 0.1654886917202519 T T T

0.4548845265301958 0.1913327312891121 0.1650052573853759 T T T

0.0713816105017817 0.2000894690254296 0.1651077522714112 T T T

0.5685007349635373 0.3647253899400383 0.1654658715001314 T T T

0.1260485514010364 0.3729261678063850 0.1666700704778584 T T T

0.5654088322328757 0.5158574885342300 0.1654332302701938 T T T

0.2779457440974846 0.5219750657735774 0.1666638216772630 T T T

0.4505247552270770 0.5748862242947465 0.1649991513111377 T T T

0.1303441370033695 0.0847605507688406 0.3318857690979825 T T T

0.2807422271622758 0.0801910902916472 0.3314225332692044 T T T

0.4548086160371863 0.1913887952360119 0.3317451236882045 T T T

0.0709242332424266 0.1990866088476540 0.3324163200796819 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5685682638865113 | 0.3648241538431070 | 0.3314103439098274 | T | T | T |
| 0.1261573469086047 | 0.3716409347204836 | 0.3327588001775877 | T | T | T |
| 0.5659260872439296 | 0.5160770278327799 | 0.3317991496139291 | T | T | T |
| 0.2792271548474385 | 0.5217954940603735 | 0.3329395955970335 | T | T | T |
| 0.4515716697792083 | 0.5754450964271384 | 0.3323585731875941 | T | T | T |
| 0.1975344873903866 | 0.0674586670094298 | 0.4150700029770583 | T | T | T |
| 0.0859157097512512 | 0.1301622985830315 | 0.4158016076546291 | T | T | T |
| 0.3704313930474585 | 0.1234724548672633 | 0.4153082614764457 | T | T | T |
| 0.0846885611692432 | 0.2822119758521525 | 0.4161020895461999 | T | T | T |
| 0.5239086619642925 | 0.2751844805022096 | 0.4152996252207430 | T | T | T |
| 0.1940205059503590 | 0.4558976380034333 | 0.4177552889460656 | T | T | T |
| 0.5825950776580175 | 0.4484860935749629 | 0.4150002755810916 | T | T | T |
| 0.3685615448283835 | 0.5619708569756405 | 0.4161564552943537 | T | T | T |
| 0.5205931712563948 | 0.5606353993288028 | 0.4157107462703477 | T | T | T |
| 0.1976244309131669 | 0.0674278492317240 | 0.5819278117904922 | T | T | T |
| 0.0860155594168753 | 0.1300511057218509 | 0.5818605675694288 | T | T | T |
| 0.3704911587679073 | 0.1234346402739237 | 0.5814977627746120 | T | T | T |
| 0.0851654307557723 | 0.2824277160988332 | 0.5828210352477053 | T | T | T |
| 0.5239759703756922 | 0.2750561592759647 | 0.5814472139199467 | T | T | T |
| 0.1934478341716321 | 0.4565370901952513 | 0.5822829446041098 | T | T | T |
| 0.5826676630276281 | 0.4483345345588893 | 0.5818117048950062 | T | T | T |
| 0.3684665118954350 | 0.5613342847461957 | 0.5828847892249186 | T | T | T |
| 0.5208223116413769 | 0.5604883559196575 | 0.5817588634867636 | T | T | T |
| 0.1303546652319785 | 0.0847317258300411 | 0.6654867967914759 | T | T | T |
| 0.2807330290112726 | 0.0801619830256341 | 0.6654704748736521 | T | T | T |
| 0.4548500386555103 | 0.1913649599183017 | 0.6649120071304213 | T | T | T |
| 0.0717540442771417 | 0.1994703913096783 | 0.6659881288223027 | T | T | T |
| 0.5687079287339279 | 0.3648482590775964 | 0.6653716589656843 | T | T | T |
| 0.1254671662242357 | 0.3718311794965573 | 0.6671517013474811 | T | T | T |
| 0.5661762097310965 | 0.5161692661663969 | 0.6654053572096482 | T | T | T |
| 0.2792244154893856 | 0.5219755363082275 | 0.6671325163380486 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4514150736387424 | 0.5746571458426000 | 0.6659684528342305 | T | T | T |
| 0.1306180951283377 | 0.0850755358112598 | 0.8319048800143585 | T | T | T |
| 0.2808767639060123 | 0.0802714949011646 | 0.8314813974845446 | T | T | T |
| 0.4549454809150754 | 0.1912599094908193 | 0.8317273475026448 | T | T | T |
| 0.0727981447559487 | 0.2004065054672926 | 0.8324303043264589 | T | T | T |
| 0.5685571648501945 | 0.3646891620030271 | 0.8314208488181322 | T | T | T |
| 0.1237348138856303 | 0.3722232634989743 | 0.8315986764180859 | T | T | T |
| 0.5659324271378757 | 0.5159193818767429 | 0.8317866953272098 | T | T | T |
| 0.2789478464460285 | 0.5230311176413242 | 0.8315354658676245 | T | T | T |
| 0.4505206740486447 | 0.5734496387204374 | 0.8323202690232850 | T | T | T |
| 0.1979206077384277 | 0.0678737219203744 | 0.9152362470187915 | T | T | T |
| 0.0870564408558691 | 0.1311415747901789 | 0.9159547187754957 | T | T | T |
| 0.3706430235407988 | 0.1233992768360135 | 0.9152977532567895 | T | T | T |
| 0.0866172540281246 | 0.2841152174428223 | 0.9154943530595308 | T | T | T |
| 0.5240538985161874 | 0.2749664570079959 | 0.9152908603890840 | T | T | T |
| 0.1829220499801296 | 0.4681561975823886 | 0.9138649539468665 | T | T | T |
| 0.5823061821575587 | 0.4481014037144803 | 0.9152004288484196 | T | T | T |
| 0.3666789098019207 | 0.5593270789015893 | 0.9152806555362770 | T | T | T |
| 0.5198810139789806 | 0.5594955945462737 | 0.9159091475188246 | T | T | T |
| 0.1848494628635854 | 0.6214134019489236 | 0.9257779175943645 | T | T | T |
| 0.1241021545870686 | 0.5171765416858879 | 0.8868817548182859 | T | T | T |
| 0.1502904490802366 | 0.6243664005560302 | 0.0173430459791590 | T | T | T |

OOH\_CNT(10,0) #### KPOINTS: 2x2x2 #### E= -631.47358999 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C O H

80 2 1

Selective dynamics

Direct

0.2425344424073613 0.0611980655286894 0.0851676260366928 T T T

0.1125041563216803 0.0856818971313900 0.0851080170384507 T T T

0.4083907941310657 0.1399490802978065 0.0855201558378238 T T T

0.5445557639589775 0.2907363730561526 0.0855580602416133 T T T

0.1095638017714381 0.3606383142097037 0.0831943154390528 T T T

0.2453162960543837 0.5108568624094475 0.0832431068874624 T T T

0.5440229234644186 0.5633024716622206 0.0851951396277731 T T T

0.4108477531049193 0.5830380831523051 0.0842452611002702 T T T

0.0646536236631443 0.1997632913301492 0.0840860898296784 T T T

0.5965795025982785 0.4531494847402093 0.0852357285062340 T T T

0.1692121577970884 0.0604436345321349 0.1683556087653380 T T T

0.4841561006500005 0.2097010702609734 0.1690340284861481 T T T

0.1680242170545588 0.4426294043675679 0.1677891544824727 T T T

0.4851140590651982 0.5857102538323504 0.1682810505544597 T T T

0.3252226994676296 0.0888885197974504 0.1686525237472981 T T T

0.0764151392041781 0.1333793725794013 0.1681487665948753 T T T

0.0759892177264686 0.2772282867443929 0.1670042252358049 T T T

0.5832041125568477 0.3745157056104386 0.1687107112427600 T T T

0.5827150104043094 0.5181456214630810 0.1684586864276085 T T T

0.3290744400130511 0.5575526649035391 0.1671374665679189 T T T

0.3252185509586566 0.0889552483914120 0.3354839060591416 T T T

0.0760549035581038 0.1333919046555266 0.3347435763337629 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0755776231876359 | 0.2769838426095531 | 0.3340933853380844 | T | T | T |
| 0.5831506044469484 | 0.3744901452788204 | 0.3355247959152039 | T | T | T |
| 0.5826427885249706 | 0.5183184311177126 | 0.3352200224026314 | T | T | T |
| 0.3292058711533036 | 0.5579458231675095 | 0.3341891971719778 | T | T | T |
| 0.1689972020043739 | 0.0604924734665338 | 0.3351003408421969 | T | T | T |
| 0.4841794620862703 | 0.2096594736021654 | 0.3353868866436905 | T | T | T |
| 0.1689781003715532 | 0.4419446213187890 | 0.3323462859463029 | T | T | T |
| 0.4850181048550919 | 0.5859769443099319 | 0.3348653056732179 | T | T | T |
| 0.0636050171398347 | 0.1992505543841449 | 0.4177201981950278 | T | T | T |
| 0.5963184951525210 | 0.4530468485556991 | 0.4188742641528829 | T | T | T |
| 0.2425813601780558 | 0.0614907271530511 | 0.4187777313634091 | T | T | T |
| 0.1122131190066910 | 0.0855165219051287 | 0.4180726733400911 | T | T | T |
| 0.4083931116585905 | 0.1401191079159264 | 0.4187153807591946 | T | T | T |
| 0.5443784965543684 | 0.2906543018423230 | 0.4187337857977568 | T | T | T |
| 0.1104730500411454 | 0.3604312100896603 | 0.4168875591736448 | T | T | T |
| 0.2456314866558612 | 0.5101555693285067 | 0.4168497391164571 | T | T | T |
| 0.5441077673817706 | 0.5634964742087654 | 0.4182177103124449 | T | T | T |
| 0.4111443322060903 | 0.5839484889276346 | 0.4178236251474600 | T | T | T |
| 0.2425606309476593 | 0.0613794420738513 | 0.5851436687275082 | T | T | T |
| 0.1125865668343593 | 0.0860629210772366 | 0.5850984260689034 | T | T | T |
| 0.4083930550322846 | 0.1400375279911553 | 0.5854363896849505 | T | T | T |
| 0.5444245301512136 | 0.2906995978961014 | 0.5854654403110309 | T | T | T |
| 0.1101073096208305 | 0.3616675608945426 | 0.5834897478264077 | T | T | T |
| 0.2441970478063047 | 0.5101207925004437 | 0.5834562006749053 | T | T | T |
| 0.5435538338107131 | 0.5630588421962668 | 0.5852265628053703 | T | T | T |
| 0.4100547645338742 | 0.5832033233921486 | 0.5850055041652060 | T | T | T |
| 0.0641032131661920 | 0.2002734212726945 | 0.5849054614171998 | T | T | T |
| 0.5964497096464285 | 0.4531060396667048 | 0.5852276157691271 | T | T | T |
| 0.1694045402201332 | 0.0608991404264193 | 0.6684756816908006 | T | T | T |
| 0.4842095985652202 | 0.2096430813176090 | 0.6690076089547089 | T | T | T |
| 0.1666902011766864 | 0.4436826283460848 | 0.6642698673249354 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4843850379223008 | 0.5850387916241870 | 0.6684188921250933 | T | T | T |
| 0.3252286351878129 | 0.0889282453207627 | 0.6685640810791063 | T | T | T |
| 0.0769569527310745 | 0.1341034369915053 | 0.6682761810466249 | T | T | T |
| 0.0747793282147986 | 0.2774162223919261 | 0.6673489115543084 | T | T | T |
| 0.5831325354574763 | 0.3744789286706549 | 0.6686288905880957 | T | T | T |
| 0.5822785364412540 | 0.5178823046241399 | 0.6685748496028586 | T | T | T |
| 0.3284985857422931 | 0.5582074005215176 | 0.6674253990072920 | T | T | T |
| 0.3253064896376750 | 0.0889151508250463 | 0.8353995075792664 | T | T | T |
| 0.0772395651463928 | 0.1341933388300312 | 0.8345750665861289 | T | T | T |
| 0.0771587754490447 | 0.2787503289388017 | 0.8348223701542328 | T | T | T |
| 0.5831380952433270 | 0.3743782200995168 | 0.8354592210741133 | T | T | T |
| 0.5823724348935140 | 0.5179439791789370 | 0.8351950588380825 | T | T | T |
| 0.3276255488243031 | 0.5558056848043637 | 0.8349555841742896 | T | T | T |
| 0.1694081747491348 | 0.0608239116710308 | 0.8350948365812273 | T | T | T |
| 0.4844183438923951 | 0.2094598996736599 | 0.8353916844713806 | T | T | T |
| 0.1561044192878155 | 0.4515546597590728 | 0.8355859920393155 | T | T | T |
| 0.4844344867112734 | 0.5849144712037135 | 0.8346785116059882 | T | T | T |
| 0.0656554735002487 | 0.2005708295044462 | 0.9177228966734680 | T | T | T |
| 0.5962903871231066 | 0.4529029234086250 | 0.9188080194885665 | T | T | T |
| 0.2427364354679971 | 0.0615084227893222 | 0.9187421742383329 | T | T | T |
| 0.1127061386994306 | 0.0859057710494790 | 0.9181266849105661 | T | T | T |
| 0.4085374413291815 | 0.1398960880778065 | 0.9187403636841797 | T | T | T |
| 0.5445797715143442 | 0.2905426906434087 | 0.9187772750004757 | T | T | T |
| 0.1079719467321770 | 0.3607239562146516 | 0.9182754334130874 | T | T | T |
| 0.2448958591371531 | 0.5118665666666518 | 0.9183205572096367 | T | T | T |
| 0.5438326002916521 | 0.5631250241563879 | 0.9182179420419098 | T | T | T |
| 0.4101914044528793 | 0.5819457620452978 | 0.9178901571629948 | T | T | T |
| 0.1337764353157376 | 0.5824023134175471 | 0.8047531198996278 | T | T | T |
| 0.0904236366540161 | 0.4868665575384308 | 0.8591566503743245 | T | T | T |
| 0.1516051794914795 | 0.6140140963536426 | 0.9047934200420350 | T | T | T |

OOH\_CNT(11,0) #### KPOINTS: 2x2x2 #### E= -695.47443460 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C O H

88 2 1

Selective dynamics

Direct

0.1539723010027676 0.0552091093363089 0.0845089360892236 T T T

0.2981773943752472 0.0734003436632061 0.0849174787227511 T T T

0.0677643272555900 0.1258923714732258 0.0844486985531445 T T T

0.4527927075275489 0.1749628523042728 0.0853867436487152 T T T

0.0632306020519701 0.2596937668678510 0.0834521112477210 T T T

0.5675646225040455 0.3253579667279153 0.0849622768119685 T T T

0.1363339611083647 0.4167588014183736 0.0824378760203541 T T T

0.6054423578898419 0.4763634895391389 0.0845434452455238 T T T

0.2763976192944430 0.5472416036463671 0.0823940962460362 T T T

0.5538604932909303 0.5790324192485991 0.0845609530478485 T T T

0.4315381834547279 0.6032725700674449 0.0834704194642903 T T T

0.2217151964870520 0.0532526547827740 0.1680895159488237 T T T

0.1012520903469376 0.0804224348186462 0.1677994988285863 T T T

0.3776326189779032 0.1153922384797805 0.1685680848339675 T T T

0.0543651601926055 0.1868786668760098 0.1674866832379284 T T T

0.5178998283253926 0.2467671017954065 0.1685606021032752 T T T

0.0910741073648785 0.3376397164494369 0.1663863928094394 T T T

0.5970803518262945 0.4038328767767324 0.1681055116983145 T T T

0.1999508708501622 0.4899274966459220 0.1668926153968817 T T T

0.5904523688496477 0.5364758120986660 0.1678853349701152 T T T

0.3557430883872722 0.5846216497058229 0.1664094449256586 T T T

0.4998202203795666 0.6022735043775976 0.1675593790380014 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2216474235568445 | 0.0532132137929503 | 0.3350929568954090 | T | T | T |
| 0.1013488351061138 | 0.0806261771540558 | 0.3345249173893527 | T | T | T |
| 0.3775607950838533 | 0.1153513148383585 | 0.3349777421882743 | T | T | T |
| 0.0542412400784314 | 0.1870432104059717 | 0.3337989380708333 | T | T | T |
| 0.5178957320009836 | 0.2468374250704773 | 0.3349867280500871 | T | T | T |
| 0.0906853551165684 | 0.3376791278198042 | 0.3334198812551839 | T | T | T |
| 0.5971391131277696 | 0.4039109969786196 | 0.3351501324839333 | T | T | T |
| 0.2005018726047718 | 0.4893081617317448 | 0.3317286484656872 | T | T | T |
| 0.5902635848443453 | 0.5364335304760214 | 0.3345716544566941 | T | T | T |
| 0.3556702089733528 | 0.5850686341246116 | 0.3334411605092480 | T | T | T |
| 0.4995943887437536 | 0.6023701532113133 | 0.3339021340615598 | T | T | T |
| 0.1541119211374027 | 0.0553441178768194 | 0.4182238937565436 | T | T | T |
| 0.2981318746008432 | 0.0735479074852513 | 0.4184632583408831 | T | T | T |
| 0.0678826937451920 | 0.1260231396903531 | 0.4174253601101551 | T | T | T |
| 0.4527203658894640 | 0.1750300822966862 | 0.4183442848665981 | T | T | T |
| 0.0625424852379241 | 0.2596031115992826 | 0.4168752730627704 | T | T | T |
| 0.5673966299923878 | 0.3254231411287944 | 0.4184485207752017 | T | T | T |
| 0.1368720964690326 | 0.4166094760309237 | 0.4162444182714408 | T | T | T |
| 0.6053110354200176 | 0.4762594984684919 | 0.4182726823441804 | T | T | T |
| 0.2763826298426558 | 0.5468811475942628 | 0.4162352254700101 | T | T | T |
| 0.5536537240118068 | 0.5788759925281052 | 0.4174867092034702 | T | T | T |
| 0.4316019898379749 | 0.6039574094815275 | 0.4170161172084879 | T | T | T |
| 0.1541356994341787 | 0.0554692290144678 | 0.5844696932303612 | T | T | T |
| 0.2982278927029351 | 0.0735002904460948 | 0.5849420087571564 | T | T | T |
| 0.0680813127004791 | 0.1263801638017722 | 0.5845531366643808 | T | T | T |
| 0.4528196846414622 | 0.1749203256331723 | 0.5854470177071531 | T | T | T |
| 0.0630072282505777 | 0.2603504811288450 | 0.5841389354086334 | T | T | T |
| 0.5674090852436111 | 0.3253192730418276 | 0.5849383534450165 | T | T | T |
| 0.1366887613483730 | 0.4177790403990834 | 0.5825934972386055 | T | T | T |
| 0.6052747129278331 | 0.4762833890073508 | 0.5845413537052543 | T | T | T |
| 0.2753001788874302 | 0.5471117623281676 | 0.5826059218423902 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5533052978735986 | 0.5786923453213392 | 0.5846109736727467 | T | T | T |
| 0.4307967793522867 | 0.6033859838951513 | 0.5842995466228456 | T | T | T |
| 0.2217885342550797 | 0.0533381936534737 | 0.6680830183737262 | T | T | T |
| 0.1015449198757302 | 0.0807680753617598 | 0.6678200501141782 | T | T | T |
| 0.3776993532428748 | 0.1153304065736471 | 0.6686457099583051 | T | T | T |
| 0.0549523187839207 | 0.1874698152726587 | 0.6675488710275942 | T | T | T |
| 0.5179618807110883 | 0.2466944095524496 | 0.6686017375389360 | T | T | T |
| 0.0902971527275495 | 0.3381177354645367 | 0.6664788140934375 | T | T | T |
| 0.5969881077890938 | 0.4037594864417521 | 0.6680830996477901 | T | T | T |
| 0.1988701327715826 | 0.4912941009001928 | 0.6637468105522585 | T | T | T |
| 0.5900979934788031 | 0.5362046603126780 | 0.6679283467025806 | T | T | T |
| 0.3552157212016965 | 0.5850959792374388 | 0.6666370320967721 | T | T | T |
| 0.4991167941433081 | 0.6015638512950960 | 0.6676502398286628 | T | T | T |
| 0.2216787592224453 | 0.0530831137460942 | 0.8350499655332172 | T | T | T |
| 0.1014040610659438 | 0.0805315730045944 | 0.8344011306784909 | T | T | T |
| 0.3776556175361624 | 0.1153133821208792 | 0.8349885180608826 | T | T | T |
| 0.0552785882562927 | 0.1875610178016814 | 0.8337031168653134 | T | T | T |
| 0.5180178019860716 | 0.2467367762065650 | 0.8349996819064447 | T | T | T |
| 0.0923478484628948 | 0.3389001736873665 | 0.8341314687877354 | T | T | T |
| 0.5972190920312047 | 0.4038101751832422 | 0.8350880099525627 | T | T | T |
| 0.1911005951124520 | 0.5008978581642493 | 0.8351138780915721 | T | T | T |
| 0.5903049782891664 | 0.5362970330968430 | 0.8344469115149242 | T | T | T |
| 0.3541717592201451 | 0.5827392214371243 | 0.8342996635065658 | T | T | T |
| 0.4990849193195139 | 0.6013423094799184 | 0.8337976094589744 | T | T | T |
| 0.1540449987448810 | 0.0551877384577840 | 0.9181736014929419 | T | T | T |
| 0.2981761220262888 | 0.0733951306778711 | 0.9184130758067670 | T | T | T |
| 0.0680852930623383 | 0.1260958719312316 | 0.9174263566164423 | T | T | T |
| 0.4527788364584830 | 0.1749956449181647 | 0.9183160187371456 | T | T | T |
| 0.0641409386263325 | 0.2602339661998565 | 0.9169671192491328 | T | T | T |
| 0.5675990760850230 | 0.3253478428639583 | 0.9184431256059981 | T | T | T |
| 0.1348265869738931 | 0.4169971160112943 | 0.9176027443492355 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6054073890569566 | 0.4762323739029333 | 0.9181920052594218 | T | T | T |
| 0.2762203379204032 | 0.5482635420177627 | 0.9176095777143713 | T | T | T |
| 0.5536599681544615 | 0.5787272374780407 | 0.9175464260916902 | T | T | T |
| 0.4308127226790630 | 0.6021546186881470 | 0.9170408622347639 | T | T | T |
| 0.1940747874082202 | 0.6382975318019926 | 0.8089665951646939 | T | T | T |
| 0.1408114866753889 | 0.5479284484683631 | 0.8587390729142722 | T | T | T |
| 0.2192121916717909 | 0.6653361974672264 | 0.9087925600550882 | T | T | T |

OOH\_CNT(12,0) #### KPOINTS: 1x1x2 #### E= -758.88828382 eV

1.000000000000000

15.588499999999998 -9.000000000000000 0.000000000000000

0.000000000000000 18.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 8.457919999999997

C O H

96 2 1

Selective dynamics

Direct

0.6558002487316048 0.5352448326812763 0.4140711468176763 T T T

0.6560229105178333 0.5353167238824391 0.9141130914011482 T T T

0.4672802324022772 0.6487781097861580 0.4141136762486828 T T T

0.4668209386322962 0.6473923604750738 0.9143086734771132 T T T

0.3917124180770915 0.1093558485899235 0.4143270947637727 T T T

0.3917278093051592 0.1091353995818067 0.9142969165504774 T T T

0.1122596006252658 0.0730459491425512 0.4138267493912300 T T T

0.1124864925405962 0.0731594522566633 0.9140013851570358 T T T

0.6353232879649753 0.3897953777656067 0.4142953700182735 T T T

0.6355256178900414 0.3898237021317977 0.9142328034758960 T T T

0.5931798560804491 0.6292814279193406 0.4137813553400229 T T T

0.5932869194933953 0.6291519910009181 0.9138953642821634 T T T

0.1638690024803500 0.4717483229595021 0.4159092146260382 T T T

0.1501903569886028 0.4807614234595538 0.9126345875202645 T T T

0.0724542482229810 0.3154770525570706 0.4144380653733503 T T T

0.0732206070234961 0.3169273727627199 0.9139229722711931 T T T

0.2356284767573812 0.0496614951307684 0.4141408571895984 T T T

0.2355746349232410 0.0494662240687122 0.9141718773707203 T T T

0.5378713773724648 0.2336983866461666 0.4139579950764305 T T T

0.5376888424164051 0.2338279479289622 0.9139794656678216 T T T

0.3117517729277977 0.5916567771336624 0.4144379099969167 T T T

0.3104399858571711 0.5899970434069094 0.9136891952416779 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0540718761448775 | 0.1709300864611311 | 0.4141948691544257 | T | T | T |
| 0.0553373267936255 | 0.1718270619302076 | 0.9144425448692838 | T | T | T |
| 0.5931248888302841 | 0.6290249340954944 | 0.0809635279892149 | T | T | T |
| 0.5934216568341240 | 0.6292841732994653 | 0.5810272427569108 | T | T | T |
| 0.0548321385117224 | 0.1715190939288684 | 0.0808183712094047 | T | T | T |
| 0.0543346886222627 | 0.1709345757463119 | 0.5808016582648385 | T | T | T |
| 0.3111272515875770 | 0.5923218534028759 | 0.0813000797825199 | T | T | T |
| 0.3117192203613961 | 0.5910367361521830 | 0.5815445336628732 | T | T | T |
| 0.1124796932977575 | 0.0732306688698271 | 0.0810722239166770 | T | T | T |
| 0.1123207755258757 | 0.0729491304451526 | 0.5810756325606649 | T | T | T |
| 0.6559514367481475 | 0.5352331255472946 | 0.0809048930316564 | T | T | T |
| 0.6559533512274260 | 0.5352631887963258 | 0.5808716276556045 | T | T | T |
| 0.2356577723332801 | 0.0496340233254471 | 0.0809582814675363 | T | T | T |
| 0.2356520287388492 | 0.0496006953503368 | 0.5809579139289059 | T | T | T |
| 0.1612642649409714 | 0.4734360504725279 | 0.0835753686024287 | T | T | T |
| 0.1630293927048268 | 0.4722756136236607 | 0.5811306811750573 | T | T | T |
| 0.3917372125772650 | 0.1091624669338705 | 0.0809137487027080 | T | T | T |
| 0.3917548544239546 | 0.1093213909742378 | 0.5809423059835805 | T | T | T |
| 0.4669425271808126 | 0.6478800123787686 | 0.0806860652144373 | T | T | T |
| 0.4674710460284933 | 0.6485865210254690 | 0.5807664709734451 | T | T | T |
| 0.5377203831106063 | 0.2338024141578274 | 0.0811783687796981 | T | T | T |
| 0.5378724852134203 | 0.2337165731982844 | 0.5812121261040959 | T | T | T |
| 0.0710629698903970 | 0.3156863472033046 | 0.0814838239902120 | T | T | T |
| 0.0729837442858888 | 0.3157274316387153 | 0.5815664963515388 | T | T | T |
| 0.6354660347012173 | 0.3898360897124204 | 0.0808343032901781 | T | T | T |
| 0.6352897180248097 | 0.3897461625909469 | 0.5808765904448365 | T | T | T |
| 0.2325506513215910 | 0.5390007117958757 | 0.1647469633197486 | T | T | T |
| 0.2336531976754582 | 0.5392548245480654 | 0.6654103038903019 | T | T | T |
| 0.0539507496558475 | 0.2402936608443042 | 0.1637082323843570 | T | T | T |
| 0.0548167151959346 | 0.2399871124350662 | 0.6644286153671499 | T | T | T |
| 0.3122730251519789 | 0.0699536294590334 | 0.1639955120762582 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3122452230507194 | 0.0698778131065960 | 0.6639728968726704 | T | T | T |
| 0.3900115449671162 | 0.6284992443956056 | 0.1635283569040063 | T | T | T |
| 0.3907656526885548 | 0.6280913538753107 | 0.6643856003685399 | T | T | T |
| 0.6343038965678720 | 0.5908156480375107 | 0.1641931320460802 | T | T | T |
| 0.6345666266160022 | 0.5910197259599657 | 0.6642059807687930 | T | T | T |
| 0.4687025610790638 | 0.1652210753318839 | 0.1642288358506950 | T | T | T |
| 0.4687556552564440 | 0.1652786005140936 | 0.6642700406684711 | T | T | T |
| 0.0743804253385393 | 0.1145897959492785 | 0.1639810855241549 | T | T | T |
| 0.0741544031384680 | 0.1141676392362685 | 0.6640601819771871 | T | T | T |
| 0.1082087264869299 | 0.3958692539350791 | 0.1647417519251379 | T | T | T |
| 0.1080137282287007 | 0.3950214183341546 | 0.6653969183049946 | T | T | T |
| 0.5948064003036714 | 0.3102387161242093 | 0.1641961487006151 | T | T | T |
| 0.5948482758857898 | 0.3101607210088326 | 0.6642483565392119 | T | T | T |
| 0.5360025629688732 | 0.6483788491028742 | 0.1638793533387095 | T | T | T |
| 0.5364942087654065 | 0.6487785177966168 | 0.6639647812484994 | T | T | T |
| 0.1671305816554906 | 0.0505957916114883 | 0.1642836647380302 | T | T | T |
| 0.1671150089411713 | 0.0505243237599264 | 0.6642712843094769 | T | T | T |
| 0.6561080770386686 | 0.4665849157047695 | 0.1639932477624413 | T | T | T |
| 0.6560107900391853 | 0.4665660301616040 | 0.6638961404942666 | T | T | T |
| 0.0740575595852457 | 0.1140824460247730 | 0.3310065861874310 | T | T | T |
| 0.0744443607422883 | 0.1144273008189683 | 0.8310429803909294 | T | T | T |
| 0.5363976743631567 | 0.6487935499059204 | 0.3309280504881456 | T | T | T |
| 0.5363223659741698 | 0.6484614289390012 | 0.8309179650909302 | T | T | T |
| 0.6343140944751656 | 0.5908268832147000 | 0.3306728606999186 | T | T | T |
| 0.6345838442325418 | 0.5909603117544712 | 0.8307484555363308 | T | T | T |
| 0.4686906119824694 | 0.1652591985929436 | 0.3309258085918946 | T | T | T |
| 0.4687008669831664 | 0.1653007757189066 | 0.8309526431175641 | T | T | T |
| 0.0536953323656119 | 0.2394837410269151 | 0.3313045524785372 | T | T | T |
| 0.0556010831947160 | 0.2407091412751418 | 0.8313299613394967 | T | T | T |
| 0.1671753990530322 | 0.0505633688780041 | 0.3307412929702494 | T | T | T |
| 0.1672004335867152 | 0.0505459794899129 | 0.8307781507206635 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3908552828307257 | 0.6290921728354389 | 0.3311777221954301 | T | T | T |
| 0.3902129271296587 | 0.6270262359499039 | 0.8312134491586765 | T | T | T |
| 0.5948149799461160 | 0.3101933804627607 | 0.3308922761012298 | T | T | T |
| 0.5948063451304501 | 0.3101763442950669 | 0.8309084133202697 | T | T | T |
| 0.1088799703729091 | 0.3947920914778220 | 0.3314147366678895 | T | T | T |
| 0.1057927362383889 | 0.3951561557822706 | 0.8305421844768528 | T | T | T |
| 0.2339865359612911 | 0.5388471498757619 | 0.3315255867364679 | T | T | T |
| 0.2329274296715819 | 0.5405173346261883 | 0.8304797354022296 | T | T | T |
| 0.3122869415145592 | 0.0700133417154673 | 0.3311961686904842 | T | T | T |
| 0.3122546389833943 | 0.0697630013857413 | 0.8312215493575997 | T | T | T |
| 0.6560174288217501 | 0.4665479535301935 | 0.3311554292275256 | T | T | T |
| 0.6560995476184878 | 0.4665595438477321 | 0.8311048433700834 | T | T | T |
| 0.1280274831242424 | 0.6046354912661821 | 0.9283038892834680 | T | T | T |
| 0.0858561924958959 | 0.5118858410715409 | 0.8874779192556170 | T | T | T |
| 0.0944748697340816 | 0.6015808206813510 | 0.0206438866440484 | T | T | T |

OOH\_CNT(13,0) #### KPOINTS: 1x1x2 #### E= -1230.18307403 eV

1.000000000000000

24.248699999999995 -14.000000000000000 0.000000000000000

0.000000000000000 28.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 12.838699999999993

C O H

156 2 1

Selective dynamics

Direct

0.4410427687885271 0.4067267876101954 0.0279344697662327 T T T

0.4529936027464589 0.3696989469077334 0.1947120456772386 T T T

0.4531256793247966 0.3697605939544518 0.3055935651821469 T T T

0.3834173727971654 0.4499278388312482 0.0278251224080317 T T T

0.4408829589016111 0.4066437391141779 0.1390068911462787 T T T

0.4170496614116314 0.4335948358406574 0.1945243074523376 T T T

0.4169011474242391 0.4334616568268330 0.3057208048087396 T T T

0.2933989521897344 0.4448262545933983 0.0272605437722286 T T T

0.3831366510752270 0.4497082310963593 0.1388791088289559 T T T

0.3408741389838598 0.4532252262179041 0.1943472639989795 T T T

0.3402289987162432 0.4526944588657068 0.3057712309831609 T T T

0.1923180638497524 0.3944404544586897 0.0269731665092389 T T T

0.2932984891953845 0.4447708665579393 0.1383875698438003 T T T

0.2427091444610990 0.4248318798289494 0.1935922425400093 T T T

0.2421267076410146 0.4253365741600548 0.3047464751051635 T T T

0.1028141319307479 0.3090309988281422 0.0272248517496917 T T T

0.1923112470230398 0.3944184698047217 0.1376619761548759 T T T

0.1447463326778535 0.3551897438448818 0.1935531361100814 T T T

0.1446929019689516 0.3562653176815794 0.3046850756490578 T T T

0.0446536162416949 0.2083207917654908 0.0277546496226635 T T T

0.1028375647196652 0.3091311161646375 0.1383195687715266 T T T

0.0689010215405685 0.2594641154517055 0.1942662805652666 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0694787589573597 | 0.2599603602394471 | 0.3056811569053451 | T | T | T |
| 0.0322226189655796 | 0.1151717663669840 | 0.0279136568480236 | T | T | T |
| 0.0448521093637859 | 0.2085131909968409 | 0.1387917052244143 | T | T | T |
| 0.0326259661000382 | 0.1594852275697752 | 0.1944866906284479 | T | T | T |
| 0.0328585032780055 | 0.1596703386418641 | 0.3056878283157071 | T | T | T |
| 0.0687105993862546 | 0.0516135373706913 | 0.0280032080872560 | T | T | T |
| 0.0323757975474176 | 0.1153253673051897 | 0.1389903577045528 | T | T | T |
| 0.0446715681678748 | 0.0785179845647824 | 0.1947150708101022 | T | T | T |
| 0.0446062649100635 | 0.0784769944558476 | 0.3055941557521686 | T | T | T |
| 0.1443944692338392 | 0.0312783243211140 | 0.0281927995934238 | T | T | T |
| 0.0686249949383220 | 0.0515505171181802 | 0.1391248938214747 | T | T | T |
| 0.1024248828975752 | 0.0354601559770822 | 0.1947616478896458 | T | T | T |
| 0.1023484964488717 | 0.0353965543747165 | 0.3057920569308385 | T | T | T |
| 0.2426019731695618 | 0.0594303099110858 | 0.0281958476048495 | T | T | T |
| 0.1443754006189474 | 0.0312821290147840 | 0.1391339562942388 | T | T | T |
| 0.1920661555408864 | 0.0394799375117222 | 0.1948111011664079 | T | T | T |
| 0.1920380429047875 | 0.0394929606434493 | 0.3058951676992564 | T | T | T |
| 0.3409197300105424 | 0.1295534130870285 | 0.0282034740946439 | T | T | T |
| 0.2426094417445108 | 0.0594294894347836 | 0.1392264899187392 | T | T | T |
| 0.2932188960850937 | 0.0900631187498379 | 0.1949580410982797 | T | T | T |
| 0.2932306568240579 | 0.0900435867899923 | 0.3058852169729112 | T | T | T |
| 0.4166693508081622 | 0.2254800676498571 | 0.0282177097139259 | T | T | T |
| 0.3408959557892370 | 0.1295346208195676 | 0.1392544136676886 | T | T | T |
| 0.3828024346262932 | 0.1755153785715001 | 0.1948458869195427 | T | T | T |
| 0.3827958723255511 | 0.1755545881190438 | 0.3059149943835285 | T | T | T |
| 0.4524121242401931 | 0.3252996834401918 | 0.0280465818714967 | T | T | T |
| 0.4166491548458892 | 0.2254648991933451 | 0.1391559409219862 | T | T | T |
| 0.4402908703991329 | 0.2764356886281849 | 0.1947802281779870 | T | T | T |
| 0.4403949205743379 | 0.2764934399134353 | 0.3058150579720235 | T | T | T |
| 0.4525361681085203 | 0.3253576847323515 | 0.1391418754272938 | T | T | T |
| 0.4409947469444230 | 0.4065712605200661 | 0.3612776389345507 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4534255351166766 | 0.3698419228229198 | 0.5280603666751335 | T | T | T |
| 0.4533507016744086 | 0.3698343901693189 | 0.6390287540711757 | T | T | T |
| 0.3826901373361395 | 0.4489349707159249 | 0.3613530411486625 | T | T | T |
| 0.4411432143959080 | 0.4066070595660338 | 0.4722351593556335 | T | T | T |
| 0.4170182421419330 | 0.4333168428748556 | 0.5277957503171030 | T | T | T |
| 0.4172129076697907 | 0.4335321717175465 | 0.6388860129779509 | T | T | T |
| 0.2929127765050790 | 0.4447632492159914 | 0.3607538158572711 | T | T | T |
| 0.3826058424406175 | 0.4486698374905486 | 0.4721229306403200 | T | T | T |
| 0.3401119414676770 | 0.4517830601839168 | 0.5277495559620841 | T | T | T |
| 0.3405559950986581 | 0.4524262216296330 | 0.6384548984654708 | T | T | T |
| 0.1914903107948478 | 0.3968280295608859 | 0.3585564787925287 | T | T | T |
| 0.2922252495652221 | 0.4436177411125978 | 0.4723819821383951 | T | T | T |
| 0.2428632143182737 | 0.4267915692636869 | 0.5281522715508870 | T | T | T |
| 0.2427458306655978 | 0.4258876881099116 | 0.6381343008300758 | T | T | T |
| 0.1027296374011255 | 0.3098023566992011 | 0.3606810544473808 | T | T | T |
| 0.1887455146886347 | 0.4056595334392674 | 0.4724657555472181 | T | T | T |
| 0.1432379419496705 | 0.3566602862351673 | 0.5282220778678476 | T | T | T |
| 0.1440839637198058 | 0.3560448801518784 | 0.6381492440964610 | T | T | T |
| 0.0455378524354423 | 0.2086919128257059 | 0.3613000880091623 | T | T | T |
| 0.1037615147273128 | 0.3100417487679087 | 0.4722995284445948 | T | T | T |
| 0.0701674964946812 | 0.2597148691540794 | 0.5276682814639704 | T | T | T |
| 0.0696086141010984 | 0.2595042033726933 | 0.6384083895675629 | T | T | T |
| 0.0324687674881660 | 0.1153056445108838 | 0.3612416417032299 | T | T | T |
| 0.0458779725671253 | 0.2087362053768638 | 0.4720813051951505 | T | T | T |
| 0.0329919092534820 | 0.1595639874506976 | 0.5277152610930869 | T | T | T |
| 0.0327621406166144 | 0.1594243170040402 | 0.6388051355980440 | T | T | T |
| 0.0684513396049042 | 0.0513615199378303 | 0.3613047600052381 | T | T | T |
| 0.0324028191055749 | 0.1152151793109034 | 0.4721817721168007 | T | T | T |
| 0.0444439294069105 | 0.0782608117518722 | 0.5279980953071388 | T | T | T |
| 0.0444521530678935 | 0.0782772447561906 | 0.6389450918668016 | T | T | T |
| 0.1443609568363770 | 0.0313349776778086 | 0.3615410510756448 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0683752489897345 | 0.0512632462953401 | 0.4724137876857647 | T | T | T |
| 0.1023206122144190 | 0.0353530935247230 | 0.5280604819178588 | T | T | T |
| 0.1023014207767979 | 0.0353316327555273 | 0.6390851557576823 | T | T | T |
| 0.2426129342821080 | 0.0594463144621336 | 0.3615209618175892 | T | T | T |
| 0.1443330122104354 | 0.0313202390052589 | 0.4724727256865573 | T | T | T |
| 0.1920413367369447 | 0.0395175790989504 | 0.5281303641170696 | T | T | T |
| 0.1920398284016104 | 0.0395204669018730 | 0.6392338099929943 | T | T | T |
| 0.3408861379039030 | 0.1295431181914407 | 0.3615375374579378 | T | T | T |
| 0.2426202229085771 | 0.0594564784583212 | 0.4725808927592091 | T | T | T |
| 0.2932302693256567 | 0.0900831401896691 | 0.5283006296508906 | T | T | T |
| 0.2932262928930854 | 0.0900522964245408 | 0.6392114440818182 | T | T | T |
| 0.4166098635945770 | 0.2255207612604079 | 0.3615594869759010 | T | T | T |
| 0.3408868678343283 | 0.1295563969078299 | 0.4725787011319202 | T | T | T |
| 0.3827847947812892 | 0.1755809415319401 | 0.5281549741562520 | T | T | T |
| 0.3827832115649233 | 0.1755723647967933 | 0.6392357607314748 | T | T | T |
| 0.4528475907356265 | 0.3254703022547693 | 0.3613312858245457 | T | T | T |
| 0.4166203935785762 | 0.2255455207803146 | 0.4724932824533363 | T | T | T |
| 0.4404244966768805 | 0.2764955656404774 | 0.5281022739971827 | T | T | T |
| 0.4404543537204116 | 0.2765116790668440 | 0.6391374580531267 | T | T | T |
| 0.4529708289027406 | 0.3254951095756344 | 0.4724493808213517 | T | T | T |
| 0.4412121339912533 | 0.4066656545597613 | 0.6946761787084151 | T | T | T |
| 0.4529744536339924 | 0.3696793383597385 | 0.8614215345870220 | T | T | T |
| 0.4528979918355821 | 0.3697085947622257 | 0.9723448068709916 | T | T | T |
| 0.3831114711463661 | 0.4492219405221595 | 0.6943271344840207 | T | T | T |
| 0.4410653113083518 | 0.4066777201603257 | 0.8056487790348754 | T | T | T |
| 0.4173670285053047 | 0.4338832357683983 | 0.8611077257669101 | T | T | T |
| 0.4173784870037337 | 0.4339687010673825 | 0.9722785840877379 | T | T | T |
| 0.2930949051805790 | 0.4443621888528895 | 0.6940298205182609 | T | T | T |
| 0.3833172152364973 | 0.4496519870323878 | 0.8051813487723330 | T | T | T |
| 0.3411019898030473 | 0.4533194172609719 | 0.8607913061994821 | T | T | T |
| 0.3411585294957939 | 0.4534630219538935 | 0.9718120347083837 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1918008591404350 | 0.3959782903841506 | 0.6946432975261775 | T | T | T |
| 0.2933078580413147 | 0.4447584676194271 | 0.8051757634892122 | T | T | T |
| 0.2429151850150222 | 0.4253008297577445 | 0.8607017837947567 | T | T | T |
| 0.2428969652537980 | 0.4250347712939919 | 0.9714284034720058 | T | T | T |
| 0.1031439812170701 | 0.3092840317727326 | 0.6940145096238561 | T | T | T |
| 0.1920735604108686 | 0.3951895090952406 | 0.8046007680134738 | T | T | T |
| 0.1444706772316397 | 0.3552416582298615 | 0.8607260176945907 | T | T | T |
| 0.1446471381199141 | 0.3550604799260728 | 0.9714177742423817 | T | T | T |
| 0.0452534456649406 | 0.2083922041365092 | 0.6942771591566761 | T | T | T |
| 0.1028942921086766 | 0.3091703843282145 | 0.8051627611927428 | T | T | T |
| 0.0688981781958677 | 0.2592766986285214 | 0.8607805239519599 | T | T | T |
| 0.0687840333398249 | 0.2592592306112274 | 0.9717771294713153 | T | T | T |
| 0.0322852770863664 | 0.1150874329700344 | 0.6945566472842679 | T | T | T |
| 0.0449254235037798 | 0.2083356094596557 | 0.8051470460682556 | T | T | T |
| 0.0323323349033912 | 0.1592837376325655 | 0.8610232303945232 | T | T | T |
| 0.0322531866335575 | 0.1592994536364740 | 0.9722146106020012 | T | T | T |
| 0.0684039755663657 | 0.0512809479399547 | 0.6946612077880726 | T | T | T |
| 0.0322559967457507 | 0.1151417445912812 | 0.8055276434642255 | T | T | T |
| 0.0446603983269134 | 0.0784933502117251 | 0.8613437997003474 | T | T | T |
| 0.0446775194732986 | 0.0785785532203927 | 0.9722984265007980 | T | T | T |
| 0.1443537725416879 | 0.0313306557219238 | 0.6948293353350306 | T | T | T |
| 0.0685044192670554 | 0.0514005894900125 | 0.8057742698948956 | T | T | T |
| 0.1023910663435829 | 0.0354029928411465 | 0.8614302241644994 | T | T | T |
| 0.1024529062573681 | 0.0354766750591573 | 0.9724600946814209 | T | T | T |
| 0.2426149458450422 | 0.0594634060218076 | 0.6948610505231669 | T | T | T |
| 0.1443555222968028 | 0.0312887360931562 | 0.8057893328647584 | T | T | T |
| 0.1920585566480117 | 0.0394835597081267 | 0.8614900935353059 | T | T | T |
| 0.1920537309428974 | 0.0394406311601789 | 0.9725462245489538 | T | T | T |
| 0.3408750825781716 | 0.1295505417487550 | 0.6948637994007031 | T | T | T |
| 0.2425969995411806 | 0.0594450490927388 | 0.8059011692069399 | T | T | T |
| 0.2932170645112315 | 0.0900783211733835 | 0.8616013070386580 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2932228476904429 | 0.0900569047389561 | 0.9725440483545381 | T | T | T |
| 0.4166109859142438 | 0.2255245567103028 | 0.6948575904767248 | T | T | T |
| 0.3408900540582472 | 0.1295477885580481 | 0.8058930102576393 | T | T | T |
| 0.3828078686014235 | 0.1755263005260601 | 0.8614925602710015 | T | T | T |
| 0.3828706560863527 | 0.1755291758156217 | 0.9725557077293454 | T | T | T |
| 0.4528950846626061 | 0.3254754617794189 | 0.6947404293770431 | T | T | T |
| 0.4166400008309457 | 0.2254944639686459 | 0.8058050545645628 | T | T | T |
| 0.4403360993314676 | 0.2764401565931739 | 0.8614809930004789 | T | T | T |
| 0.4402516357713950 | 0.2764436658094050 | 0.9725045642755801 | T | T | T |
| 0.4527371561184731 | 0.3254198975717419 | 0.8058423738911868 | T | T | T |
| 0.1696273090815661 | 0.4484732692623807 | 0.4843039444581906 | T | T | T |
| 0.2113265212612307 | 0.5014031355337607 | 0.4379096757453564 | T | T | T |
| 0.2331456906465952 | 0.5201427248583825 | 0.4992059439788969 | T | T | T |

### 1.2.2 OOH adsorbate on N-doped CNT

OOH\_N-CNT(5,5) ### KPOINTS: 2x2x3 ### E= -473.10504767 eV

1.000000000000000

13.8564000000000007 -8.000000000000000 0.000000000000000

0.000000000000000 16.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.394779999999999

C N O H

59 1 2 1

Selective dynamics

Direct

0.5647281080975531 0.4267908226384622 0.0832798799913229 T T T

0.5647152356894428 0.4267848250470022 0.4160876106196335 T T T

0.5646107161554624 0.4266759801138147 0.7496724738332446 T T T

0.4839731181345001 0.5467395874903662 0.0831902888382703 T T T

0.4839895668604993 0.5467619227972749 0.4163421364699734 T T T

0.4847066303054746 0.5466121012943956 0.7497713351651450 T T T

0.3959714886824152 0.5488161268759751 0.0834277344937010 T T T

0.3959919380363749 0.5488300497635744 0.4161186566177117 T T T

0.3961370100642350 0.5467341424214055 0.7497947276716129 T T T

0.1148155634872372 0.3443138633307222 0.0831957592843478 T T T

0.1152334338870442 0.3443184483247969 0.4161603323038368 T T T

0.1011220927895466 0.3488603323970776 0.7493352466876111 T T T

0.0781449468559403 0.1546950668577542 0.0828858519620781 T T T

0.0781032676310698 0.1546332861146929 0.4164569831356610 T T T

0.0776989142122260 0.1549278141542934 0.7497502487654258 T T T

0.1174447866342985 0.0923121057799007 0.0830267512677074 T T T

0.1173947940686944 0.0922462485005312 0.4164183358464689 T T T

0.1175838715186807 0.0930507694228365 0.7497832631660607 T T T

0.2868678910611778 0.0821354840516675 0.0831626214589808 T T T

0.2868593561524828 0.0821170388750337 0.4163030169144390 T T T

0.2869875539482138 0.0822979186351257 0.7497294086321689 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3894268471512151 | 0.1387435366981743 | 0.0830579713375993 | T | T | T |
| 0.3894180580909959 | 0.1387248642408924 | 0.4163078536385653 | T | T | T |
| 0.3894753726939050 | 0.1390111356330273 | 0.7496847364748640 | T | T | T |
| 0.5424212337536786 | 0.3287980541741679 | 0.0830880295642736 | T | T | T |
| 0.5424207871466649 | 0.3287907567392402 | 0.4162239174665072 | T | T | T |
| 0.5427000195091075 | 0.3288093782783802 | 0.7496436529884333 | T | T | T |
| 0.1934590474293720 | 0.4420090364502980 | 0.0816997011173087 | T | T | T |
| 0.1936132488733713 | 0.4420564214800066 | 0.4177052359160781 | T | T | T |
| 0.2429261833638926 | 0.4818523240239158 | 0.2496901236996135 | T | T | T |
| 0.2437181921282741 | 0.4781751775553664 | 0.5846902334930827 | T | T | T |
| 0.2436500834165305 | 0.4780313428719757 | 0.9147731920615542 | T | T | T |
| 0.5597204558257366 | 0.4692276333979152 | 0.2496949183782475 | T | T | T |
| 0.5596370395890182 | 0.4690211745653540 | 0.5829032531479160 | T | T | T |
| 0.5596451437780963 | 0.4690143696054175 | 0.9164788530013822 | T | T | T |
| 0.1501013163358985 | 0.0735807194733002 | 0.2497337266232879 | T | T | T |
| 0.1506073891559128 | 0.0742781888799526 | 0.5833068119288288 | T | T | T |
| 0.1506078188655137 | 0.0742686871283876 | 0.9161988220036512 | T | T | T |
| 0.2365123408553155 | 0.0683900793227025 | 0.2497411799695871 | T | T | T |
| 0.2366452773353209 | 0.0689193635518070 | 0.5832088857730822 | T | T | T |
| 0.2366411215044149 | 0.0688795968177985 | 0.9162649670800699 | T | T | T |
| 0.5184634131367544 | 0.5302718824323200 | 0.2497554355029375 | T | T | T |
| 0.5186829220529516 | 0.5299727814831706 | 0.5828235820703904 | T | T | T |
| 0.5186505171322343 | 0.5299241141218836 | 0.9166932353789796 | T | T | T |
| 0.0908675339029099 | 0.2927005660420475 | 0.2497407647355206 | T | T | T |
| 0.0886058920505957 | 0.2925836529293204 | 0.5804853142709727 | T | T | T |
| 0.0879133337617565 | 0.2925129724496842 | 0.9186376430660962 | T | T | T |
| 0.4376431599506500 | 0.1796632943042043 | 0.2496805558985243 | T | T | T |
| 0.4377640889742955 | 0.1799079345010573 | 0.5829970090502502 | T | T | T |
| 0.4377881106013003 | 0.1799016671891524 | 0.9163401057664334 | T | T | T |
| 0.5155241121150704 | 0.2767341788177324 | 0.2496596572941092 | T | T | T |
| 0.5158003048594473 | 0.2767552526432173 | 0.5830263132209343 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5158236905737106 | 0.2767597683091189 | 0.9162771670472465 | T | T | T |
| 0.0717499062886797 | 0.1957566387916164 | 0.2497203155257876 | T | T | T |
| 0.0736324006387906 | 0.1980803311273071 | 0.5831628730304255 | T | T | T |
| 0.0733830585213740 | 0.1979672102935879 | 0.9161684751951081 | T | T | T |
| 0.3458310755822230 | 0.5360469884159154 | 0.2497435039079256 | T | T | T |
| 0.3456404613768207 | 0.5329092855420238 | 0.5838788070652895 | T | T | T |
| 0.3455858550553713 | 0.5328258212243908 | 0.9156991887671095 | T | T | T |
| 0.1968252883401995 | 0.4409477030453550 | 0.7496799792869301 | T | T | T |
| 0.0368498862373763 | 0.3918727312440520 | 0.7480228574755136 | T | T | T |
| 0.9360377821179539 | 0.3127239961655537 | 0.7374821942148189 | T | T | T |
| 0.9189599456547062 | 0.3037954531525198 | 0.8652862934393644 | T | T | T |

OOH\_N-CNT(6,6) ### KPOINTS: 2x2x3 ### E= -569.32602591 eV

1.000000000000000

14.7224000000000004 -8.500000000000000 0.000000000000000

0.0000000000000000 17.000000000000000 0.000000000000000

0.0000000000000000 0.000000000000000 7.3992800000000001

C N O H

71 1 2 1

Selective dynamics

Direct

0.6147661959491845 0.4959844987709034 0.0834238202969639 T T T

0.6148170221800557 0.4960290692477829 0.4165496612902370 T T T

0.6151573243054803 0.4961414638574620 0.7500192304452727 T T T

0.5293916474544856 0.6010745816903417 0.0831410999028298 T T T

0.5294699290018240 0.6010814652673299 0.4166986939678021 T T T

0.5283934680330955 0.6003182491871681 0.7499695575390644 T T T

0.4493076577698631 0.6076382622677636 0.0829884115955069 T T T

0.4493529283474721 0.6075360461089676 0.4166881472794918 T T T

0.4490690601681825 0.6080418522169115 0.7499295086253310 T T T

0.1719979087908417 0.4538620162208834 0.0819803675034223 T T T

0.1719857713017349 0.4537847557628311 0.4177579690265134 T T T

0.0689363847129940 0.2627669794366692 0.0834991094139099 T T T

0.0689440132135402 0.2627718148415121 0.4164520334829244 T T T

0.0712048722888450 0.2625088260192632 0.7500091628966502 T T T

0.0599815721559570 0.1748949555273470 0.0833480032278113 T T T

0.0599445004657209 0.1748710547295786 0.4166929726499605 T T T

0.0602684384936610 0.1743066532506426 0.7500281489074612 T T T

0.1385334742650346 0.0633298416874805 0.0836695157653222 T T T

0.1385382386099626 0.0633385582169531 0.4164404566969645 T T T

0.1385639855720176 0.0634079720591394 0.7500636494215852 T T T

0.2180991038760527 0.0556030123178619 0.0834631331887897 T T T

0.2180991182811541 0.0556052514389675 0.4166595851230656 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2180669092284271 | 0.0555980513924401 | 0.7500751408535046 | T | T | T |
| 0.4087156649218380 | 0.1394104393312239 | 0.0834325898431759 | T | T | T |
| 0.4087167113681492 | 0.1394052173800598 | 0.4166809135365577 | T | T | T |
| 0.4086995613970708 | 0.1394748182015917 | 0.7500655342071739 | T | T | T |
| 0.4962440397153803 | 0.2186496741946644 | 0.0834611345322488 | T | T | T |
| 0.4962467693712791 | 0.2186515526197124 | 0.4166461889742932 | T | T | T |
| 0.4963291003078459 | 0.2186054209550350 | 0.7500534275153623 | T | T | T |
| 0.6070756041839637 | 0.4087574868450847 | 0.0834691345603243 | T | T | T |
| 0.6070881544355466 | 0.4087818912885716 | 0.4165661087870610 | T | T | T |
| 0.6071659836042771 | 0.4087829570202602 | 0.7500324859420038 | T | T | T |
| 0.2603756284815962 | 0.5333458312779688 | 0.0831191439744291 | T | T | T |
| 0.2604243177979500 | 0.5331160921021417 | 0.4163157990502496 | T | T | T |
| 0.2533773037982587 | 0.5449169099217180 | 0.7496870947504500 | T | T | T |
| 0.0676331513726487 | 0.1369531791982108 | 0.2500212551946636 | T | T | T |
| 0.0677933271356243 | 0.1366735830117146 | 0.5830692390532544 | T | T | T |
| 0.0678074322180171 | 0.1366848934469702 | 0.9170015843632405 | T | T | T |
| 0.1072827802511312 | 0.0803065306637535 | 0.2500469845374818 | T | T | T |
| 0.1072908055451899 | 0.0801893155399395 | 0.5831901748553363 | T | T | T |
| 0.1072776856942204 | 0.0801753090029572 | 0.9169117151751318 | T | T | T |
| 0.5623224186435335 | 0.5863330493129028 | 0.2499113486818251 | T | T | T |
| 0.5616248025856256 | 0.5853916438156815 | 0.5834867128255047 | T | T | T |
| 0.5616085121892754 | 0.5853981964486185 | 0.9164655921883276 | T | T | T |
| 0.1359005857013006 | 0.4070509853997379 | 0.2498486596366647 | T | T | T |
| 0.1394452042527517 | 0.4066193369386109 | 0.5846659423722590 | T | T | T |
| 0.1394327440385472 | 0.4066539668839891 | 0.9151878709050474 | T | T | T |
| 0.2642865499948857 | 0.0649253853145711 | 0.2500603789312268 | T | T | T |
| 0.2642950939181581 | 0.0649639643599718 | 0.5835054057827835 | T | T | T |
| 0.2642927092929465 | 0.0649617768004416 | 0.9166336195257201 | T | T | T |
| 0.3607813866201089 | 0.1074549708234705 | 0.2500556393770985 | T | T | T |
| 0.3606863897451620 | 0.1075692659032636 | 0.5834826651169686 | T | T | T |
| 0.3606800169151456 | 0.1075686839629124 | 0.9166503774324847 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0837812195462323 | 0.3104410138039186 | 0.2499683431639966 | T | T | T |
| 0.0870335867957766 | 0.3107133669460949 | 0.5840867553652155 | T | T | T |
| 0.0870225259388378 | 0.3107267694836385 | 0.9158782037131498 | T | T | T |
| 0.3084802932889668 | 0.5621714311970825 | 0.2497209117959542 | T | T | T |
| 0.3080996307818852 | 0.5640971650582269 | 0.5807508770195605 | T | T | T |
| 0.3080149561391254 | 0.5644154014659281 | 0.9188454968752948 | T | T | T |
| 0.5340119679349012 | 0.2644267993055473 | 0.2500475369158560 | T | T | T |
| 0.5339396140625400 | 0.2644556512298887 | 0.5834832828508218 | T | T | T |
| 0.5339492320130842 | 0.2644411251998882 | 0.9166120398891852 | T | T | T |
| 0.5904396281576887 | 0.3606620102833952 | 0.2500395863536373 | T | T | T |
| 0.5901135899237377 | 0.3605678526897538 | 0.5833900281342856 | T | T | T |
| 0.5901323276849653 | 0.3605511891121204 | 0.9166646912503399 | T | T | T |
| 0.6055890691967589 | 0.5330088488378006 | 0.2499587809645203 | T | T | T |
| 0.6052776399725677 | 0.5327156601388112 | 0.5834864479069599 | T | T | T |
| 0.6052439434074859 | 0.5327010918395203 | 0.9165211118526021 | T | T | T |
| 0.4042824211971161 | 0.6001769692950863 | 0.2498216667789565 | T | T | T |
| 0.4026381880371561 | 0.5987344083642430 | 0.5833206751513145 | T | T | T |
| 0.4025084171850973 | 0.5988873004738272 | 0.9163667344206374 | T | T | T |
| 0.1737200020738397 | 0.4511645381363327 | 0.7499210912086828 | T | T | T |
| 0.2717345979320510 | 0.6948125151003846 | 0.7527531559009210 | T | T | T |
| 0.2035540878895722 | 0.5974440746348083 | 0.7484802441661351 | T | T | T |
| 0.2766131008776234 | 0.7094372579217959 | 0.6244102375932382 | T | T | T |

OOH\_N-CNT(7,7) ### KPOINTS: 1x1x3 ### E= -665.15190614 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C N O H

83 1 2 1

Selective dynamics

Direct

0.1810396860537605 0.0472750510181762 0.0848514710856177 T T T

0.2635905893084743 0.0549659143201763 0.0848865401938020 T T T

0.0700241382815668 0.1152841160354630 0.0845864198492281 T T T

0.4445224358073474 0.1497569417064167 0.0849832912254460 T T T

0.0510405564246507 0.1829539097230007 0.0845020325441937 T T T

0.5259939946080237 0.2260201602716649 0.0849219861601783 T T T

0.0911706601948532 0.3558469581489467 0.0856796506351174 T T T

0.6391654624793107 0.4050596220863459 0.0849621428346946 T T T

0.1442111010727724 0.4461441972428949 0.0863031800168579 T T T

0.6594702320997308 0.4921653936481431 0.0849583985947981 T T T

0.3023403393657552 0.5982050818650290 0.0831788462081256 T T T

0.6160472368222181 0.6224882054267897 0.0850136523522426 T T T

0.3926721262987839 0.6383282757444029 0.0854824411039043 T T T

0.5571851082291319 0.6532868450824011 0.0851109950808440 T T T

0.0514736832907370 0.2227766452968614 0.2514581978088543 T T T

0.5619120124080332 0.2689272891947621 0.2515703872506945 T T T

0.0725208137321171 0.3098264543811592 0.2515137587792353 T T T

0.6191946425289089 0.3591289037868905 0.2515888138699169 T T T

0.1451939884560844 0.0543425444428180 0.2515130168213416 T T T

0.3087234400065762 0.0696394457387066 0.2515448161915980 T T T

0.0893261461422373 0.0888175929627657 0.2514666317638691 T T T

0.3999508518648825 0.1175780424198421 0.2515661849826814 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6591078287452778 | 0.5318759912664681 | 0.2515738212831242 | T | T | T |
| 0.2504692105402181 | 0.5774513504369577 | 0.2525808541999825 | T | T | T |
| 0.6372830175046958 | 0.5976530113823181 | 0.2515565638254330 | T | T | T |
| 0.4381389565796101 | 0.6523202163395726 | 0.2517530898375379 | T | T | T |
| 0.5200762179316065 | 0.6589792166376094 | 0.2516201200387879 | T | T | T |
| 0.1810297505073294 | 0.0472814691099127 | 0.4182036351098831 | T | T | T |
| 0.2636028574615757 | 0.0550143912264211 | 0.4182270951002582 | T | T | T |
| 0.0699854133494494 | 0.1152587743361148 | 0.4182981942773851 | T | T | T |
| 0.4445197433490834 | 0.1497795390361312 | 0.4181636769316991 | T | T | T |
| 0.0510879327093862 | 0.1829775901630318 | 0.4183628747258249 | T | T | T |
| 0.5259951112285519 | 0.2260265606179014 | 0.4182293639449061 | T | T | T |
| 0.0910780888677201 | 0.3558295379054053 | 0.4173773275649419 | T | T | T |
| 0.6391461568812065 | 0.4050504557401030 | 0.4182408724816522 | T | T | T |
| 0.1440502758700307 | 0.4461006785727690 | 0.4169200617980756 | T | T | T |
| 0.6594501984549498 | 0.4921496578312231 | 0.4182071262269851 | T | T | T |
| 0.3025942895483403 | 0.5971961835466145 | 0.4210174850989282 | T | T | T |
| 0.6159752101995370 | 0.6224148358444170 | 0.4181103255018755 | T | T | T |
| 0.3926734512505624 | 0.6377838947647364 | 0.4182545466872560 | T | T | T |
| 0.5571462418063806 | 0.6532208419291368 | 0.4181371258509918 | T | T | T |
| 0.1450524355414293 | 0.0541574672731449 | 0.5849826477177800 | T | T | T |
| 0.3087347520003955 | 0.0696721072676377 | 0.5849584716747138 | T | T | T |
| 0.0890964918742986 | 0.0885783269909364 | 0.5850765062047888 | T | T | T |
| 0.3999224392893945 | 0.1175455125451762 | 0.5849080612497322 | T | T | T |
| 0.0513598086236259 | 0.2232197331779402 | 0.5847292153731063 | T | T | T |
| 0.5618466734452698 | 0.2689780803876176 | 0.5850075850081448 | T | T | T |
| 0.0708877193770684 | 0.3102255694925058 | 0.5849141755139882 | T | T | T |
| 0.6189132963636707 | 0.3591401528939458 | 0.5850529445069267 | T | T | T |
| 0.1755845846061864 | 0.4902657226391545 | 0.5837328767871075 | T | T | T |
| 0.6592355510567455 | 0.5319263638938539 | 0.5849581267992576 | T | T | T |
| 0.2582229010591856 | 0.5661556385347229 | 0.5850743096879070 | T | T | T |
| 0.6371450959720636 | 0.5975299845330214 | 0.5849016193844760 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4381000557159876 | 0.6511421799387058 | 0.5849040452222597 | T | T | T |
| 0.5205590899555457 | 0.6589395169979705 | 0.5848929022417877 | T | T | T |
| 0.0697550053144708 | 0.1151665728138708 | 0.7514735296882770 | T | T | T |
| 0.0508724956398003 | 0.1831557376718746 | 0.7514451848880586 | T | T | T |
| 0.5261457349965205 | 0.2259771483415024 | 0.7515974335863300 | T | T | T |
| 0.0885131283284084 | 0.3557119973319443 | 0.7515701444786944 | T | T | T |
| 0.6393342740771836 | 0.4051110346183201 | 0.7516017344619811 | T | T | T |
| 0.1412363029639286 | 0.4464965736266338 | 0.7516437362660334 | T | T | T |
| 0.1809731034986006 | 0.0471909405963349 | 0.7515320469444012 | T | T | T |
| 0.2636553902829614 | 0.0550734882138206 | 0.7515664518389753 | T | T | T |
| 0.4445412412385141 | 0.1496884405030725 | 0.7515850361588459 | T | T | T |
| 0.6598973331680469 | 0.4924199752871497 | 0.7515766867603941 | T | T | T |
| 0.3030302444086105 | 0.5954197005169144 | 0.7518723363998472 | T | T | T |
| 0.6160016417721387 | 0.6223207243033537 | 0.7515885168361547 | T | T | T |
| 0.3939594971271740 | 0.6386848464447430 | 0.7517878203945052 | T | T | T |
| 0.5572731243086119 | 0.6534474662563451 | 0.7516972718862567 | T | T | T |
| 0.1451008738482043 | 0.0542016063672140 | 0.9180453101328980 | T | T | T |
| 0.3087299467015276 | 0.0696476054847030 | 0.9181745761335829 | T | T | T |
| 0.0891600153804839 | 0.0886326972993877 | 0.9178502415902551 | T | T | T |
| 0.3999206209470241 | 0.1175428130885841 | 0.9182539415644178 | T | T | T |
| 0.0512608013260907 | 0.2231824872632337 | 0.9181640113544783 | T | T | T |
| 0.5618255775631779 | 0.2689949844690651 | 0.9181825526542882 | T | T | T |
| 0.0708856678088177 | 0.3102206283549894 | 0.9181432312541862 | T | T | T |
| 0.6189142531838643 | 0.3591491654575633 | 0.9181792674280932 | T | T | T |
| 0.1756314380052013 | 0.4904014649844494 | 0.9196099250990283 | T | T | T |
| 0.6592849513239093 | 0.5319621935077904 | 0.9182015834642561 | T | T | T |
| 0.2580650553448066 | 0.5666412410420614 | 0.9187812856739540 | T | T | T |
| 0.6372065896975164 | 0.5975786580619983 | 0.9182150434091436 | T | T | T |
| 0.4380765252228108 | 0.6513098909788431 | 0.9187332142674915 | T | T | T |
| 0.5205034401099928 | 0.6589363184543233 | 0.9185064414747824 | T | T | T |
| 0.1770882664035262 | 0.4879803043747051 | 0.2516371154183041 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2621036365866834 | 0.7164765370208703 | 0.2849470163985120 | T | T | T |
| 0.2006853349598902 | 0.6247265123472313 | 0.2567273673184305 | T | T | T |
| 0.2683883953191544 | 0.7379521011202349 | 0.1619594415643939 | T | T | T |

OOH\_N-CNT(8,8) #### KPOINTS: 1x1x3 #### E= -760.70100066 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C N O H

95 1 2 1

Selective dynamics

Direct

0.2521008959129992 0.0403667862207413 0.0839924548216201 T T T

0.1158216923398571 0.0498248419539354 0.0839685491481151 T T T

0.3328476510963644 0.0679997486612471 0.0840368491649302 T T T

0.0712019046488661 0.0871780043345854 0.0839335920949507 T T T

0.4929799202632975 0.1762904747182458 0.0841065792589798 T T T

0.0433519405505761 0.2124026632534198 0.0838125088977288 T T T

0.5618018580712463 0.2494399799630128 0.0840455451798089 T T T

0.0601514167036403 0.2902755843512699 0.0837443185112013 T T T

0.6543434791812681 0.4120953986400019 0.0839635824327871 T T T

0.1453888090567446 0.4525255220061405 0.0839663775575364 T T T

0.6709190026924527 0.4900072447705661 0.0839990956005892 T T T

0.2133636656238699 0.5270643517979802 0.0826958621598036 T T T

0.6382806686870450 0.6121440594441263 0.0839975462534929 T T T

0.3742757930222298 0.6299174975287302 0.0839691073205364 T T T

0.5918339521242320 0.6475662018528989 0.0840421531886092 T T T

0.4548465670928794 0.6561957758432806 0.0837719339986959 T T T

0.2136909204024166 0.0344335136771934 0.2506617894657260 T T T

0.1449635600933827 0.0390366770094303 0.2506417708858391 T T T

0.3741901048516908 0.0890955349883316 0.2506868449745880 T T T

0.4546617255626794 0.1435824354700109 0.2506927370323334 T T T

0.0421315677308486 0.1760667590765920 0.2506111438786625 T T T

0.6709978798526871 0.5258547778103584 0.2506350498647171 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2521765258980492 | 0.5590687128590452 | 0.2505557756973751 | T | T | T |
| 0.6544946393448612 | 0.5872655797635460 | 0.2506007503217745 | T | T | T |
| 0.5622032709743927 | 0.6578213981422907 | 0.2505297470572669 | T | T | T |
| 0.0561860150908268 | 0.1130446661947198 | 0.2505728775011307 | T | T | T |
| 0.5915026029392950 | 0.2891646652194717 | 0.2507181742845946 | T | T | T |
| 0.0748564104469762 | 0.3305799238710006 | 0.2506450299973124 | T | T | T |
| 0.6380837034742278 | 0.3710457800041265 | 0.2506902564248501 | T | T | T |
| 0.1183259371526139 | 0.4123931853963154 | 0.2506594247277621 | T | T | T |
| 0.3331366978589389 | 0.6108029043554595 | 0.2505612743700895 | T | T | T |
| 0.4932603933479139 | 0.6621462929027671 | 0.2505205705409614 | T | T | T |
| 0.2521022559247511 | 0.0403772832405478 | 0.4172623476016704 | T | T | T |
| 0.1158552806268540 | 0.0498725213353356 | 0.4172701555709874 | T | T | T |
| 0.3328366541830665 | 0.0679985101062099 | 0.4172765959073698 | T | T | T |
| 0.0711800198026317 | 0.0871769696750388 | 0.4173034573857792 | T | T | T |
| 0.4929640493163161 | 0.1762765401534703 | 0.4173647740630292 | T | T | T |
| 0.0431885353465601 | 0.2123518366272629 | 0.4175494683904503 | T | T | T |
| 0.5618083702564376 | 0.2494445747985579 | 0.4174425015503292 | T | T | T |
| 0.0598690740121214 | 0.2902237975482660 | 0.4176176451879965 | T | T | T |
| 0.6543490749739489 | 0.4121082679741100 | 0.4173626203135847 | T | T | T |
| 0.1450835453020814 | 0.4526258521390439 | 0.4174308584465714 | T | T | T |
| 0.6709281455742278 | 0.4900109697587962 | 0.4172607625990607 | T | T | T |
| 0.2132748553024439 | 0.5270976980694775 | 0.4184938862145034 | T | T | T |
| 0.6383093749382875 | 0.6121497948426609 | 0.4171716860326702 | T | T | T |
| 0.3742685147973301 | 0.6299388947221585 | 0.4171346057646865 | T | T | T |
| 0.5917994707265763 | 0.6475139141596467 | 0.4169994062973825 | T | T | T |
| 0.4548601043145921 | 0.6562196252096252 | 0.4172102487292588 | T | T | T |
| 0.2136289937818531 | 0.0342704823681864 | 0.5839689998196326 | T | T | T |
| 0.1450880484030833 | 0.0390571066961118 | 0.5838915505920634 | T | T | T |
| 0.3742403551444982 | 0.0892143823174710 | 0.5839385445754199 | T | T | T |
| 0.0565309444151517 | 0.1133590819472101 | 0.5840171732543572 | T | T | T |
| 0.4546644915425713 | 0.1435983406239429 | 0.5840324517169394 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0426016285562010 | 0.1763629790151118 | 0.5841028644034211 | T | T | T |
| 0.5914820089208020 | 0.2892243419987485 | 0.5841629294582079 | T | T | T |
| 0.0750791941570475 | 0.3318150407485365 | 0.5841947892490817 | T | T | T |
| 0.6380779237360231 | 0.3710433864987185 | 0.5840892797149368 | T | T | T |
| 0.1157846306566385 | 0.4132716659218935 | 0.5817054840557202 | T | T | T |
| 0.6708956859071052 | 0.5258311523795871 | 0.5838855367368476 | T | T | T |
| 0.2525214151800326 | 0.5565961413234233 | 0.5850803147597429 | T | T | T |
| 0.6545210147746779 | 0.5873132209425700 | 0.5839054663834605 | T | T | T |
| 0.3331614764595184 | 0.6085036226928425 | 0.5846100909846286 | T | T | T |
| 0.5620992701707523 | 0.6575253771877561 | 0.5837606241886693 | T | T | T |
| 0.4933232208648163 | 0.6617570897945082 | 0.5836194185546310 | T | T | T |
| 0.2520639477848425 | 0.0402886308269204 | 0.7506228934953939 | T | T | T |
| 0.1160827434354177 | 0.0500563899942893 | 0.7506203158125492 | T | T | T |
| 0.3328762553105588 | 0.0680947781706378 | 0.7506423542099814 | T | T | T |
| 0.4929420276158955 | 0.1762174102875232 | 0.7507305059696974 | T | T | T |
| 0.0437493161436063 | 0.2131276647895392 | 0.7506476134344640 | T | T | T |
| 0.1351778148697794 | 0.4600510352473908 | 0.7511382155591867 | T | T | T |
| 0.6383221276103049 | 0.6121740919560370 | 0.7506133797107016 | T | T | T |
| 0.5916867050270047 | 0.6473463717822957 | 0.7505198553200996 | T | T | T |
| 0.0715427854527942 | 0.0874145412666264 | 0.7505979760361726 | T | T | T |
| 0.5617721046634032 | 0.2494238778896519 | 0.7507392280755713 | T | T | T |
| 0.0591239663390362 | 0.2903837420397714 | 0.7506781547128673 | T | T | T |
| 0.6543716357236489 | 0.4121168936949826 | 0.7506837697560380 | T | T | T |
| 0.6708336909367284 | 0.4900042109067069 | 0.7506381533480793 | T | T | T |
| 0.3747460021076280 | 0.6284507161217752 | 0.7505442760925755 | T | T | T |
| 0.4551133481507517 | 0.6558167962428644 | 0.7504554409497511 | T | T | T |
| 0.2136417212439933 | 0.0342971339838033 | 0.9173130263602068 | T | T | T |
| 0.1451076388950102 | 0.0390509497846179 | 0.9173610482221035 | T | T | T |
| 0.3742378934873379 | 0.0892261137822781 | 0.9173844736466771 | T | T | T |
| 0.0566094362522625 | 0.1134059291373324 | 0.9171061537756301 | T | T | T |
| 0.4546631091790967 | 0.1435982248660816 | 0.9174231164351079 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0427797107542396 | 0.1764512823696691 | 0.9171075911489551 | T | T | T |
| 0.5914825173328828 | 0.2892273594132074 | 0.9173382951001298 | T | T | T |
| 0.0755942972226773 | 0.3318642531874813 | 0.9172161319570473 | T | T | T |
| 0.6380787810566153 | 0.3710433428265452 | 0.9172748253382661 | T | T | T |
| 0.1164194163719242 | 0.4130917861555466 | 0.9199509151049480 | T | T | T |
| 0.6708815117735156 | 0.5258256125241519 | 0.9173094192604887 | T | T | T |
| 0.2525868305326844 | 0.5566234055704855 | 0.9159976168670443 | T | T | T |
| 0.6545007887523646 | 0.5872850089666001 | 0.9173194966940664 | T | T | T |
| 0.3331799721964229 | 0.6084864004610944 | 0.9164663684555103 | T | T | T |
| 0.5621374489461931 | 0.6576002886191509 | 0.9173086927253546 | T | T | T |
| 0.4933297132639374 | 0.6617625263152341 | 0.9173423780722545 | T | T | T |
| 0.2154734131987687 | 0.5260114390230314 | 0.7506355354402096 | T | T | T |
| 0.0096670713485471 | 0.4502336489533440 | 0.7700994348113569 | T | T | T |
| 0.0928229459255207 | 0.5054646499200645 | 0.7538058097409752 | T | T | T |
| 0.9940925109362664 | 0.4449260880256034 | 0.6438417272430688 | T | T | T |

OOH\_N-CNT(9,9) #### KPOINTS: 1x1x3 #### E= -856.12425541 eV

1.0000000000000000

18.1865334800000014 -10.5000000000000000 0.0000000000000000

0.0000000000000000 21.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4005503900000003

C N O H

107 1 2 1

Selective dynamics

Direct

0.1975855526911425 0.0286287210197086 0.0832000622414196 T T T

0.1352728176531283 0.0383409135782853 0.0832540240916598 T T T

0.3469205743570196 0.0652854402282742 0.0831997916488112 T T T

0.4249568623496627 0.1085292686013674 0.0830939924831354 T T T

0.0525021257766110 0.1111930444111398 0.0832261830133312 T T T

0.0359433659304195 0.1690454286901582 0.0832088591313593 T T T

0.5683783791002719 0.2328916539502633 0.0830129704573538 T T T

0.6255494747075879 0.3076727546512751 0.0829910645134060 T T T

0.0531222011043368 0.3125346417925159 0.0829795115831814 T T T

0.0838593867014806 0.3898167255577022 0.0856111783134916 T T T

0.6951749071046219 0.4631226900720092 0.0830840703757593 T T T

0.7050335564009238 0.5352441366208193 0.0831412234888539 T T T

0.2011438824810305 0.5353945648539215 0.0821347530115640 T T T

0.2736812864572198 0.5960885491805005 0.0826782819051318 T T T

0.6722101031595036 0.6506339123723556 0.0832130667720383 T T T

0.6299918252599623 0.6865027022192929 0.0832786671069166 T T T

0.4289304012623371 0.6829868278178163 0.0837075320544703 T T T

0.5042623715123202 0.7028284341141759 0.0836069908504874 T T T

0.2326991852660826 0.0308477561368951 0.2498916458100957 T T T

0.3077942622621836 0.0494409973523098 0.2498823591054592 T T T

0.4632731671314118 0.1354817840335353 0.2497961979283572 T T T

0.5353123416251538 0.1978733018397864 0.2497432688345843 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0431826551672942 | 0.2739185975542265 | 0.2494601666159581 | T | T | T |
| 0.1087678182704586 | 0.4280532537105119 | 0.2497667437430439 | T | T | T |
| 0.1667344525745884 | 0.5028948450749340 | 0.2490914749174364 | T | T | T |
| 0.3114868845006514 | 0.6235615524849152 | 0.2501787965480370 | T | T | T |
| 0.3895637021431981 | 0.6667662053060442 | 0.2500513270604315 | T | T | T |
| 0.1087034083118283 | 0.0502062314005488 | 0.2499111537135153 | T | T | T |
| 0.0672995132096193 | 0.0869594323201897 | 0.2498890906866399 | T | T | T |
| 0.0342834958398422 | 0.2022300288012930 | 0.2496568333998473 | T | T | T |
| 0.6490164295076755 | 0.3467529427257618 | 0.2497032853432849 | T | T | T |
| 0.6838940692275400 | 0.4248193273792065 | 0.2497687515878968 | T | T | T |
| 0.7034122399930016 | 0.5684674928342187 | 0.2499022342315640 | T | T | T |
| 0.6871399599185215 | 0.6265846561064208 | 0.2499727512361589 | T | T | T |
| 0.6031243707884089 | 0.6979205611416653 | 0.2500810177419428 | T | T | T |
| 0.5397881780647329 | 0.7060243860652121 | 0.2502748947147829 | T | T | T |
| 0.1974906640101333 | 0.0285091359761778 | 0.4165381247498424 | T | T | T |
| 0.1351077618800802 | 0.0381613953350115 | 0.4165796461911920 | T | T | T |
| 0.3469333068840512 | 0.0653092585996418 | 0.4164885775502868 | T | T | T |
| 0.4249824623347976 | 0.1085424703624981 | 0.4164473449184366 | T | T | T |
| 0.0526630232130659 | 0.1112410373081148 | 0.4165674045199287 | T | T | T |
| 0.0361833112152674 | 0.1691849052732660 | 0.4165283078542911 | T | T | T |
| 0.5683760222813866 | 0.2328214640140684 | 0.4164304311514174 | T | T | T |
| 0.6255572235976621 | 0.3076711396890934 | 0.4164194611835828 | T | T | T |
| 0.0538234698866897 | 0.3115016328740443 | 0.4167056042795712 | T | T | T |
| 0.0873271376207910 | 0.3891203244077449 | 0.4166668241077076 | T | T | T |
| 0.6952832697355807 | 0.4631443214127264 | 0.4164222194876379 | T | T | T |
| 0.7050210064910810 | 0.5352504491660123 | 0.4164521463345315 | T | T | T |
| 0.2003195548803093 | 0.5372551488560923 | 0.4168623926048069 | T | T | T |
| 0.2732014605385710 | 0.5979212367628337 | 0.4168620342312052 | T | T | T |
| 0.6724985529912497 | 0.6509013021986324 | 0.4165669532627946 | T | T | T |
| 0.6302489062701021 | 0.6867732942348334 | 0.4166389351276154 | T | T | T |
| 0.4286879964116778 | 0.6830233948624300 | 0.4168249892587357 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5042054916268801 | 0.7028982084279347 | 0.4167583466578008 | T | T | T |
| 0.2327357149434586 | 0.0308876686781892 | 0.5831533845911225 | T | T | T |
| 0.3078156168961717 | 0.0494292283932121 | 0.5831263309252157 | T | T | T |
| 0.1086543609333021 | 0.0501605995862393 | 0.5832576059839362 | T | T | T |
| 0.0672557642927605 | 0.0869127761274077 | 0.5833162477264633 | T | T | T |
| 0.4632639027362676 | 0.1354819831462729 | 0.5831034594311065 | T | T | T |
| 0.5353022897419699 | 0.1978609447897484 | 0.5830816083113566 | T | T | T |
| 0.0343931350305146 | 0.2021498365524765 | 0.5834977125011429 | T | T | T |
| 0.0434731397945998 | 0.2737998051323085 | 0.5836879866672074 | T | T | T |
| 0.6490281342341384 | 0.3467740556628012 | 0.5831303556557407 | T | T | T |
| 0.6838977305657871 | 0.4248208180020284 | 0.5830837926679890 | T | T | T |
| 0.1088928994493956 | 0.4280224584370211 | 0.5834469755489978 | T | T | T |
| 0.1661957147542083 | 0.5031723821833347 | 0.5849366290057233 | T | T | T |
| 0.7033868968911088 | 0.5684592391937503 | 0.5831036508011215 | T | T | T |
| 0.6871596979651692 | 0.6265851726443582 | 0.5831573959608443 | T | T | T |
| 0.3114453939637231 | 0.6235678941066420 | 0.5835713511925240 | T | T | T |
| 0.3895357945240824 | 0.6667040094190366 | 0.5836214336295187 | T | T | T |
| 0.6031216725924191 | 0.6979414999768444 | 0.5832490322789345 | T | T | T |
| 0.5397715031000266 | 0.7060056740430776 | 0.5831914008911129 | T | T | T |
| 0.1976138016545994 | 0.0286813926472603 | 0.7498629878653567 | T | T | T |
| 0.1352686597301499 | 0.0383347696433944 | 0.7498732549563529 | T | T | T |
| 0.3469172212109983 | 0.0652678614144658 | 0.7498162756418700 | T | T | T |
| 0.4249448648523820 | 0.1085305800214099 | 0.7498217919830524 | T | T | T |
| 0.5683736642088676 | 0.2328828960471719 | 0.7497910937565986 | T | T | T |
| 0.0536259175548682 | 0.3122796023545237 | 0.7502411455965803 | T | T | T |
| 0.0845175800459259 | 0.3892843356718951 | 0.7471504721482171 | T | T | T |
| 0.2007667352514468 | 0.5357500081817077 | 0.7518201970315721 | T | T | T |
| 0.2735508858418710 | 0.5962121786053748 | 0.7511064537705495 | T | T | T |
| 0.4289092021914641 | 0.6829487889383614 | 0.7499051724136092 | T | T | T |
| 0.0525135489192462 | 0.1111779508648846 | 0.7500670259555980 | T | T | T |
| 0.0360494192352171 | 0.1690665478807963 | 0.7501265546215461 | T | T | T |

|                     |                    |                    |   |   |   |
|---------------------|--------------------|--------------------|---|---|---|
| 0.6255567372034898  | 0.3076821943073863 | 0.7498209975262009 | T | T | T |
| 0.6951668385076587  | 0.4631089769718234 | 0.7498148593140485 | T | T | T |
| 0.7050017257368648  | 0.5352310331770354 | 0.7498414578744421 | T | T | T |
| 0.6722490958055525  | 0.6506670753623881 | 0.7499380967644699 | T | T | T |
| 0.6300264083131436  | 0.6865580160347238 | 0.7499655707360484 | T | T | T |
| 0.5042429370211290  | 0.7028245181869082 | 0.7498853979945369 | T | T | T |
| 0.2327774059826034  | 0.0309566276491124 | 0.9165361492715306 | T | T | T |
| 0.3078189211839083  | 0.0494031830591007 | 0.9165166145731177 | T | T | T |
| 0.1087332736191591  | 0.0502993372297463 | 0.9165602907603470 | T | T | T |
| 0.0670843120839401  | 0.0867502738096523 | 0.9166456571042706 | T | T | T |
| 0.4632847899328247  | 0.1354718707050557 | 0.9164477054845347 | T | T | T |
| 0.5353161267450282  | 0.1978910169072126 | 0.9164045658958887 | T | T | T |
| 0.0340279691873681  | 0.2024809124761699 | 0.9166944707426151 | T | T | T |
| 0.0418037549836925  | 0.2735981248829351 | 0.9167930019832675 | T | T | T |
| 0.6490448577226444  | 0.3467538358950047 | 0.9164295852556416 | T | T | T |
| 0.6838640733568799  | 0.4248181855492549 | 0.9164292918260790 | T | T | T |
| 0.0960183469181852  | 0.4330854736980618 | 0.9157093347368028 | T | T | T |
| 0.7035982983407572  | 0.5685751922409007 | 0.9164713769219845 | T | T | T |
| 0.6871849954790328  | 0.6265869120896804 | 0.9165141701972953 | T | T | T |
| 0.3123432646823169  | 0.6227151958313526 | 0.9168182268098242 | T | T | T |
| 0.3899816207222495  | 0.6666864359884954 | 0.9168108744716202 | T | T | T |
| 0.6030434334664959  | 0.6978511088533740 | 0.9166349782946612 | T | T | T |
| 0.5397055457109132  | 0.7058542756107010 | 0.9167160149025306 | T | T | T |
| 0.1682975884333057  | 0.5027344542240455 | 0.9170267889228974 | T | T | T |
| 0.0427018817106222  | 0.5058841189542143 | 0.0310402244027839 | T | T | T |
| 0.0375136035457647  | 0.4531716722142800 | 0.8890065356720577 | T | T | T |
| -0.0002244991827962 | 0.4737731379849832 | 0.1034250223167457 | T | T | T |

OOH\_N-CNT(10,10) ### KPOINTS: 1x1x3 ### E= -951.37658812 eV

1.000000000000000

19.0525588799999994 -11.000000000000000 0.000000000000000

0.000000000000000 22.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.401084169999999

C N O H

119 1 2 1

Selective dynamics

Direct

0.1871389983227904 0.0234550628217670 0.0849845808643522 T T T

0.2541674829370738 0.0283954744519868 0.0850703584722676 T T T

0.0818354899578896 0.0617439107176956 0.0847772701229446 T T T

0.4014850773210427 0.0835692355785388 0.0850472714821766 T T T

0.0488403116223938 0.1032776523072834 0.0847300578386950 T T T

0.4750873818771861 0.1312377590306014 0.0851678127764661 T T T

0.0280988568631963 0.2204568113665113 0.0843903499480292 T T T

0.6067288416943736 0.2572056576695527 0.0852393009823725 T T T

0.0398993980150520 0.2901506258010011 0.0842809514203071 T T T

0.6588483110667840 0.3295697853555326 0.0852212762927363 T T T

0.1029963797359765 0.4374444674784160 0.0845180803444174 T T T

0.7245147932944702 0.4780459951918846 0.0852314222824436 T T T

0.1556382445263377 0.5099256801511759 0.0838412320881569 T T T

0.7352580499002030 0.5474009645935960 0.0852481139211255 T T T

0.2879867358331996 0.6336913908716790 0.0848525581248686 T T T

0.7126741447487280 0.6635980848359402 0.0851283811896976 T T T

0.3613634629553229 0.6824791090598198 0.0847654909366743 T T T

0.6800426975101709 0.7054571760478884 0.0851093098472031 T T T

0.5090102458605952 0.7404560295574844 0.0851273328311547 T T T

0.5760188585941016 0.7453860467795097 0.0850710939204311 T T T

0.0378601353872744 0.1288352053881071 0.2514858812481117 T T T

0.5766634606724153 0.2226909476467616 0.2518969736872638 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0511309386511475 | 0.3262759118877306 | 0.2514972297533865 | T | T | T |
| 0.0833998452373709 | 0.4003194385603167 | 0.2515143471212268 | T | T | T |
| 0.1859396379169654 | 0.5439662158681795 | 0.2516034794366124 | T | T | T |
| 0.7351255196673151 | 0.5798293816677866 | 0.2518601536080019 | T | T | T |
| 0.2525515724780134 | 0.6061715806879211 | 0.2516004770022464 | T | T | T |
| 0.3988247909301983 | 0.7025081971236030 | 0.2516381203349732 | T | T | T |
| 0.6586623421164185 | 0.7214398098928922 | 0.2517543685233324 | T | T | T |
| 0.6064634277025348 | 0.7416120059265978 | 0.2517137893839065 | T | T | T |
| 0.1565435543559272 | 0.0270663345336290 | 0.2516435311720871 | T | T | T |
| 0.2900503753125225 | 0.0367270476029965 | 0.2516899116531000 | T | T | T |
| 0.1035583713731129 | 0.0461326077938825 | 0.2515883084457429 | T | T | T |
| 0.3639434602720245 | 0.0643976855093558 | 0.2517730464001682 | T | T | T |
| 0.5106268650726401 | 0.1594324848171371 | 0.2518630562887572 | T | T | T |
| 0.0275947820657783 | 0.1877338603142094 | 0.2513264343256541 | T | T | T |
| 0.6805265432744474 | 0.3669227293600365 | 0.2519542671622390 | T | T | T |
| 0.7134734325898712 | 0.4414611003878382 | 0.2519618522690710 | T | T | T |
| 0.7237793925230976 | 0.6380911334273902 | 0.2517860406967125 | T | T | T |
| 0.4730031948110371 | 0.7317717562192536 | 0.2516186625278183 | T | T | T |
| 0.1872260388395706 | 0.0235993570591656 | 0.4183100863965776 | T | T | T |
| 0.2542109573846902 | 0.0284357649378643 | 0.4183630866977375 | T | T | T |
| 0.0816120221341064 | 0.0615564774540967 | 0.4182255750048101 | T | T | T |
| 0.4014462962723236 | 0.0835317767381397 | 0.4184778182239181 | T | T | T |
| 0.0485913304935265 | 0.1030643161387299 | 0.4182532794372817 | T | T | T |
| 0.4750633850108861 | 0.1312197610416039 | 0.4184868794467279 | T | T | T |
| 0.0280731149516393 | 0.2203311598680339 | 0.4183599150377769 | T | T | T |
| 0.6067280974436517 | 0.2572106263377309 | 0.4186380101855389 | T | T | T |
| 0.0401096156181602 | 0.2900318894901756 | 0.4184876436692760 | T | T | T |
| 0.6588657678613896 | 0.3296085987256466 | 0.4186610122737379 | T | T | T |
| 0.1030103296135869 | 0.4374343648953756 | 0.4183390008420500 | T | T | T |
| 0.7245132519811991 | 0.4780512864978094 | 0.4186486451754368 | T | T | T |
| 0.1549841953193525 | 0.5101486682584309 | 0.4196747143137953 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7352676495766154 | 0.5474269421485138 | 0.4185806871921619 | T | T | T |
| 0.2879413845915744 | 0.6336916754686955 | 0.4183341868267255 | T | T | T |
| 0.7126211805375866 | 0.6635543871736471 | 0.4184691634554002 | T | T | T |
| 0.3613499998378947 | 0.6824378553357301 | 0.4184660098104013 | T | T | T |
| 0.6800055841038006 | 0.7054027563466825 | 0.4184257590934846 | T | T | T |
| 0.5090594305487288 | 0.7405702666766102 | 0.4181374615845587 | T | T | T |
| 0.5760465902992535 | 0.7455074337178241 | 0.4183707802876300 | T | T | T |
| 0.1567377106724825 | 0.0273048771887002 | 0.5849865405264931 | T | T | T |
| 0.2900502309097168 | 0.0367036373235989 | 0.5850341944742147 | T | T | T |
| 0.1036918289838851 | 0.0462874807679697 | 0.5849320941884335 | T | T | T |
| 0.3639320185432786 | 0.0643726376024287 | 0.5851437525117018 | T | T | T |
| 0.0375208685468763 | 0.1286528734669952 | 0.5848862632857114 | T | T | T |
| 0.5106225879742158 | 0.1594806715327169 | 0.5851774945708262 | T | T | T |
| 0.0272155913131451 | 0.1875103518462788 | 0.5849181663506763 | T | T | T |
| 0.5766548127943079 | 0.2226797326805830 | 0.5853045488072266 | T | T | T |
| 0.0503678623764687 | 0.3268904261422940 | 0.5849517274762958 | T | T | T |
| 0.6805263956301123 | 0.3669730033453229 | 0.5853689048101139 | T | T | T |
| 0.0800770572351258 | 0.4004772294304743 | 0.5819701457253093 | T | T | T |
| 0.7134898193460272 | 0.4414798002671650 | 0.5853120513000589 | T | T | T |
| 0.1863985119763956 | 0.5427971271163848 | 0.5864461897336324 | T | T | T |
| 0.7350574053672283 | 0.5798206473371579 | 0.5852417363320591 | T | T | T |
| 0.2530199673692904 | 0.6048423857155799 | 0.5858199934358816 | T | T | T |
| 0.7237652551648807 | 0.6380804975238820 | 0.5852191052300562 | T | T | T |
| 0.3990501501638052 | 0.7024521155276080 | 0.5847730898840263 | T | T | T |
| 0.6585419302161664 | 0.7213157848436489 | 0.5850596071617203 | T | T | T |
| 0.4730795102580428 | 0.7316950018132753 | 0.5847876348358579 | T | T | T |
| 0.6063391426730819 | 0.7414534849818313 | 0.5849933406248001 | T | T | T |
| 0.0818645356676766 | 0.0618578208884356 | 0.7515193588898269 | T | T | T |
| 0.0485824683540680 | 0.1030247748046612 | 0.7514646118093553 | T | T | T |
| 0.6067120461325414 | 0.2571574409950408 | 0.7520150907787438 | T | T | T |
| 0.0898605090206853 | 0.4419473476158663 | 0.7506279381159191 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7352171847391670 | 0.5473884917700415 | 0.7518264991640300 | T | T | T |
| 0.2889192139371676 | 0.6331807724652000 | 0.7515311578780361 | T | T | T |
| 0.3617594912918375 | 0.6824118295210181 | 0.7515797637995029 | T | T | T |
| 0.6800682112611158 | 0.7054650219577110 | 0.7516977195739231 | T | T | T |
| 0.5759556989575346 | 0.7453063983025915 | 0.7516231914743811 | T | T | T |
| 0.1872257244177812 | 0.0235962530280235 | 0.7515968630995613 | T | T | T |
| 0.2541167283631560 | 0.0283464970093522 | 0.7516677626547734 | T | T | T |
| 0.4014910865914951 | 0.0835415140657688 | 0.7517906784006982 | T | T | T |
| 0.4750936600114909 | 0.1312719563712300 | 0.7518826383798890 | T | T | T |
| 0.0275489340929733 | 0.2205706596012828 | 0.7514922151539833 | T | T | T |
| 0.0381934602779427 | 0.2897512580645482 | 0.7515298787385694 | T | T | T |
| 0.6588331431767731 | 0.3295696776954222 | 0.7520471293436308 | T | T | T |
| 0.7245320553364120 | 0.4780663189378768 | 0.7519361126039130 | T | T | T |
| 0.7127503909293961 | 0.6636362101782211 | 0.7517535504248127 | T | T | T |
| 0.5089939194864663 | 0.7402734523330142 | 0.7516413890280410 | T | T | T |
| 0.1566475684907200 | 0.0271375825455141 | 0.9181808729625484 | T | T | T |
| 0.2900201616284060 | 0.0366951785467420 | 0.9183545294646023 | T | T | T |
| 0.1037893843194421 | 0.0463632188074284 | 0.9181816212499885 | T | T | T |
| 0.3639407385838665 | 0.0644026033877325 | 0.9183945810481290 | T | T | T |
| 0.0377731975180483 | 0.1288441260041322 | 0.9180554781736643 | T | T | T |
| 0.5106190560484990 | 0.1594787728994528 | 0.9185683540396822 | T | T | T |
| 0.0272893705958338 | 0.1875941373006559 | 0.9179738482470803 | T | T | T |
| 0.5766595618086612 | 0.2226836910278818 | 0.9186165684761276 | T | T | T |
| 0.0499628869805649 | 0.3270952400323775 | 0.9178180097951547 | T | T | T |
| 0.6805353613238994 | 0.3669748950800239 | 0.9186426612623946 | T | T | T |
| 0.0796489834850036 | 0.4009296909768485 | 0.9204770418122186 | T | T | T |
| 0.7134975838248538 | 0.4414855281793520 | 0.9185261719900297 | T | T | T |
| 0.1868266889262069 | 0.5424787679003013 | 0.9169090727725702 | T | T | T |
| 0.7350385788442328 | 0.5797989399558765 | 0.9184718085412710 | T | T | T |
| 0.2531466905052346 | 0.6047236631024768 | 0.9173494115476903 | T | T | T |
| 0.7237684226129178 | 0.6381133376167993 | 0.9185005686381500 | T | T | T |

|                     |                    |                     |   |   |   |
|---------------------|--------------------|---------------------|---|---|---|
| 0.3990384038985657  | 0.7023994518714822 | 0.9184300377334927  | T | T | T |
| 0.6585150997222476  | 0.7213071260342900 | 0.9184142940606745  | T | T | T |
| 0.4730588631040404  | 0.7315685969781055 | 0.9184402605917303  | T | T | T |
| 0.6062868061157544  | 0.7413264015933200 | 0.9183190295482504  | T | T | T |
| 0.1570793191998628  | 0.5099529805882365 | 0.7517469810431255  | T | T | T |
| 0.0363441554469818  | 0.5095699134710807 | 0.8636680939166534  | T | T | T |
| 0.0316631884714022  | 0.4582659078354372 | 0.7253893048797819  | T | T | T |
| -0.0017688184819546 | 0.4788190676112289 | -0.0559306240536508 | T | T | T |

OOH\_N-CNT(8,0) ### KPOINTS: 2x2x2 ### E= -502.08539350 eV

1.000000000000000

12.9903810600000007 -7.500000000000000 0.000000000000000

0.000000000000000 15.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 8.5305455000000006

C N O H

63 1 2 1

Selective dynamics

Direct

0.0795973745952095 0.1963587371412754 0.0823018617305401 T T T

0.4987795775950843 0.2596384668566566 0.0822099053488451 T T T

0.1379676496218351 0.3804524725169972 0.0810159100071198 T T T

0.5612174643829000 0.4439172475415627 0.0825870251042423 T T T

0.1540292703294655 0.0839563645967084 0.0825471266386147 T T T

0.3274380704117518 0.1084382087107854 0.0821838036823081 T T T

0.3074546881793113 0.5287115760427569 0.0812366570289739 T T T

0.4802351377178786 0.5503441716695959 0.0824031410569559 T T T

0.2334439333812802 0.0776445230330873 0.1659460456921194 T T T

0.1002909928110975 0.1255380684651158 0.1659593436639064 T T T

0.4207887876969577 0.1729237546714691 0.1657276498328929 T T T

0.2127641624160851 0.4695874018882226 0.1670796867696667 T T T

0.5372932856407795 0.5120578768668401 0.1660253358356026 T T T

0.4000737402142744 0.5550423954178314 0.1651006011548181 T T T

0.0932401031617243 0.2849409027774451 0.1649533444596213 T T T

0.5481786328672675 0.3554706572537724 0.1660026954059062 T T T

0.0935891684962766 0.2857679464962653 0.3326374733351984 T T T

0.5482154820402044 0.3552860537898262 0.3322373167600284 T T T

0.2335714926959978 0.0776558228130578 0.3322835845239982 T T T

0.1006970707992716 0.1260910835534114 0.3319405139475080 T T T

0.4210012422384581 0.1726119043659687 0.3324600558017223 T T T

0.2120954764109407 0.4705168925025396 0.3308553992669037 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5369373260482846 | 0.5118131688772716 | 0.3319556659366027 | T | T | T |
| 0.3993147836242978 | 0.5547464743123529 | 0.3329503207172038 | T | T | T |
| 0.1548497604815327 | 0.0850187446938938 | 0.4156738847305656 | T | T | T |
| 0.3276301722740019 | 0.1084477326932268 | 0.4159600374116678 | T | T | T |
| 0.3072242507411506 | 0.5302047571589540 | 0.4170761717940011 | T | T | T |
| 0.4791192562094792 | 0.5491896199859474 | 0.4156892184684103 | T | T | T |
| 0.0810286312850636 | 0.1975653727351834 | 0.4155653582028926 | T | T | T |
| 0.4988504766366805 | 0.2594334157437016 | 0.4159529602572535 | T | T | T |
| 0.1363336974820560 | 0.3811745193274159 | 0.4167242834168884 | T | T | T |
| 0.5603757999961344 | 0.4433642752493504 | 0.4156854537976951 | T | T | T |
| 0.0824222576726269 | 0.1983101492903956 | 0.5818959538692584 | T | T | T |
| 0.4989549200431662 | 0.2593385701813703 | 0.5822362549698357 | T | T | T |
| 0.1355770425121709 | 0.3811428927730436 | 0.5819521889987199 | T | T | T |
| 0.5605332721960001 | 0.4432467377614958 | 0.5824401041163987 | T | T | T |
| 0.1548700248783853 | 0.0849425791760579 | 0.5823931656853630 | T | T | T |
| 0.3276182476960855 | 0.1083333238993248 | 0.5821809041348397 | T | T | T |
| 0.3072939176848452 | 0.5301410333507077 | 0.5824148731287979 | T | T | T |
| 0.4782225401487432 | 0.5477045174554338 | 0.5817919684520172 | T | T | T |
| 0.2337522132723290 | 0.0778384969894342 | 0.6660012756224643 | T | T | T |
| 0.1019298792192663 | 0.1270717290120044 | 0.6658610203315199 | T | T | T |
| 0.4209982779967429 | 0.1725706582276745 | 0.6658105637189806 | T | T | T |
| 0.2037209129344582 | 0.4831442182177220 | 0.6658944973109298 | T | T | T |
| 0.5359376455121067 | 0.5106786988536627 | 0.6659381894354988 | T | T | T |
| 0.3966945030466563 | 0.5500125515447279 | 0.6645704791543087 | T | T | T |
| 0.0977350155663204 | 0.2875820172462404 | 0.6646276183388573 | T | T | T |
| 0.5480986474076209 | 0.3550881327626908 | 0.6660570270690737 | T | T | T |
| 0.0959262119216757 | 0.2862953577432482 | 0.8321439987950543 | T | T | T |
| 0.5480375975639605 | 0.3552012827859153 | 0.8322202919436291 | T | T | T |
| 0.2336302509653184 | 0.0778122468221514 | 0.8322664499189896 | T | T | T |
| 0.1010045378577377 | 0.1263920315142052 | 0.8321018950292428 | T | T | T |
| 0.4210133377525007 | 0.1725099291797213 | 0.8324806720433284 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5365288737442783 | 0.5114789330230789 | 0.8322208488673241 | T | T | T |
| 0.3981806971246317 | 0.5519966996406191 | 0.8322841413136460 | T | T | T |
| 0.1544796901795837 | 0.0846198865146290 | 0.9158275526701184 | T | T | T |
| 0.3275477019795508 | 0.1084448329838988 | 0.9160269850815728 | T | T | T |
| 0.3069412468553769 | 0.5257023028361699 | 0.9157402859531196 | T | T | T |
| 0.4792228646522706 | 0.5493509700539603 | 0.9160318377215607 | T | T | T |
| 0.0805807162253748 | 0.1971999873035465 | 0.9158575223411018 | T | T | T |
| 0.4987700146342398 | 0.2594841723792173 | 0.9160073673167307 | T | T | T |
| 0.1405410650812217 | 0.3802964869589573 | 0.9158476841900287 | T | T | T |
| 0.5605916827570151 | 0.4435681022158764 | 0.9158762741597641 | T | T | T |
| 0.2118737151747322 | 0.4710464566593421 | 0.8365948118836790 | T | T | T |
| 0.2259709567053431 | 0.6509440071354013 | 0.6876170307526740 | T | T | T |
| 0.1523167441937721 | 0.5425753542300222 | 0.6407667087486848 | T | T | T |
| 0.1887458183611949 | 0.6567540435295840 | 0.7767337251522102 | T | T | T |

OOH\_N-CNT(9,0) ### KPOINTS: 2x2x2 ### E= -566.21609688 eV

1.0000000000000000

13.8564064600000005 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5367054200000005

C N O H

71 1 2 1

Selective dynamics

Direct

0.1979623649513790 0.0677444398259596 0.0847669500371225 T T T

0.0886293452337732 0.1325755382470785 0.0843014118180942 T T T

0.3707630621285432 0.1237547580956419 0.0847161460991064 T T T

0.0914959259502551 0.2868302064599500 0.0854803996394798 T T T

0.5245488917809118 0.2750662880209213 0.0846360620788147 T T T

0.1802417720140433 0.4706509767557938 0.0842872583414488 T T T

0.5817727970585757 0.4479582728655706 0.0847830506318102 T T T

0.3643551116162970 0.5581983056160782 0.0854046258391597 T T T

0.5169376147010006 0.5574880205084043 0.0843906825626462 T T T

0.1308404334118199 0.0852262926790036 0.1683623937157389 T T T

0.2809717465843368 0.0802967114847272 0.1685746029130017 T T T

0.4551612906528458 0.1915043628480285 0.1680506678031785 T T T

0.0763686441457119 0.2031524498422479 0.1681775234724321 T T T

0.5692238935757740 0.3648910861192549 0.1686627498882006 T T T

0.1245635342979130 0.3742012697017826 0.1686813099681087 T T T

0.5637657944866411 0.5147715669168176 0.1682514601600997 T T T

0.2769591191536215 0.5264911822836376 0.1681517697660421 T T T

0.4474169267077517 0.5715009959970980 0.1681200990486265 T T T

0.1307366621127966 0.0851906678113550 0.3347513675959649 T T T

0.2808530632827259 0.0803143909489177 0.3345256339494708 T T T

0.4550566593380411 0.1916554014844505 0.3349622403331924 T T T

0.0750991222752537 0.2024525737348827 0.3348828498866661 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5692832381123476 | 0.3650986044246595 | 0.3344719891392370 | T | T | T |
| 0.1250834070106243 | 0.3744960671659455 | 0.3332745894010117 | T | T | T |
| 0.5637962801767328 | 0.5148790254080261 | 0.3347729597606641 | T | T | T |
| 0.2768982595428632 | 0.5262248506285083 | 0.3327970544794567 | T | T | T |
| 0.4481357489024866 | 0.5727814291845549 | 0.3347839262806198 | T | T | T |
| 0.1976952186784404 | 0.0675410026076014 | 0.4181635880059369 | T | T | T |
| 0.0874039141627432 | 0.1316702104321663 | 0.4186849569954739 | T | T | T |
| 0.3706352232386746 | 0.1238478504974962 | 0.4183960571415362 | T | T | T |
| 0.0880088898842522 | 0.2853602859323056 | 0.4177696110783390 | T | T | T |
| 0.5245784432581152 | 0.2752763327796001 | 0.4184326069515316 | T | T | T |
| 0.1902150158863535 | 0.4611360178598576 | 0.4194394316356959 | T | T | T |
| 0.5819759984215357 | 0.4482974778173737 | 0.4181777822443394 | T | T | T |
| 0.3659701464216628 | 0.5619632520920570 | 0.4175667461749236 | T | T | T |
| 0.5177148682593351 | 0.5585516555017729 | 0.4185237356850661 | T | T | T |
| 0.1977098188351239 | 0.0677740888649119 | 0.5849648134526088 | T | T | T |
| 0.0871374402990606 | 0.1314617618158408 | 0.5842397272840797 | T | T | T |
| 0.3706467077966583 | 0.1241623846782453 | 0.5846379823016987 | T | T | T |
| 0.0876385019737468 | 0.2847837396178258 | 0.5852998172470730 | T | T | T |
| 0.5244039223420912 | 0.2754131744610960 | 0.5845859993678061 | T | T | T |
| 0.1911252314998074 | 0.4601761315519199 | 0.5826116411008387 | T | T | T |
| 0.5817448976688193 | 0.4483314855384675 | 0.5849287285316205 | T | T | T |
| 0.3665293790419514 | 0.5622140010265720 | 0.5850896945330669 | T | T | T |
| 0.5179306536729946 | 0.5588896490014634 | 0.5842475149321114 | T | T | T |
| 0.1303698272363253 | 0.0849249256540954 | 0.6683011849693620 | T | T | T |
| 0.2809634087554891 | 0.0807876419117085 | 0.6685549981314609 | T | T | T |
| 0.4550575638825718 | 0.1918685193973023 | 0.6680309553066269 | T | T | T |
| 0.0740722920325669 | 0.2017413509605706 | 0.6677693292931588 | T | T | T |
| 0.5689486149264488 | 0.3651361406415720 | 0.6687153532984781 | T | T | T |
| 0.1262649031859384 | 0.3742835137434581 | 0.6694491874509798 | T | T | T |
| 0.5639051150083058 | 0.5151810247979643 | 0.6682141964525887 | T | T | T |
| 0.2771387270864947 | 0.5246252299550331 | 0.6694656622902798 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4489166865077747 | 0.5738628981242144 | 0.6676454758767989 | T | T | T |
| 0.1306629415752423 | 0.0852935860243456 | 0.8346098098638151 | T | T | T |
| 0.2809877216066349 | 0.0807692655214091 | 0.8344661764597227 | T | T | T |
| 0.4550150378063087 | 0.1917946468300169 | 0.8349413045066731 | T | T | T |
| 0.0750913998803864 | 0.2026188216635743 | 0.8347077528276986 | T | T | T |
| 0.5688890877836026 | 0.3650390790266521 | 0.8344489603612857 | T | T | T |
| 0.1288191634812757 | 0.3744608287251917 | 0.8341238480807905 | T | T | T |
| 0.5636865997096299 | 0.5150028263618432 | 0.8347009617159127 | T | T | T |
| 0.2769905293123978 | 0.5219694930039483 | 0.8340993532436536 | T | T | T |
| 0.4480158022237462 | 0.5728521159894843 | 0.8346601597995585 | T | T | T |
| 0.1978687494393089 | 0.0678308074076146 | 0.9180660279563899 | T | T | T |
| 0.0880045487619959 | 0.1321918162617060 | 0.9187019036135405 | T | T | T |
| 0.3706946755956658 | 0.1238652468954569 | 0.9184833088728106 | T | T | T |
| 0.0901124870856307 | 0.2860069642357144 | 0.9181222617033538 | T | T | T |
| 0.5245287951614251 | 0.2752355867518016 | 0.9185642690664456 | T | T | T |
| 0.5817299734060324 | 0.4481673114642812 | 0.9181140118202092 | T | T | T |
| 0.3653194898136381 | 0.5596401525865655 | 0.9181221744010051 | T | T | T |
| 0.5172982604010551 | 0.5581264851881750 | 0.9186024761417390 | T | T | T |
| 0.1907794399842755 | 0.4606539369801921 | 0.9144145210818256 | T | T | T |
| 0.1723046634905968 | 0.6146226695136561 | 0.0467839903127316 | T | T | T |
| 0.1193732444315456 | 0.5139186403868091 | 0.1068044349715605 | T | T | T |
| 0.1964252698813205 | 0.6495822368598287 | 0.1450237408564284 | T | T | T |

OOH\_N-CNT(10,0) #### KPOINTS: 2x2x2 #### E= -630.60129807 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C N O H

79 1 2 1

Selective dynamics

Direct

0.2408641166148365 0.0606983454015999 0.0820738252293157 T T T

0.1111756734846166 0.0855743715383486 0.0821899373252288 T T T

0.4067216679193965 0.1388697988957418 0.0821951836748935 T T T

0.5428571208317902 0.2892026063243374 0.0822071440129015 T T T

0.1156280308339778 0.3650315956521497 0.0796674626363568 T T T

0.2464063856037903 0.5175491310921730 0.0840734705031796 T T T

0.5424211142255478 0.5620291317642295 0.0822148276279731 T T T

0.4122516363336957 0.5870557843581438 0.0823391636956444 T T T

0.0670777101739936 0.2022615211520147 0.0821130400191248 T T T

0.5946666606063238 0.4516302534402612 0.0821550318785567 T T T

0.1676174954084675 0.0598436516214605 0.1653440677566355 T T T

0.4826267379300593 0.2084635072218800 0.1654364488698811 T T T

0.1726895185953626 0.4471775660760673 0.1651195119507128 T T T

0.4840823027099728 0.5858975249255048 0.1651355955020643 T T T

0.3233461671150800 0.0881709980659586 0.1652893733658087 T T T

0.0766017148551782 0.1345932782892033 0.1654024508672215 T T T

0.0801007431414165 0.2809456903648908 0.1637603593867332 T T T

0.5817848011847451 0.3731915496154942 0.1654731662847802 T T T

0.5804548513652460 0.5163098512301856 0.1653012512191033 T T T

0.3302873721253603 0.5642423339506124 0.1654256601011894 T T T

0.3233027791671278 0.0883016432848238 0.3322287897292993 T T T

0.0762914009553511 0.1344725030720494 0.3318977358802169 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0790790564200237 | 0.2803554544471918 | 0.3315955883803660 | T | T | T |
| 0.5819602954413687 | 0.3731924262838020 | 0.3320785818851073 | T | T | T |
| 0.5806803705798566 | 0.5163631704303012 | 0.3323253906602422 | T | T | T |
| 0.3307708638486858 | 0.5636991947177253 | 0.3327980794886329 | T | T | T |
| 0.1674201709038718 | 0.0597138603803513 | 0.3320461494510609 | T | T | T |
| 0.4826781554921896 | 0.2084618147428761 | 0.3321179991325744 | T | T | T |
| 0.1724018410466917 | 0.4458099801610449 | 0.3323184264886802 | T | T | T |
| 0.4847911411024639 | 0.5862785171527236 | 0.3324236351949941 | T | T | T |
| 0.0659849482498954 | 0.2017839333750205 | 0.4144527392868520 | T | T | T |
| 0.5946863766289303 | 0.4517239571024796 | 0.4153692028111808 | T | T | T |
| 0.2408444966038155 | 0.0606415537695556 | 0.4154818445669466 | T | T | T |
| 0.1110573758764664 | 0.0854721084628811 | 0.4150516725540367 | T | T | T |
| 0.4067291932608539 | 0.1391267924863141 | 0.4154177772991233 | T | T | T |
| 0.5431076000520483 | 0.2892870256902560 | 0.4153047002891375 | T | T | T |
| 0.1149776724416721 | 0.3641277760199368 | 0.4157103871844419 | T | T | T |
| 0.2471612060763531 | 0.5152176158358216 | 0.4169738930927328 | T | T | T |
| 0.5429090660990700 | 0.5625717251712476 | 0.4154703632220915 | T | T | T |
| 0.4124734421526139 | 0.5867353487685387 | 0.4156383817332184 | T | T | T |
| 0.2408264358649016 | 0.0604696132125775 | 0.5821159762899601 | T | T | T |
| 0.1110941009716169 | 0.0853078540798907 | 0.5820824655084221 | T | T | T |
| 0.4067188502770434 | 0.1389376994411024 | 0.5821180421173069 | T | T | T |
| 0.5430102516131762 | 0.2891611842258461 | 0.5823087525774570 | T | T | T |
| 0.1159311143735969 | 0.3638586424134351 | 0.5830641605421268 | T | T | T |
| 0.2471596260892753 | 0.5158099451923323 | 0.5836672449037678 | T | T | T |
| 0.5432816668470308 | 0.5625311599486671 | 0.5821629670548543 | T | T | T |
| 0.4125436250839229 | 0.5861875686850204 | 0.5826536978507931 | T | T | T |
| 0.0664947937980992 | 0.2016343190304316 | 0.5816667259547399 | T | T | T |
| 0.5948671042591518 | 0.4516433671355785 | 0.5821275895458061 | T | T | T |
| 0.1675795639297409 | 0.0596477336839210 | 0.6653806798185721 | T | T | T |
| 0.4826792946198604 | 0.2083898870378498 | 0.6654511214635389 | T | T | T |
| 0.1732494854250400 | 0.4452544613808915 | 0.6668203822376167 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4846733478887090 | 0.5854989709405379 | 0.6657589648221141 | T | T | T |
| 0.3233947354070636 | 0.0879773065154607 | 0.6652410938290800 | T | T | T |
| 0.0766871751735524 | 0.1343508244543844 | 0.6651159630392761 | T | T | T |
| 0.0815973231799227 | 0.2801337415407397 | 0.6650655281284034 | T | T | T |
| 0.5818588044210178 | 0.3732088118544844 | 0.6654275570537495 | T | T | T |
| 0.5811542572255162 | 0.5165862595586315 | 0.6652663035526214 | T | T | T |
| 0.3315865690077973 | 0.5639934274675198 | 0.6669667999877437 | T | T | T |
| 0.3233620910740201 | 0.0879605153239889 | 0.8322352723038633 | T | T | T |
| 0.0768072210152351 | 0.1344251576033117 | 0.8318343731567310 | T | T | T |
| 0.0842057553839380 | 0.2814074338555367 | 0.8318734656941386 | T | T | T |
| 0.5817554985450065 | 0.3731445354787897 | 0.8320897929601850 | T | T | T |
| 0.5810802893687727 | 0.5164644883596021 | 0.8323240801594667 | T | T | T |
| 0.3315864835636194 | 0.5648079390233686 | 0.8310195365989554 | T | T | T |
| 0.1675514243140268 | 0.0596109470425483 | 0.8320204171463075 | T | T | T |
| 0.4826335146673424 | 0.2083004409553112 | 0.8321639609953394 | T | T | T |
| 0.4838251868105485 | 0.5843744699707935 | 0.8323218165990467 | T | T | T |
| 0.0680024963566313 | 0.2022936917305388 | 0.9156813876379746 | T | T | T |
| 0.5947971205665700 | 0.4516611311368395 | 0.9155123778088760 | T | T | T |
| 0.2409361870366415 | 0.0606344613884241 | 0.9154046488149910 | T | T | T |
| 0.1111319183556332 | 0.0852453173103319 | 0.9151838114340084 | T | T | T |
| 0.4068265419687749 | 0.1388413015132391 | 0.9154360450605018 | T | T | T |
| 0.5428609463027827 | 0.2892343983546314 | 0.9152661208841968 | T | T | T |
| 0.1201451399398165 | 0.3646892937444324 | 0.9143354880054050 | T | T | T |
| 0.2420038401832185 | 0.5293400705663857 | 0.9115949056602723 | T | T | T |
| 0.5425158344717527 | 0.5618027915823693 | 0.9156342002924920 | T | T | T |
| 0.4107023570319817 | 0.5840856564821229 | 0.9150743904515009 | T | T | T |
| 0.1723056060229567 | 0.4455325862227117 | 0.8304235753229500 | T | T | T |
| 0.2734434350341448 | 0.6847158728977617 | 0.9086493988995977 | T | T | T |
| 0.2015719255031201 | 0.5898240890063048 | 0.8833158479646597 | T | T | T |
| 0.2525117875692082 | 0.6978257403161537 | 0.0060647596323387 | T | T | T |



OOH\_N-CNT(11,0) ### KPOINTS: 2x2x2 ### E= -694.62324215 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C N O H

87 1 2 1

Selective dynamics

Direct

0.1525400614325957 0.0553956294136809 0.0816955945254269 T T T

0.2968381676062174 0.0738247392542199 0.0816839231202775 T T T

0.0670105916070427 0.1269763124463710 0.0820129221586825 T T T

0.4516244022225361 0.1752257446473137 0.0819424151351620 T T T

0.0628144488748886 0.2612194799711525 0.0818941276814453 T T T

0.5683593573968986 0.3249479758030083 0.0817579354316339 T T T

0.1399813322431523 0.4183262390715350 0.0810293746936612 T T T

0.6096241866723346 0.4768274615174725 0.0817500755112483 T T T

0.2800951125280540 0.5461226713570534 0.0811514875426528 T T T

0.5583350832189258 0.5798478542584615 0.0821444186739387 T T T

0.4355303672315408 0.6037403590869298 0.0820462685754564 T T T

0.2200907435276430 0.0529985906758535 0.1651050139783903 T T T

0.1003915326604568 0.0813470950208775 0.1652154224738507 T T T

0.3762899651635525 0.1159599916197574 0.1652591730967650 T T T

0.0541758784206068 0.1883644263319823 0.1652545286878073 T T T

0.5173055117524352 0.2466361322778869 0.1652968070845330 T T T

0.0921021104589351 0.3396209821933851 0.1647713265007121 T T T

0.6001311894606781 0.4038374105584193 0.1651659724893290 T T T

0.2034912462180676 0.4909607239474983 0.1665693057432724 T T T

0.5948779477914464 0.5371588417844714 0.1653400834298886 T T T

0.3593243720399548 0.5844315542818915 0.1649712942765511 T T T

0.5037976304495415 0.6024875271298021 0.1653857675412731 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2201536595222566 | 0.0529838842267509 | 0.3319117847774849 | T | T | T |
| 0.1004694243432069 | 0.0813109898953469 | 0.3316777117960265 | T | T | T |
| 0.3763236814653828 | 0.1159167737764631 | 0.3317504010792879 | T | T | T |
| 0.0546635175202002 | 0.1887690611394223 | 0.3315487460109749 | T | T | T |
| 0.5173617281495883 | 0.2465920947042861 | 0.3318104698998124 | T | T | T |
| 0.0924777543680127 | 0.3402767023495269 | 0.3321003460943843 | T | T | T |
| 0.6001113197888475 | 0.4037971766616739 | 0.3319823272795249 | T | T | T |
| 0.2025652879308289 | 0.4921889981729005 | 0.3310714829865279 | T | T | T |
| 0.5948780587320058 | 0.5371248897995199 | 0.3317660252646430 | T | T | T |
| 0.3587204242934484 | 0.5843343733061420 | 0.3324336672142130 | T | T | T |
| 0.5034331795327468 | 0.6021969661434489 | 0.3316434318073049 | T | T | T |
| 0.1527908725600836 | 0.0556012703111303 | 0.4152586494795945 | T | T | T |
| 0.2969051857504194 | 0.0738807149610585 | 0.4152754433298645 | T | T | T |
| 0.0677437094150801 | 0.1275390271220094 | 0.4150135072343481 | T | T | T |
| 0.4517004413185130 | 0.1751555779810089 | 0.4151768319766320 | T | T | T |
| 0.0641613199733123 | 0.2619839392760166 | 0.4151883323378666 | T | T | T |
| 0.5682857121896463 | 0.3249253526331888 | 0.4152998187599399 | T | T | T |
| 0.1383194746529476 | 0.4193369947025721 | 0.4162103698878151 | T | T | T |
| 0.6093933392965154 | 0.4766731040961457 | 0.4153606483582561 | T | T | T |
| 0.2794676540813333 | 0.5482533243607508 | 0.4166914384643348 | T | T | T |
| 0.5577443828600130 | 0.5792992526995927 | 0.4150863958527710 | T | T | T |
| 0.4347703250543902 | 0.6028337410184491 | 0.4153257331661686 | T | T | T |
| 0.1529165925730607 | 0.0557786663701566 | 0.5816530293961873 | T | T | T |
| 0.2970029480663330 | 0.0739230774264894 | 0.5817424661744169 | T | T | T |
| 0.0680234751135788 | 0.1277985457334233 | 0.5819421212371420 | T | T | T |
| 0.4518326436704871 | 0.1750068782420889 | 0.5819250453937894 | T | T | T |
| 0.0652847077479604 | 0.2624313145707352 | 0.5815568855451837 | T | T | T |
| 0.5682225936623480 | 0.3248278476060510 | 0.5817959046635220 | T | T | T |
| 0.1372082995538202 | 0.4192217903434084 | 0.5817072512732091 | T | T | T |
| 0.6092602777006753 | 0.4765385051536454 | 0.5817350303963977 | T | T | T |
| 0.2795587155331637 | 0.5489204112083752 | 0.5822347544922923 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5575002685318192 | 0.5790245237080736 | 0.5820190793679501 | T | T | T |
| 0.4341307307590356 | 0.6015583324212214 | 0.5816055204031965 | T | T | T |
| 0.2203982804840549 | 0.0534014005529775 | 0.6651680918922176 | T | T | T |
| 0.1008824704436660 | 0.0817315107008864 | 0.6652867951553573 | T | T | T |
| 0.3764680365471898 | 0.1158298471390338 | 0.6652293409016351 | T | T | T |
| 0.0559943359494169 | 0.1895808990997950 | 0.6653531750503128 | T | T | T |
| 0.5174314106181939 | 0.2464772934438277 | 0.6652328177368290 | T | T | T |
| 0.0949058699732609 | 0.3411986480308206 | 0.6643345943189617 | T | T | T |
| 0.5997267548194114 | 0.4035931063027631 | 0.6652352179591818 | T | T | T |
| 0.1939575862130198 | 0.5030990466601752 | 0.6665802001497780 | T | T | T |
| 0.5944584529315228 | 0.5367294665452825 | 0.6653812586066336 | T | T | T |
| 0.3573334255043091 | 0.5813973246205739 | 0.6643124173708327 | T | T | T |
| 0.5024799984498005 | 0.6008709550755370 | 0.6654233843756652 | T | T | T |
| 0.2202509691740159 | 0.0532467984849346 | 0.8318490676972623 | T | T | T |
| 0.1006924252320417 | 0.0816787408990667 | 0.8317560664651287 | T | T | T |
| 0.3763956912195565 | 0.1158424407706103 | 0.8316783403039092 | T | T | T |
| 0.0550703484377616 | 0.1891922322771855 | 0.8318987133824608 | T | T | T |
| 0.5174564111242331 | 0.2465141604601142 | 0.8317112308619704 | T | T | T |
| 0.0936218865881113 | 0.3405173091317855 | 0.8317888822763529 | T | T | T |
| 0.5998752160227735 | 0.4037054620574124 | 0.8319316830667297 | T | T | T |
| 0.5945248971159416 | 0.5368917731009025 | 0.8317791144185321 | T | T | T |
| 0.3582802842957432 | 0.5826081183384799 | 0.8318795202231920 | T | T | T |
| 0.5029280815866496 | 0.6016103095846878 | 0.8319832663927736 | T | T | T |
| 0.1527286853716246 | 0.0556707696644958 | 0.9152625899534366 | T | T | T |
| 0.2968963459767214 | 0.0738775051502952 | 0.9152408425138621 | T | T | T |
| 0.0674626155644225 | 0.1274977212520772 | 0.9151961355794640 | T | T | T |
| 0.4516657458101264 | 0.1752075678036940 | 0.9151898264966222 | T | T | T |
| 0.0636273582124984 | 0.2619500906736668 | 0.9154852428638391 | T | T | T |
| 0.5683219685929132 | 0.3249140290806375 | 0.9152853522476411 | T | T | T |
| 0.1416157208257445 | 0.4181185229728770 | 0.9153715709337951 | T | T | T |
| 0.6093883376045588 | 0.4767221773551396 | 0.9153311442888340 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2800569102334218 | 0.5442637681398089 | 0.9153259839831989 | T | T | T |
| 0.5577747797655163 | 0.5794109930249256 | 0.9153139310681194 | T | T | T |
| 0.4346803132737547 | 0.6028620545794919 | 0.9156015410256656 | T | T | T |
| 0.2035831482229222 | 0.4909453956366768 | 0.8352827358634448 | T | T | T |
| 0.2024165774548260 | 0.6393175850619138 | 0.7036555554428304 | T | T | T |
| 0.1456916086665904 | 0.5484586107207848 | 0.6510413655571673 | T | T | T |
| 0.1654241070050670 | 0.6420045208365349 | 0.7836291138233392 | T | T | T |

OOH\_N-CNT(12,0) ### KPOINTS: 1x1x2 ### E= -757.96797912 eV

1.0000000000000000

15.588499999999998 -9.000000000000000 0.000000000000000

0.0000000000000000 18.000000000000000 0.000000000000000

0.0000000000000000 0.000000000000000 8.457919999999997

C N O H

95 1 2 1

Selective dynamics

Direct

0.6549357678929631 0.5372229977768510 0.4166435214610759 T T T

0.6549144250710730 0.5372711597815182 0.9165284868214222 T T T

0.4650851012880008 0.6484814007458276 0.4164278029821305 T T T

0.4650659963300188 0.6483620272932531 0.9166166467634825 T T T

0.3911663038796866 0.1095451863101615 0.4163384580062576 T T T

0.3911499774539857 0.1096409920903687 0.9164454156061280 T T T

0.1082473856634179 0.0670259768658611 0.4165959484901258 T T T

0.1081499612701581 0.0669815451708459 0.9165142870470748 T T T

0.6330322373502668 0.3911065381381459 0.4163289607209281 T T T

0.6329701200430494 0.3910690160257919 0.9162817012151008 T T T

0.5922847814904728 0.6309844002901670 0.4163398272872328 T T T

0.5925885939054794 0.6314473227529781 0.9163603129806033 T T T

0.1644155936798690 0.4692273742542328 0.4176403162409458 T T T

0.1678790350873863 0.4674159201492423 0.9168298335425455 T T T

0.0740902076990757 0.3117907051271975 0.4162590819369011 T T T

0.0738785200557769 0.3117987602790488 0.9164525142115671 T T T

0.2345778563448126 0.0486261096935977 0.4162521512886606 T T T

0.2345898495461195 0.0486355406121615 0.9162786942857927 T T T

0.5366733796133702 0.2346486443302044 0.4163577243172381 T T T

0.5366895902482691 0.2346457535773690 0.9163899110540776 T T T

0.3094054414710383 0.5943515016916571 0.4181046074766944 T T T

0.3099603001442427 0.5894463077646441 0.9167984117333101 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0500942098378192 | 0.1646822693382398 | 0.4162423873356441 | T | T | T |
| 0.0498532537579534 | 0.1646315327074542 | 0.9162686400565128 | T | T | T |
| 0.5928701509534484 | 0.6316473165778566 | 0.0833938243695045 | T | T | T |
| 0.5921488058977060 | 0.6307708786348192 | 0.5833542399507277 | T | T | T |
| 0.0496767001467733 | 0.1644386773518656 | 0.0832529383966353 | T | T | T |
| 0.0502272952729404 | 0.1646715273667465 | 0.5831957615023332 | T | T | T |
| 0.3100164943041525 | 0.5917441680826715 | 0.0824366870149739 | T | T | T |
| 0.3096474434738998 | 0.5950612026503865 | 0.5837537910237459 | T | T | T |
| 0.1080543141191560 | 0.0667901275539307 | 0.0830474150261992 | T | T | T |
| 0.1082185860597120 | 0.0669591709628485 | 0.5829946578294180 | T | T | T |
| 0.6550642014233405 | 0.5373041250813637 | 0.0830402350562970 | T | T | T |
| 0.6550420935999457 | 0.5372139712536049 | 0.5830720904274689 | T | T | T |
| 0.2345069581347616 | 0.0485179513237270 | 0.0833345065286320 | T | T | T |
| 0.2346057984154619 | 0.0486986193736635 | 0.5833438509585758 | T | T | T |
| 0.1660710972553655 | 0.4679357694136560 | 0.0823263044749921 | T | T | T |
| 0.1635513202554925 | 0.4689133613061436 | 0.5831454003204494 | T | T | T |
| 0.3911073205312635 | 0.1096815317769916 | 0.0831496553106814 | T | T | T |
| 0.3911567026525299 | 0.1094237992895564 | 0.5830809173420022 | T | T | T |
| 0.4658047524896386 | 0.6493215270123409 | 0.0836311342231501 | T | T | T |
| 0.4645061567217804 | 0.6472312938451218 | 0.5831569585756895 | T | T | T |
| 0.5366831327870620 | 0.2347063839506920 | 0.0831480388634566 | T | T | T |
| 0.5366911523438738 | 0.2345554277239522 | 0.5831029264676594 | T | T | T |
| 0.0729545970900648 | 0.3112788035924843 | 0.0834023135384848 | T | T | T |
| 0.0751945659624828 | 0.3119784886094119 | 0.5831193239102985 | T | T | T |
| 0.6330929240158489 | 0.3911355096147806 | 0.0833321788412054 | T | T | T |
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| 0.3114845253136954 | 0.0698206258376757 | 0.1663937848454447 | T | T | T |

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| 0.3114724677140863 | 0.0697500248297599 | 0.6664330278117322 | T | T | T |
| 0.3894163225886524 | 0.6293893660702671 | 0.1661000551159956 | T | T | T |
| 0.3876688210416110 | 0.6264858220217385 | 0.6656259735175106 | T | T | T |
| 0.6334311213788518 | 0.5928837413320174 | 0.1663192400711337 | T | T | T |
| 0.6335271744248091 | 0.5928322060040361 | 0.6664243033163388 | T | T | T |
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| 0.0690306798087181 | 0.1074501667215028 | 0.8332374021653154 | T | T | T |
| 0.5351071843006736 | 0.6503422876184156 | 0.3330363143851331 | T | T | T |
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| 0.6335185561595310 | 0.5928988606429598 | 0.3333926655346344 | T | T | T |
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| 0.4679068482152314 | 0.1658170229502401 | 0.3332710846577791 | T | T | T |
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| 0.3888142120384644 | 0.6293628511654205 | 0.3338882728727579 | T | T | T |
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| 0.5929802175518750 | 0.3115913535304266 | 0.3331188379629882 | T | T | T |
| 0.5930152040505100 | 0.3115579433439699 | 0.8330328689492495 | T | T | T |
| 0.1122685113012105 | 0.3910735370185863 | 0.3335079375184977 | T | T | T |
| 0.1138392982207469 | 0.3909097132898856 | 0.8333565787421585 | T | T | T |
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| 0.3114952300899076 | 0.0697549373319748 | 0.8330965229372196 | T | T | T |
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| 0.2332929150300688 | 0.5375609695738636 | 0.8361463157396390 | T | T | T |
| 0.2357240027669198 | 0.6879841025979893 | 0.7212798463533558 | T | T | T |
| 0.1788924160790993 | 0.6004972237608499 | 0.6556288496081046 | T | T | T |
| 0.2022633399821378 | 0.6850897493585076 | 0.8138087507972139 | T | T | T |

OOH\_N-CNT(13,0) ### KPOINTS: 1x1x2 ### E= -1229.31215901 eV

1.000000000000000

24.248699999999995 -14.000000000000000 0.000000000000000

0.000000000000000 28.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 12.838699999999993

C N O H

155 1 2 1

Selective dynamics

Direct

0.4408426618055287 0.4066441941457000 0.0279063660071211 T T T

0.4529699922729918 0.3697375454778261 0.1945137788734683 T T T

0.4530538000856808 0.3697713629630059 0.3056014743310536 T T T

0.3832089029342107 0.4498702297304888 0.0279198778366024 T T T

0.4409667076222366 0.4066637587565985 0.1389265876691161 T T T

0.4172350536674632 0.4338108590548311 0.1945200982691156 T T T

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0.2931917186804020 0.4450227471255636 0.0281506904568792 T T T

0.3832584742650381 0.4496907434597369 0.1390122112805030 T T T

0.3408850411272487 0.4529828113221018 0.1948379580002206 T T T

0.3401777114427526 0.4520691424152452 0.3057178196238151 T T T

0.1921025885217452 0.3952284659423402 0.0281865601713520 T T T

0.2932277792870993 0.4444904189106218 0.1395416868320814 T T T

0.2425890018514761 0.4241744110601895 0.1950593735023510 T T T

0.2422806925442018 0.4230409253607498 0.3058226933302180 T T T

0.1029057087461538 0.3094227558437415 0.0281543310421701 T T T

0.1922926081816810 0.3947320353499087 0.1386122778104697 T T T

0.1453142015659688 0.3550108824110463 0.1950256034848750 T T T

0.1460098078246408 0.3547943683723800 0.3057411077509125 T T T

0.0448759348916039 0.2085600816115368 0.0279479328170440 T T T

0.1031389757949911 0.3091299451167698 0.1394806920825823 T T T

0.0691802422106272 0.2594073922157029 0.1948320181364832 T T T

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|--------------------|--------------------|--------------------|---|---|---|
| 0.0699736145603724 | 0.2597670047770651 | 0.3057058506683539 | T | T | T |
| 0.0324336088735161 | 0.1153896655272495 | 0.0279492489194757 | T | T | T |
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| 0.0327719937954132 | 0.1596779730990474 | 0.3057300417129483 | T | T | T |
| 0.0687479062187606 | 0.0517483357480387 | 0.0279337848761763 | T | T | T |
| 0.0323653266139419 | 0.1153009414219064 | 0.1389972620759614 | T | T | T |
| 0.0446817627045785 | 0.0786136488912273 | 0.1945849720790003 | T | T | T |
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| 0.2426406577284285 | 0.0595545701365391 | 0.1390171361695138 | T | T | T |
| 0.2931943326204698 | 0.0901353167639568 | 0.1945935811340611 | T | T | T |
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| 0.4402217918031827 | 0.2764271592084355 | 0.9723557972099186 | T | T | T |
| 0.4524908536861191 | 0.3254002524915944 | 0.8057580908353574 | T | T | T |
| 0.1922253740281148 | 0.3949881056025830 | 0.3590782048954446 | T | T | T |
| 0.1690322738273903 | 0.4463693584219989 | 0.4766591538118338 | T | T | T |
| 0.2126660034810992 | 0.5000274764687068 | 0.4335235113604246 | T | T | T |
| 0.2313993969830672 | 0.5188178062585348 | 0.4974083623766994 | T | T | T |

### 1.2.3 OOH adsorbate on B-doped CNT

OOH\_B-CNT(5,5) ### KPOINTS: 2x2x3 ### E= -472.49864401 eV

1.0000000000000000

13.8564000000000007 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3947799999999999

C B O H

59 1 2 1

Selective dynamics

Direct

0.5605310612199377 0.4222899115854742 0.0876631139893960 T T T

0.5605505589049028 0.4223039124611705 0.4207833582144551 T T T

0.5598446073947696 0.4219021695899863 0.7542473413943898 T T T

0.4791854135385381 0.5419449699626122 0.0878484905873459 T T T

0.4792148455809995 0.5419730160986319 0.4204929873623754 T T T

0.4759805041533904 0.5404852286349547 0.7542141795310127 T T T

0.3940846467094690 0.5487806772291062 0.0880401210859946 T T T

0.3942180998809874 0.5490223645597698 0.4203442833905963 T T T

0.3912954834597211 0.5484388362706759 0.7541224727399469 T T T

0.1180770323330507 0.3457875562974817 0.0881999313145307 T T T

0.1184480377309335 0.3458281130873672 0.4207996763201593 T T T

0.1111826156795637 0.3435781434746616 0.7544584643436575 T T T

0.0828991110073681 0.1549481419832554 0.0882197872119728 T T T

0.0828407551214527 0.1548745630121660 0.4205642165953034 T T T

0.0817178339880449 0.1542405420926430 0.7544179505723169 T T T

0.1216914601274951 0.0918195860668283 0.0879880814772636 T T T

0.1216574867827186 0.0917752647814931 0.4206677518910478 T T T

0.1213821442679299 0.0914489039888410 0.7543779981005443 T T T

0.2896835190823319 0.0787644487124612 0.0877826031518691 T T T

0.2896788954822312 0.0787765505324982 0.4208406201636498 T T T

0.2895619531087552 0.0785014196424109 0.7543294675040060 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3924596983191126 | 0.1344890276492812 | 0.0879121902992121 | T | T | T |
| 0.3924436331028733 | 0.1345038378114882 | 0.4207269227718133 | T | T | T |
| 0.3924531624283875 | 0.1344983347767985 | 0.7543161807754835 | T | T | T |
| 0.5423137566390729 | 0.3255084411466863 | 0.0877454776477528 | T | T | T |
| 0.5423000089988842 | 0.3255107826249318 | 0.4207993213670954 | T | T | T |
| 0.5423358512335826 | 0.3254269138127128 | 0.7542774193352383 | T | T | T |
| 0.1940944141413598 | 0.4446288361343805 | 0.0899273326365758 | T | T | T |
| 0.1944142688990390 | 0.4445252187499044 | 0.4185863273889986 | T | T | T |
| 0.2430119938365103 | 0.4834610181248712 | 0.2541891518696165 | T | T | T |
| 0.2406243548888176 | 0.4900265833105502 | 0.5812855414077512 | T | T | T |
| 0.2406116559682890 | 0.4899559790747591 | 0.9272360410954770 | T | T | T |
| 0.5548343111520524 | 0.4640182252019219 | 0.2541989786621788 | T | T | T |
| 0.5531343539732453 | 0.4633357563052124 | 0.5878561011545663 | T | T | T |
| 0.5531073462802036 | 0.4633229527725291 | 0.9205855165155639 | T | T | T |
| 0.1538365413236482 | 0.0726070662937184 | 0.2543109626876121 | T | T | T |
| 0.1542418475517743 | 0.0730478890129835 | 0.5878205862318056 | T | T | T |
| 0.1542661091365515 | 0.0730583737112160 | 0.9208558238145709 | T | T | T |
| 0.2396955119637347 | 0.0660179516925150 | 0.2543262575269761 | T | T | T |
| 0.2396543425859912 | 0.0661551020643972 | 0.5878495026691264 | T | T | T |
| 0.2396555109645579 | 0.0661306956202555 | 0.9208140376489800 | T | T | T |
| 0.5133259054233811 | 0.5248805217446386 | 0.2541943243016945 | T | T | T |
| 0.5107755278230919 | 0.5230783350091298 | 0.5879064449614662 | T | T | T |
| 0.5107522334517567 | 0.5230621904807553 | 0.9205248651977046 | T | T | T |
| 0.0942586745979951 | 0.2940743405812579 | 0.2544530946932815 | T | T | T |
| 0.0933887845120830 | 0.2929027625084930 | 0.5902838221925365 | T | T | T |
| 0.0930686062916089 | 0.2928572772374472 | 0.9186649102788839 | T | T | T |
| 0.4407109778029886 | 0.1753321959307128 | 0.2543086725891965 | T | T | T |
| 0.4405774080742478 | 0.1757510115581895 | 0.5876673324699695 | T | T | T |
| 0.4406021210709959 | 0.1757433204522381 | 0.9209367936436703 | T | T | T |
| 0.5173822053756417 | 0.2734942489885867 | 0.2542802409353765 | T | T | T |
| 0.5170328472248998 | 0.2734414456266799 | 0.5876823570713510 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5170513104532488 | 0.2734322708029759 | 0.9209020166759238 | T | T | T |
| 0.0764347655433170 | 0.1962964492534546 | 0.2544100609344998 | T | T | T |
| 0.0770664939422233 | 0.1966622722448986 | 0.5880195813746457 | T | T | T |
| 0.0770524324203657 | 0.1967290205418836 | 0.9208348790838782 | T | T | T |
| 0.3456590764096580 | 0.5384739452665392 | 0.2541571889204679 | T | T | T |
| 0.3422233364499134 | 0.5375245686838593 | 0.5848482977387178 | T | T | T |
| 0.3420926754106388 | 0.5372727409894891 | 0.9233723641528654 | T | T | T |
| 0.1741543718499804 | 0.4608724883302489 | 0.7544959365092793 | T | T | T |
| 0.1162516430640882 | 0.5112603865836621 | 0.7744801192722199 | T | T | T |
| 0.0469570370898880 | 0.4834832387337478 | 0.6209779776939978 | T | T | T |

OOH\_B-CNT(6,6) ### KPOINTS: 2x2x3 ### E= -568.70321821 eV

1.0000000000000000

14.7224000000000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3992800000000001

C B O H

71 1 2 1

Selective dynamics

Direct

0.6132289671175670 0.4930796734785570 0.0834992981029030 T T T

0.6132148791307652 0.4930589174889908 0.4166820131124149 T T T

0.6133119259786584 0.4931918529299453 0.7501041572620497 T T T

0.5278743179030977 0.5983730286301484 0.0836550970963443 T T T

0.5278400608763139 0.5983415710163210 0.4162490022830976 T T T

0.5282477862407144 0.5989867799622259 0.7499698859629684 T T T

0.4476103383347146 0.6051640044227741 0.0836337363972667 T T T

0.4476242322226037 0.6052075193878453 0.4160968478709258 T T T

0.4478885476306374 0.6063554504811541 0.7498839804464343 T T T

0.1682120944710830 0.4488127818977115 0.0849770051833763 T T T

0.1682788739641210 0.4487475597572091 0.4143232185958373 T T T

0.0680456495099866 0.2589670156285578 0.0836315024611382 T T T

0.0680520890945870 0.2589376085978484 0.4157896190211057 T T T

0.0679261847283163 0.2611108860932451 0.7496726834114317 T T T

0.0634561954110113 0.1732388666589055 0.0834679005590432 T T T

0.0633529761813403 0.1731736101779585 0.4161206168832158 T T T

0.0645831904063438 0.1757877814852427 0.7498085926568218 T T T

0.1449415890084964 0.0644614768474214 0.0833779468701788 T T T

0.1449757178063489 0.0645208602573593 0.4166628732841469 T T T

0.1454052927615173 0.0650841745084118 0.7499998694813383 T T T

0.2236575379025189 0.0550463409463822 0.0835451102830422 T T T

0.2236793729785864 0.0550997872577434 0.4167041499291635 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2236367381033338 | 0.0550260361613072 | 0.7501113520567423 | T | T | T |
| 0.4137728563388864 | 0.1353967953539931 | 0.0836681064538318 | T | T | T |
| 0.4137813727160486 | 0.1353699947761626 | 0.4166807985439230 | T | T | T |
| 0.4137133748692658 | 0.1356743114725453 | 0.7501818717845049 | T | T | T |
| 0.5008019067081622 | 0.2155883982967148 | 0.0836874976381655 | T | T | T |
| 0.5007869723310715 | 0.2155866015567220 | 0.4166480399195149 | T | T | T |
| 0.5009687378434393 | 0.2156175359901910 | 0.7501637244265146 | T | T | T |
| 0.6070036139393343 | 0.4063034553129515 | 0.0836363926594913 | T | T | T |
| 0.6070532100147698 | 0.4063136273136288 | 0.4166469254589227 | T | T | T |
| 0.6069085297152335 | 0.4062186928980414 | 0.7501424011683909 | T | T | T |
| 0.2566483864439024 | 0.5288524878822638 | 0.0833872179575661 | T | T | T |
| 0.2566556359509287 | 0.5287639444732497 | 0.4161792047678716 | T | T | T |
| 0.2577711104938042 | 0.5366603496306622 | 0.7497755063300402 | T | T | T |
| 0.0724625616450271 | 0.1361737637027535 | 0.2498281902377517 | T | T | T |
| 0.0735864041962216 | 0.1377787848302047 | 0.5833802829752249 | T | T | T |
| 0.0737109434067101 | 0.1378537575125804 | 0.9163121219601997 | T | T | T |
| 0.1136433410749064 | 0.0809801414070964 | 0.2499688961373621 | T | T | T |
| 0.1142904737823694 | 0.0822245652410592 | 0.5834840688948257 | T | T | T |
| 0.1143277217739687 | 0.0822417823904836 | 0.9164767386236615 | T | T | T |
| 0.5603821391098270 | 0.5832026627482050 | 0.2499810461608457 | T | T | T |
| 0.5602541377304063 | 0.5830740516214624 | 0.5834553155645472 | T | T | T |
| 0.5603045595011127 | 0.5831215193493270 | 0.9165107853913232 | T | T | T |
| 0.1341621515166058 | 0.4021727071632283 | 0.2496678848351610 | T | T | T |
| 0.1272663205475299 | 0.4037934644200952 | 0.5766034104376018 | T | T | T |
| 0.1272457587159640 | 0.4039053517073807 | 0.9224550427178647 | T | T | T |
| 0.2693466347070745 | 0.0631276838910154 | 0.2501439954769129 | T | T | T |
| 0.2694313067219594 | 0.0631942976167770 | 0.5834704079548310 | T | T | T |
| 0.2694215766529113 | 0.0631886985678676 | 0.9168158147976542 | T | T | T |
| 0.3658296052061181 | 0.1036532300493078 | 0.2501648239240538 | T | T | T |
| 0.3657786863028389 | 0.1039130399000399 | 0.5835777787520079 | T | T | T |
| 0.3657660143955323 | 0.1039328127259226 | 0.9167707516798830 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0815202637261467 | 0.3057018550668311 | 0.2496856918460766 | T | T | T |
| 0.0815913906007653 | 0.3082184169785107 | 0.5803322910313415 | T | T | T |
| 0.0815306499199188 | 0.3082648825103146 | 0.9189923795438130 | T | T | T |
| 0.3048221053049421 | 0.5586354283747580 | 0.2497631405631557 | T | T | T |
| 0.3058371570114750 | 0.5607582384211770 | 0.5852432677887142 | T | T | T |
| 0.3058120849788505 | 0.5607908417065501 | 0.9143568974071720 | T | T | T |
| 0.5374067809046096 | 0.2618141513134363 | 0.2501655699049712 | T | T | T |
| 0.5375634913438794 | 0.2618079883720426 | 0.5835131010032293 | T | T | T |
| 0.5375912340000516 | 0.2617942705230470 | 0.9168150325492418 | T | T | T |
| 0.5914353557640663 | 0.3585290074194394 | 0.2501546559177031 | T | T | T |
| 0.5912865670549255 | 0.3584006392987155 | 0.5835146509980976 | T | T | T |
| 0.5912615151494454 | 0.3583917008286672 | 0.9167890477730550 | T | T | T |
| 0.6036692051010537 | 0.5296312029341284 | 0.2500759280918315 | T | T | T |
| 0.6034310718932089 | 0.5296104771061421 | 0.5835742059469687 | T | T | T |
| 0.6034727820938377 | 0.5296475490282690 | 0.9165748029780584 | T | T | T |
| 0.4021480893710853 | 0.5975304392843203 | 0.2498388454216631 | T | T | T |
| 0.4019426142193356 | 0.5973451277871662 | 0.5833531122124612 | T | T | T |
| 0.4019190722520599 | 0.5973080138968492 | 0.9163621091636296 | T | T | T |
| 0.1499577958955403 | 0.4653258813115785 | 0.7492791823530882 | T | T | T |
| 0.0038920040474865 | 0.4597145691536439 | 0.7342342232214143 | T | T | T |
| 0.1042388893254926 | 0.5222608922736997 | 0.7478226569004178 | T | T | T |
| 0.9863392779272326 | 0.4623963325355063 | 0.8579877045424346 | T | T | T |

OOH\_B-CNT(7,7) ### KPOINTS: 1x1x3 ### E= -664.46587831 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3996889399999999

C N O H

83 1 2 1

Selective dynamics

Direct

0.1821616957140021 0.0467584281227217 0.0848254339406352 T T T

0.2646929341138564 0.0541207319285426 0.0849033385239390 T T T

0.0717713692434252 0.1159571994713309 0.0851442991444396 T T T

0.4455198453326170 0.1495730099923125 0.0849243379266802 T T T

0.0520409774763112 0.1833144926291390 0.0852926478985832 T T T

0.5268210863723883 0.2262657762333918 0.0849578105496742 T T T

0.0852994098940944 0.3553456083536953 0.0824474331782506 T T T

0.6392867020678697 0.4053945211584634 0.0849423804234986 T T T

0.1333682619241439 0.4457534044399897 0.0784858369556144 T T T

0.6598640818960508 0.4927798495173830 0.0848815231238353 T T T

0.3020958259623674 0.5972486350597178 0.0866374854675778 T T T

0.6165723557678733 0.6232728030320263 0.0847357251642276 T T T

0.3936091872124037 0.6394517978705909 0.0847199979157997 T T T

0.5576318217120015 0.6543327791029937 0.0847718432703343 T T T

0.0516141077809316 0.2239072068692917 0.2517126784729035 T T T

0.5625434718832873 0.2691173420054829 0.2515901545335710 T T T

0.0673474315725183 0.3097457141567442 0.2517901690725575 T T T

0.6194473315529410 0.3595822154145510 0.2515582603461768 T T T

0.1464027809412279 0.0540103988319188 0.2515135674472716 T T T

0.3098059799644308 0.0689302183801107 0.2516385774421738 T T T

0.0910392118518190 0.0892384713822085 0.2515669205543951 T T T

0.4011770798740089 0.1171303390528268 0.2516408001752965 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6595371587715031 | 0.5324572773540981 | 0.2514543822218650 | T | T | T |
| 0.2568725396208897 | 0.5716760783664927 | 0.2514593572183213 | T | T | T |
| 0.6377894832379483 | 0.5986054768139087 | 0.2513306613224054 | T | T | T |
| 0.4384645561649183 | 0.6533993119972941 | 0.2513233009854217 | T | T | T |
| 0.5213148366109350 | 0.6606043152000213 | 0.2512814281528514 | T | T | T |
| 0.1821382887128165 | 0.0467766728232546 | 0.4182189818841958 | T | T | T |
| 0.2646970733185484 | 0.0541997301039735 | 0.4182934039543936 | T | T | T |
| 0.0716362695017457 | 0.1158088069997929 | 0.4180737436961844 | T | T | T |
| 0.4455605066283101 | 0.1495407730715415 | 0.4183013346750660 | T | T | T |
| 0.0519832161099136 | 0.1832460259627855 | 0.4180721202769004 | T | T | T |
| 0.5268204858112155 | 0.2262418355777294 | 0.4182263336509511 | T | T | T |
| 0.0852115587514109 | 0.3551925104622871 | 0.4211030078879347 | T | T | T |
| 0.6393641832405501 | 0.4053998226036380 | 0.4181035976172563 | T | T | T |
| 0.1335358769452722 | 0.4456174852385470 | 0.4247172078376329 | T | T | T |
| 0.6597759250509647 | 0.4927202880070496 | 0.4180329031922185 | T | T | T |
| 0.3021595024539181 | 0.5969719692598237 | 0.4160553446045799 | T | T | T |
| 0.6165943050156171 | 0.6233119209957693 | 0.4178350440679353 | T | T | T |
| 0.3936874064788557 | 0.6394723456419968 | 0.4179074723030379 | T | T | T |
| 0.5577439536088874 | 0.6544826393143689 | 0.4177795669487415 | T | T | T |
| 0.1464868883950213 | 0.0541356079000178 | 0.5848616240206628 | T | T | T |
| 0.3097832495010143 | 0.0686149404163549 | 0.5849526164595290 | T | T | T |
| 0.0906046657077270 | 0.0888188214386508 | 0.5848216886135151 | T | T | T |
| 0.4010907413690856 | 0.1170450733685595 | 0.5849744913743404 | T | T | T |
| 0.0509652850318911 | 0.2217856036050376 | 0.5852378890943232 | T | T | T |
| 0.5624193888294632 | 0.2693063503298738 | 0.5849821500818936 | T | T | T |
| 0.0687220724382447 | 0.3080061850696764 | 0.5855321385215654 | T | T | T |
| 0.6194079888183773 | 0.3596134052442186 | 0.5849827766257931 | T | T | T |
| 0.1738553682699723 | 0.4872223358571633 | 0.5864185068467682 | T | T | T |
| 0.6595509382681808 | 0.5324552586424037 | 0.5848309081984965 | T | T | T |
| 0.2562958729027771 | 0.5642267077501804 | 0.5847398772391794 | T | T | T |
| 0.6375101629811981 | 0.5982186841854611 | 0.5847789050518986 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4382852550884286 | 0.6521363764325350 | 0.5850695238141186 | T | T | T |
| 0.5211425430173977 | 0.6601346041246190 | 0.5849440613636855 | T | T | T |
| 0.0709250950472348 | 0.1147679038326868 | 0.7516050160010216 | T | T | T |
| 0.0511485384313235 | 0.1820151216971219 | 0.7516805668558361 | T | T | T |
| 0.5268509098378734 | 0.2263108152149191 | 0.7515440749963795 | T | T | T |
| 0.0869459403623026 | 0.3531636469010156 | 0.7517496876070106 | T | T | T |
| 0.6395664025897478 | 0.4054720415698872 | 0.7514767188235328 | T | T | T |
| 0.1415829446184797 | 0.4435637196781512 | 0.7516443251612348 | T | T | T |
| 0.1822612517263863 | 0.0469715312404902 | 0.7515177386534297 | T | T | T |
| 0.2647569439276362 | 0.0540318967815782 | 0.7515271874359695 | T | T | T |
| 0.4454514500768930 | 0.1494898455631495 | 0.7515810612426745 | T | T | T |
| 0.6601051516489458 | 0.4929783922977890 | 0.7513807143062186 | T | T | T |
| 0.3011508979638854 | 0.5943852877590085 | 0.7514296721188900 | T | T | T |
| 0.6165850611595741 | 0.6231102288391694 | 0.7512742107421567 | T | T | T |
| 0.3935150131260428 | 0.6389566778544055 | 0.7513307164698506 | T | T | T |
| 0.5578201497096047 | 0.6545385691291022 | 0.7512666070624610 | T | T | T |
| 0.1465751248572038 | 0.0542404975498712 | 0.9182116908004468 | T | T | T |
| 0.3097568691268849 | 0.0685377064339780 | 0.9181561690008860 | T | T | T |
| 0.0907291480501553 | 0.0889600842257129 | 0.9183514925723084 | T | T | T |
| 0.4010728914897473 | 0.1170102023635021 | 0.9182176873282720 | T | T | T |
| 0.0509895731124314 | 0.2217940668370215 | 0.9181523359267609 | T | T | T |
| 0.5624498342027977 | 0.2692811774342204 | 0.9181101941462270 | T | T | T |
| 0.0688476113717969 | 0.3080894611006342 | 0.9179389305730458 | T | T | T |
| 0.6193556819817110 | 0.3596045693337983 | 0.9180488975232478 | T | T | T |
| 0.1735931665683726 | 0.4875364686035405 | 0.9167283203274661 | T | T | T |
| 0.6596848873521538 | 0.5325210188636319 | 0.9179161812148464 | T | T | T |
| 0.2562089574790605 | 0.5645993839743677 | 0.9180114101549877 | T | T | T |
| 0.6375479136706861 | 0.5982305153669869 | 0.9178127066302744 | T | T | T |
| 0.4382288579409914 | 0.6520530101017684 | 0.9175387295233526 | T | T | T |
| 0.5210646848041082 | 0.6599902226274650 | 0.9175916247573817 | T | T | T |
| 0.1558220281209726 | 0.5034991837879652 | 0.2518684466887844 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1146541851743261 | 0.6026544648262769 | 0.3915332116947198 | T | T | T |
| 0.1006647752393430 | 0.5460738807965811 | 0.2340303870722354 | T | T | T |
| 0.1514575624677399 | 0.6583522242496050 | 0.3365857152570017 | T | T | T |

OOH\_B-CNT(8,8) #### KPOINTS: 1x1x3 #### E= -760.00741172 eV

1.0000000000000000

17.3205080799999998 -10.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4003969100000004

C B O H

95 1 2 1

Selective dynamics

Direct

0.2515992964372580 0.0412422704113911 0.0828596183366618 T T T

0.1152767353830665 0.0506339864192998 0.0830139695222328 T T T

0.3323645342917451 0.0683953265403283 0.0828241010327079 T T T

0.0705078737074759 0.0879611427632349 0.0830138765701516 T T T

0.4923987581134294 0.1760478130897407 0.0827452532352090 T T T

0.0420401442978567 0.2128598575530125 0.0834817583892019 T T T

0.5613060254497826 0.2492610836170555 0.0827558329845069 T T T

0.0583114954091635 0.2907818232270625 0.0836869558498793 T T T

0.6545782443456889 0.4118944429360156 0.0827950766947833 T T T

0.1454311663508796 0.4545697863246926 0.0833192211801512 T T T

0.6725894873737989 0.4903573063859319 0.0828899460491918 T T T

0.2153880017473277 0.5281808720978279 0.0846317761771952 T T T

0.6406878528612805 0.6128299204247216 0.0828786637581490 T T T

0.3760467234506653 0.6296000830808949 0.0836993082175735 T T T

0.5931344590425889 0.6470656952158721 0.0828436981570196 T T T

0.4560792799514062 0.6547249683488683 0.0833761508814285 T T T

0.2131676979118321 0.0351378533963121 0.2495208476206381 T T T

0.1442203069121380 0.0396719812687960 0.2495841108949887 T T T

0.3735912369275390 0.0890009786615133 0.2494184942755551 T T T

0.4542555830513471 0.1433697152049988 0.2493938207529446 T T T

0.0412153891878307 0.1767646712807265 0.2498042314048636 T T T

0.6733792076726269 0.5265640265490418 0.2494801965991378 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2545248068662519 | 0.5575279549220772 | 0.2498432715651144 | T | T | T |
| 0.6571464307607062 | 0.5882850057747522 | 0.2495583284977007 | T | T | T |
| 0.5635390871870182 | 0.6568288497158288 | 0.2496530454828378 | T | T | T |
| 0.0555884887386613 | 0.1137181884853496 | 0.2497206958777127 | T | T | T |
| 0.5910602427938051 | 0.2888612166139985 | 0.2493887871829272 | T | T | T |
| 0.0732692822141908 | 0.3315338494164319 | 0.2499403978666911 | T | T | T |
| 0.6378898011462760 | 0.3708263897582180 | 0.2494143807941372 | T | T | T |
| 0.1176723276112398 | 0.4145206315723702 | 0.2499615343498352 | T | T | T |
| 0.3352441087766008 | 0.6099483717661818 | 0.2498104507979457 | T | T | T |
| 0.4943818690404611 | 0.6604192251278238 | 0.2497130382460040 | T | T | T |
| 0.2516056850991966 | 0.0412561172101824 | 0.4161355802132931 | T | T | T |
| 0.1152566076595565 | 0.0506013562320132 | 0.4162094513074783 | T | T | T |
| 0.3323629861809788 | 0.0683984000940043 | 0.4160493680781800 | T | T | T |
| 0.0704921098538390 | 0.0879424367520622 | 0.4163651929070908 | T | T | T |
| 0.4924032269420338 | 0.1760471799940987 | 0.4160365969138295 | T | T | T |
| 0.0420580730053027 | 0.2128595619410694 | 0.4161870177189397 | T | T | T |
| 0.5613088321293767 | 0.2492619351825396 | 0.4160165054762594 | T | T | T |
| 0.0583562538215910 | 0.2907842530479094 | 0.4161347047601029 | T | T | T |
| 0.6545775496919809 | 0.4118970220546116 | 0.4160402843103712 | T | T | T |
| 0.1454928289191504 | 0.4546225364903438 | 0.4166204344143115 | T | T | T |
| 0.6726095233306756 | 0.4903697691151455 | 0.4160446141424767 | T | T | T |
| 0.2154622485693682 | 0.5281886563425757 | 0.4150946517579831 | T | T | T |
| 0.6406940233137471 | 0.6128413936097044 | 0.4162787847063878 | T | T | T |
| 0.3760695870826261 | 0.6295460701479864 | 0.4158891974042864 | T | T | T |
| 0.5931433038715234 | 0.6470802024511872 | 0.4164364964556951 | T | T | T |
| 0.4560779076128378 | 0.6546591936990145 | 0.4161084410995148 | T | T | T |
| 0.2132620458622822 | 0.0353231264881398 | 0.5830591547705504 | T | T | T |
| 0.1445614085381300 | 0.0400382095086854 | 0.5830399409970152 | T | T | T |
| 0.3736203341423855 | 0.0892148184107911 | 0.5829213347994221 | T | T | T |
| 0.0555462646220586 | 0.1138265238806802 | 0.5832686303080383 | T | T | T |
| 0.4541664660745914 | 0.1434375005539171 | 0.5828894559130474 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0412377739645275 | 0.1767834756929648 | 0.5833340941852088 | T | T | T |
| 0.5909768191484484 | 0.2889917880190985 | 0.5827792751620490 | T | T | T |
| 0.0729041736873184 | 0.3315643256532338 | 0.5833200206148511 | T | T | T |
| 0.6379599588266583 | 0.3708297453940128 | 0.5828003877798846 | T | T | T |
| 0.1146163897921109 | 0.4139603707479814 | 0.5852049297244237 | T | T | T |
| 0.6728905406934910 | 0.5262377651366367 | 0.5828708587113459 | T | T | T |
| 0.2524601508158207 | 0.5646651396440687 | 0.5767242141776203 | T | T | T |
| 0.6568882064367429 | 0.5879991985583857 | 0.5828682934710746 | T | T | T |
| 0.3333786021558796 | 0.6116475282970288 | 0.5804250247023557 | T | T | T |
| 0.5626210828218580 | 0.6561494649338173 | 0.5832142697538139 | T | T | T |
| 0.4933620705802119 | 0.6597170515271794 | 0.5833152252488186 | T | T | T |
| 0.2514744297331138 | 0.0408992878129106 | 0.7494911669109321 | T | T | T |
| 0.1153400715523302 | 0.0506239354155071 | 0.7496272331588011 | T | T | T |
| 0.3323295260994475 | 0.0682173977290545 | 0.7494313267146908 | T | T | T |
| 0.4924414637535449 | 0.1759890684986401 | 0.7493816241268575 | T | T | T |
| 0.0415097309363975 | 0.2126853740099452 | 0.7498199268405987 | T | T | T |
| 0.1377502667511605 | 0.4545180501901144 | 0.7499639791608236 | T | T | T |
| 0.6403505028308429 | 0.6124968719580690 | 0.7495827840702211 | T | T | T |
| 0.5927107189997809 | 0.6465273755832469 | 0.7496469861286021 | T | T | T |
| 0.0703548436709682 | 0.0878782348913375 | 0.7497121810570568 | T | T | T |
| 0.5613499279723848 | 0.2493059245209326 | 0.7493830082396776 | T | T | T |
| 0.0571368562566519 | 0.2907656182477452 | 0.7498910992316922 | T | T | T |
| 0.6548411661659259 | 0.4119089422282015 | 0.7494155881520468 | T | T | T |
| 0.6722848901110228 | 0.4901653751784340 | 0.7494695825314676 | T | T | T |
| 0.3744584579063113 | 0.6309279957673204 | 0.7497814095826943 | T | T | T |
| 0.4543110613361355 | 0.6542416855831361 | 0.7497557692921079 | T | T | T |
| 0.2132552179005341 | 0.0353069250538821 | 0.9159609336889254 | T | T | T |
| 0.1445670689192283 | 0.0400442626223943 | 0.9161365577282800 | T | T | T |
| 0.3736220779046619 | 0.0892135959385213 | 0.9159256633757060 | T | T | T |
| 0.0555318739416057 | 0.1138252998923551 | 0.9161904066754628 | T | T | T |
| 0.4541677999566321 | 0.1434380450957958 | 0.9159110034841410 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0412100415440433 | 0.1767784210024650 | 0.9162800321688488 | T | T | T |
| 0.5909802996685389 | 0.2889920555252503 | 0.9159968880233329 | T | T | T |
| 0.0728383913076727 | 0.3315579007957702 | 0.9165148544186886 | T | T | T |
| 0.6379665527436376 | 0.3708285841051282 | 0.9159969220602581 | T | T | T |
| 0.1145488046490396 | 0.4139568245826800 | 0.9147176013062749 | T | T | T |
| 0.6728785771519813 | 0.5262273828673434 | 0.9160935802042295 | T | T | T |
| 0.2523859321241911 | 0.5644764722812630 | 0.9227538763902969 | T | T | T |
| 0.6568974544655825 | 0.5880046884976765 | 0.9162539480746625 | T | T | T |
| 0.3333237346868287 | 0.6116964477744876 | 0.9191542125753299 | T | T | T |
| 0.5626230230879287 | 0.6561702459418991 | 0.9161286819409582 | T | T | T |
| 0.4933799828015136 | 0.6597854722116709 | 0.9161802400254304 | T | T | T |
| 0.2005828026493593 | 0.5447330788390375 | 0.7496752052132600 | T | T | T |
| 0.2098325745120262 | 0.6715315876967879 | 0.7430167092288129 | T | T | T |
| 0.1543865057740973 | 0.5866597504564134 | 0.7496384069321848 | T | T | T |
| 0.2014683898766822 | 0.6857844164431118 | 0.8628373400558479 | T | T | T |

OOH\_B-CNT(9,9) ### KPOINTS: 1x1x3 ### E= -855.39313124 eV

1.000000000000000

18.1865334800000014 -10.500000000000000 0.000000000000000

0.000000000000000 21.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 7.4005503900000003

C B O H

107 1 2 1

Selective dynamics

Direct

0.1974360088648840 0.0259975770109197 0.0843950614870245 T T T

0.1346750417702855 0.0351691245293344 0.0844882403539579 T T T

0.3472326137984245 0.0641055328913852 0.0843007157218015 T T T

0.4253358360495959 0.1078862608080917 0.0841510499724452 T T T

0.0523774957145069 0.1084837265726383 0.0845067799571617 T T T

0.0363285295414911 0.1668881283986567 0.0846528393256652 T T T

0.5681730472184612 0.2332657377071624 0.0840558819068621 T T T

0.6253958409763448 0.3082005199463904 0.0840524203595501 T T T

0.0533518314333125 0.3097975946400405 0.0849224152149352 T T T

0.0832182769152201 0.3875815219238080 0.0831859841465254 T T T

0.6973029442393512 0.4638466942493532 0.0842144524921455 T T T

0.7077178081542267 0.5362584889615120 0.0843197804609088 T T T

0.1955512464343604 0.5416386900318929 0.0912706238542982 T T T

0.2694042576468194 0.5988533478644530 0.0875297202106300 T T T

0.6726095291315047 0.6500315957547005 0.0844336142336719 T T T

0.6285936535800466 0.6841014265113731 0.0845313468938030 T T T

0.4261236872099047 0.6798452221739931 0.0846009928136401 T T T

0.5013341675031366 0.6985546116736889 0.0844793560990891 T T T

0.2327467978707929 0.0286442166827479 0.2512414945109291 T T T

0.3080875604903324 0.0478470737411403 0.2511831046421475 T T T

0.4634886167324844 0.1350976027259827 0.2509149911489061 T T T

0.5352909620142763 0.1980892629712514 0.2508243425165154 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0437443125945344 | 0.2720137712909330 | 0.2520000166008290 | T | T | T |
| 0.1074408869251314 | 0.4277240478459376 | 0.2517737900165380 | T | T | T |
| 0.1649305762917760 | 0.5035246290319589 | 0.2531749332877334 | T | T | T |
| 0.3098271630119752 | 0.6236886775567415 | 0.2521099611521857 | T | T | T |
| 0.3878100049005275 | 0.6649157603337887 | 0.2517253173721726 | T | T | T |
| 0.1081979516409643 | 0.0470936030331612 | 0.2514032251713633 | T | T | T |
| 0.0669673800756452 | 0.0841293184114356 | 0.2514062224485588 | T | T | T |
| 0.0348774838722032 | 0.2001591517813880 | 0.2517911159670186 | T | T | T |
| 0.6491693040437845 | 0.3472370764085697 | 0.2508131876276085 | T | T | T |
| 0.6854263703993181 | 0.4254589712634550 | 0.2509098928858077 | T | T | T |
| 0.7059845289482777 | 0.5693865093703964 | 0.2510516903060711 | T | T | T |
| 0.6882938925251373 | 0.6266036410695227 | 0.2511034007278788 | T | T | T |
| 0.6008764757606599 | 0.6943892703611092 | 0.2511794337089944 | T | T | T |
| 0.5370373986645963 | 0.7017256269998656 | 0.2511641702875410 | T | T | T |
| 0.1974611588717878 | 0.0259323368921830 | 0.4178058487239342 | T | T | T |
| 0.1346222895597040 | 0.0351496420094219 | 0.4178881507577736 | T | T | T |
| 0.3471678125259478 | 0.0638702451320022 | 0.4176233542979927 | T | T | T |
| 0.4253385238606116 | 0.1078429868230509 | 0.4175187341024053 | T | T | T |
| 0.0525274148849611 | 0.1084672268503918 | 0.4180598557025437 | T | T | T |
| 0.0364694553374928 | 0.1669869271955182 | 0.4181654457456948 | T | T | T |
| 0.5682192319979801 | 0.2331892662515001 | 0.4174358509544586 | T | T | T |
| 0.6254304741481392 | 0.3082406254474612 | 0.4174351285828651 | T | T | T |
| 0.0537959510350872 | 0.3099369148606390 | 0.4183224620685934 | T | T | T |
| 0.0862063260115983 | 0.3886997484565088 | 0.4183857002196247 | T | T | T |
| 0.6975109962788153 | 0.4638870847439127 | 0.4175116808941460 | T | T | T |
| 0.7078109946898041 | 0.5362785675675386 | 0.4176184572379404 | T | T | T |
| 0.1993797835098349 | 0.5363673846380969 | 0.4182896344974305 | T | T | T |
| 0.2717348034501963 | 0.5978170036326209 | 0.4181857292447167 | T | T | T |
| 0.6724840736333044 | 0.6498547390436251 | 0.4177851819580868 | T | T | T |
| 0.6284098555186793 | 0.6838728097858890 | 0.4178723549818939 | T | T | T |
| 0.4268445429112961 | 0.6801796107831077 | 0.4180905873752015 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5018344823563103 | 0.6987904330593530 | 0.4180316439274643 | T | T | T |
| 0.2327652641869377 | 0.0286761494521990 | 0.5843037962891332 | T | T | T |
| 0.3080952474272284 | 0.0478880148287491 | 0.5841409754061253 | T | T | T |
| 0.1082011206234069 | 0.0470873693160360 | 0.5844390961778785 | T | T | T |
| 0.0669968235756986 | 0.0841482175134556 | 0.5846325405725903 | T | T | T |
| 0.4634848827041818 | 0.1350936354375600 | 0.5840912842803060 | T | T | T |
| 0.5352810582801172 | 0.1980828833453101 | 0.5840848262448511 | T | T | T |
| 0.0349927570741697 | 0.2002065496795698 | 0.5845967898937312 | T | T | T |
| 0.0438347258706943 | 0.2720399576899428 | 0.5845632158669984 | T | T | T |
| 0.6491896051810014 | 0.3472438394907739 | 0.5840654925660598 | T | T | T |
| 0.6854325966564488 | 0.4254610046147039 | 0.5840694108489166 | T | T | T |
| 0.1074748897193179 | 0.4278110991233265 | 0.5849956408785396 | T | T | T |
| 0.1649047377093510 | 0.5036632925853018 | 0.5834577801625627 | T | T | T |
| 0.7059736275272416 | 0.5693683812100836 | 0.5842560099735924 | T | T | T |
| 0.6882283884001053 | 0.6265399400864884 | 0.5844101764146471 | T | T | T |
| 0.3098293272975162 | 0.6236714827974996 | 0.5842401274329722 | T | T | T |
| 0.3877957153254910 | 0.6648154682523720 | 0.5845125463380129 | T | T | T |
| 0.6008176421729349 | 0.6942869543545795 | 0.5846403947179547 | T | T | T |
| 0.5369566852222610 | 0.7015634482655592 | 0.5848646916660661 | T | T | T |
| 0.1974234145458182 | 0.0259721141913895 | 0.7512049512250447 | T | T | T |
| 0.1346515512406377 | 0.0351392179573769 | 0.7513059805207069 | T | T | T |
| 0.3472351660944127 | 0.0641056810268128 | 0.7509356037591488 | T | T | T |
| 0.4253418027115733 | 0.1078786670785509 | 0.7508877734968802 | T | T | T |
| 0.5681609229203753 | 0.2332743086158238 | 0.7508094168830234 | T | T | T |
| 0.0534246930522128 | 0.3098141144637228 | 0.7516462943166248 | T | T | T |
| 0.0832903467803207 | 0.3876038191957346 | 0.7535075045944635 | T | T | T |
| 0.1953738774004251 | 0.5420857223880986 | 0.7450664251974302 | T | T | T |
| 0.2693707293528813 | 0.5989657411629588 | 0.7487815557589272 | T | T | T |
| 0.4260980838779166 | 0.6797518986310382 | 0.7516005698852098 | T | T | T |
| 0.0524159471938681 | 0.1085068568589145 | 0.7516129234389719 | T | T | T |
| 0.0364056391269412 | 0.1669289586279561 | 0.7516779008825732 | T | T | T |

|                    |                    |                     |   |   |   |
|--------------------|--------------------|---------------------|---|---|---|
| 0.6253925651060643 | 0.3082083714396509 | 0.7507939559006445  | T | T | T |
| 0.6973117296284786 | 0.4638499566081031 | 0.7507994461025626  | T | T | T |
| 0.7077548024243046 | 0.5362710501259875 | 0.7509308756939801  | T | T | T |
| 0.6725556275716491 | 0.6499652992082267 | 0.7511428929949600  | T | T | T |
| 0.6285234995273922 | 0.6840082512599392 | 0.7512340614375175  | T | T | T |
| 0.5012804893533617 | 0.6984245167192966 | 0.7515967691840177  | T | T | T |
| 0.2326330294587414 | 0.0285177811928822 | 0.9177532830114138  | T | T | T |
| 0.3081361176340443 | 0.0478561594348468 | 0.9176354292991720  | T | T | T |
| 0.1080669120241603 | 0.0469142733951607 | 0.9179298588650413  | T | T | T |
| 0.0665742627254927 | 0.0838511841330110 | 0.9180311270795036  | T | T | T |
| 0.4635544956794355 | 0.1349541334749637 | 0.9174867328241992  | T | T | T |
| 0.5353650097885714 | 0.1981013622001696 | 0.9174383942850236  | T | T | T |
| 0.0343047259952907 | 0.1998601559980819 | 0.9181940510812062  | T | T | T |
| 0.0427502602824470 | 0.2718250557199868 | 0.9182603839916086  | T | T | T |
| 0.6492852638374761 | 0.3471993203432541 | 0.9174166741124252  | T | T | T |
| 0.6854071008283608 | 0.4254709308648363 | 0.9174695584055563  | T | T | T |
| 0.0998421475476255 | 0.4260759569240957 | 0.9183452034162216  | T | T | T |
| 0.7060179122696161 | 0.5694384086971496 | 0.9176467221591350  | T | T | T |
| 0.6883260971310765 | 0.6266494617944822 | 0.9177601244287172  | T | T | T |
| 0.3079185431889115 | 0.6246656359108175 | 0.9181366265213308  | T | T | T |
| 0.3861645475210657 | 0.6642776832761517 | 0.9181214811375255  | T | T | T |
| 0.6009986943858244 | 0.6946425806759199 | 0.9179107665185005  | T | T | T |
| 0.5370064014891699 | 0.7016643031827540 | 0.9180174591897987  | T | T | T |
| 0.1457953921385816 | 0.5140632865005884 | 0.9183375726677389  | T | T | T |
| 0.1234517941188885 | 0.6184746906357135 | -0.0760878825143971 | T | T | T |
| 0.0869306725371873 | 0.5365239742347108 | 0.9198385703611321  | T | T | T |
| 0.1055869830294784 | 0.6245138621057356 | 0.0401407989998445  | T | T | T |

OOH\_B-CNT(10,10) ### KPOINTS: 1x1x3 ### E= -950.63362481 eV

1.0000000000000000

19.0525588799999994 -11.0000000000000000 0.0000000000000000

0.0000000000000000 22.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.4010841699999999

C B O H

119 1 2 1

Selective dynamics

Direct

0.1874543477437372 0.0234508058357111 0.0837444848604583 T T T

0.2544237885161305 0.0282595943662012 0.0837699783650181 T T T

0.0820793827082490 0.0616562588887324 0.0838604616921409 T T T

0.4016737966491187 0.0835273538834677 0.0836786415743412 T T T

0.0487408999908513 0.1029168280559546 0.0838879603111479 T T T

0.4752899057100626 0.1313957899581850 0.0836806465312158 T T T

0.0267241786812623 0.2193691135758191 0.0842254912827918 T T T

0.6071198732833121 0.2570348563845025 0.0836085749031232 T T T

0.0378836229412430 0.2889699102178169 0.0843917501955336 T T T

0.6591299927229928 0.3294735580760215 0.0835873024517812 T T T

0.1013142383868260 0.4380884101112058 0.0838840466817410 T T T

0.7242513879818154 0.4778697154885191 0.0836106236530199 T T T

0.1552182108052386 0.5108765768773275 0.0851630633625427 T T T

0.7355847052654169 0.5474881423677310 0.0836411103663910 T T T

0.2888981919390807 0.6334615216037437 0.0844724186177027 T T T

0.7150712445555667 0.6649300487728379 0.0836693605967825 T T T

0.3623611264476971 0.6808821220547931 0.0841034571314763 T T T

0.6827042472796346 0.7070662423575328 0.0836890278443498 T T T

0.5096337646815510 0.7386283898272519 0.0836080299271224 T T T

0.5772419739195929 0.7449074161607124 0.0836816469175561 T T T

0.0375405876096709 0.1281885892362189 0.2505192153521160 T T T

0.5770597395217472 0.2226227339760511 0.2502233225039900 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0485809532155109 | 0.3254552800200597 | 0.2505851193150411 | T | T | T |
| 0.0809973786551382 | 0.4008090645016139 | 0.2505635157874114 | T | T | T |
| 0.1872769809787651 | 0.5430363124125112 | 0.2504657439420914 | T | T | T |
| 0.7358115345016588 | 0.5800568467205216 | 0.2502864381893440 | T | T | T |
| 0.2536881675777085 | 0.6054625811775287 | 0.2505033237805284 | T | T | T |
| 0.3998902257584844 | 0.7003581885461654 | 0.2504744282154588 | T | T | T |
| 0.6610900984994088 | 0.7227894708883927 | 0.2503987110442112 | T | T | T |
| 0.6080103683436887 | 0.7417916685501266 | 0.2504310217644712 | T | T | T |
| 0.1569759161185590 | 0.0270427807349142 | 0.2503963134270930 | T | T | T |
| 0.2901600705459235 | 0.0365110345835087 | 0.2503213224522866 | T | T | T |
| 0.1039440364855178 | 0.0462718591986881 | 0.2504410903809189 | T | T | T |
| 0.3641899097046439 | 0.0642586211767028 | 0.2502895608579895 | T | T | T |
| 0.5107989416974403 | 0.1595072944208074 | 0.2502406986647874 | T | T | T |
| 0.0264713028840367 | 0.1868137063207741 | 0.2505604521209600 | T | T | T |
| 0.6805955563931568 | 0.3667807988212268 | 0.2502247096568569 | T | T | T |
| 0.7132033842354846 | 0.4413368290604470 | 0.2502406984822205 | T | T | T |
| 0.7256058490071353 | 0.6390536869658693 | 0.2503299363399281 | T | T | T |
| 0.4738415422434786 | 0.7296310892533058 | 0.2504777154366649 | T | T | T |
| 0.1874664091038592 | 0.0234728345991382 | 0.4170066049907952 | T | T | T |
| 0.2544226070261662 | 0.0282578552187464 | 0.4168919272384819 | T | T | T |
| 0.0820499753103392 | 0.0616245847544072 | 0.4170500489686467 | T | T | T |
| 0.4016744887241174 | 0.0835274507750677 | 0.4168703255541255 | T | T | T |
| 0.0487336463268279 | 0.1029051979164622 | 0.4171111967238056 | T | T | T |
| 0.4752913504375674 | 0.1313957830583555 | 0.4168144129208650 | T | T | T |
| 0.0267442182661554 | 0.2193801539348399 | 0.4169170887948966 | T | T | T |
| 0.6071204670289909 | 0.2570360877012816 | 0.4168329418893494 | T | T | T |
| 0.0378959553588220 | 0.2889731093438897 | 0.4167821683941524 | T | T | T |
| 0.6591317208044545 | 0.3294722773544727 | 0.4168612476585068 | T | T | T |
| 0.1014257723479309 | 0.4380721076898871 | 0.4172956463657685 | T | T | T |
| 0.7242598746055527 | 0.4778722816855570 | 0.4168933716751315 | T | T | T |
| 0.1554609016042030 | 0.5107394641458357 | 0.4157974948446410 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7355809367323171 | 0.5474832615134456 | 0.4169036329969728 | T | T | T |
| 0.2889890832631888 | 0.6333534360665648 | 0.4165260892570562 | T | T | T |
| 0.7150914815238418 | 0.6649566539901479 | 0.4170126347495616 | T | T | T |
| 0.3623924754045744 | 0.6808248620110816 | 0.4168916637527829 | T | T | T |
| 0.6827423340095480 | 0.7071042617459118 | 0.4170923295991796 | T | T | T |
| 0.5096223636096076 | 0.7385985442348268 | 0.4173511983805894 | T | T | T |
| 0.5772252067695551 | 0.7448757680013003 | 0.4172112339740716 | T | T | T |
| 0.1570155319485244 | 0.0272174997672857 | 0.5838790583885205 | T | T | T |
| 0.2902317577219451 | 0.0364948556774545 | 0.5836835045888450 | T | T | T |
| 0.1039890192205739 | 0.0462833128013163 | 0.5838713642705718 | T | T | T |
| 0.3641792538273389 | 0.0643006342056603 | 0.5836543659622999 | T | T | T |
| 0.0374781365254265 | 0.1283002638742189 | 0.5839817770384172 | T | T | T |
| 0.5107813773979961 | 0.1595412065715700 | 0.5836056200366438 | T | T | T |
| 0.0263557118769245 | 0.1867636639034377 | 0.5840521981984856 | T | T | T |
| 0.5770194708286190 | 0.2226080924691900 | 0.5835770910027673 | T | T | T |
| 0.0479545811817912 | 0.3252379550470633 | 0.5838806304620916 | T | T | T |
| 0.6805638789678677 | 0.3668335956715846 | 0.5835453495889447 | T | T | T |
| 0.0777573511979192 | 0.3996366991507947 | 0.5855983285514385 | T | T | T |
| 0.7131761860147172 | 0.4413341571401211 | 0.5836055412921661 | T | T | T |
| 0.1832312859523923 | 0.5478538773751297 | 0.5771956622528895 | T | T | T |
| 0.7359047490180751 | 0.5801160866320867 | 0.5835857599021907 | T | T | T |
| 0.2513425817728087 | 0.6066492999790430 | 0.5810044332304797 | T | T | T |
| 0.7256674900605571 | 0.6390709285358098 | 0.5835818535308007 | T | T | T |
| 0.3991285463934757 | 0.7000937043112229 | 0.5839844950459862 | T | T | T |
| 0.6609106333181836 | 0.7225748922145034 | 0.5837620649289320 | T | T | T |
| 0.4732643100693616 | 0.7291608413119450 | 0.5839422961975708 | T | T | T |
| 0.6078905490779565 | 0.7415874064914069 | 0.5837573417325108 | T | T | T |
| 0.0820682796506599 | 0.0616041240865205 | 0.7504550232125544 | T | T | T |
| 0.0485289974503181 | 0.1028397872521073 | 0.7505036154975840 | T | T | T |
| 0.6071288903181385 | 0.2569859793869584 | 0.7502234300611896 | T | T | T |
| 0.0935460229368341 | 0.4362300715404245 | 0.7505775633618700 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7355851278067318 | 0.5474975522173322 | 0.7502705371376318 | T | T | T |
| 0.2868378797046510 | 0.6344443745710562 | 0.7504676954877050 | T | T | T |
| 0.3607154544341384 | 0.6803573517059021 | 0.7505190330854069 | T | T | T |
| 0.6823499525105703 | 0.7066790846764257 | 0.7503914782620958 | T | T | T |
| 0.5770230829646386 | 0.7447112050281930 | 0.7504508768215299 | T | T | T |
| 0.1874580803866905 | 0.0235524477587441 | 0.7503703916646817 | T | T | T |
| 0.2544355479760949 | 0.0281627095545479 | 0.7503321215728155 | T | T | T |
| 0.4016144283731953 | 0.0834686557464566 | 0.7502765349721827 | T | T | T |
| 0.4752943173182360 | 0.1313725798730411 | 0.7502489622111763 | T | T | T |
| 0.0260740783939529 | 0.2190660692171745 | 0.7505779951474001 | T | T | T |
| 0.0367703171786764 | 0.2887869843042221 | 0.7505937967471745 | T | T | T |
| 0.6591592629810874 | 0.3295086254240609 | 0.7502205625371737 | T | T | T |
| 0.7242553027781585 | 0.4778653101044976 | 0.7502477476331463 | T | T | T |
| 0.7148628563322009 | 0.6647177210926767 | 0.7503383729880322 | T | T | T |
| 0.5094440515164130 | 0.7383314723086062 | 0.7504826165408589 | T | T | T |
| 0.1570059670569391 | 0.0271974643310498 | 0.9169021903823772 | T | T | T |
| 0.2902325053750935 | 0.0364996561495120 | 0.9169518357035740 | T | T | T |
| 0.1040084950522546 | 0.0463019664805483 | 0.9170079639830424 | T | T | T |
| 0.3641789331571009 | 0.0642994598741107 | 0.9169198491703240 | T | T | T |
| 0.0374605388188281 | 0.1282896506494798 | 0.9170483925344790 | T | T | T |
| 0.5107813510370293 | 0.1595406763969206 | 0.9168748945451478 | T | T | T |
| 0.0263201445747613 | 0.1867436562489189 | 0.9170717818881209 | T | T | T |
| 0.5770195796499104 | 0.2226068351848222 | 0.9168646723393810 | T | T | T |
| 0.0479513243076753 | 0.3252481455356229 | 0.9173044264736824 | T | T | T |
| 0.6805626518289584 | 0.3668336917568089 | 0.9169045017843318 | T | T | T |
| 0.0777176173535693 | 0.3996582117116624 | 0.9155912102882197 | T | T | T |
| 0.7131753775962312 | 0.4413332450137825 | 0.9168872575108864 | T | T | T |
| 0.1829221848280563 | 0.5480044030904161 | 0.9235393202553496 | T | T | T |
| 0.7359349552643729 | 0.5801349224028798 | 0.9169847741001670 | T | T | T |
| 0.2511422660909760 | 0.6068203922710305 | 0.9199519915654376 | T | T | T |
| 0.7256830502908654 | 0.6390729083288098 | 0.9170718677354690 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3991225561313502 | 0.7001500727951693 | 0.9170528825931821 | T | T | T |
| 0.6608833558976985 | 0.7225489064552661 | 0.9170318846339246 | T | T | T |
| 0.4732644968571098 | 0.7291941978024301 | 0.9170431423160702 | T | T | T |
| 0.6078954925210570 | 0.7415997693975342 | 0.9171124638699341 | T | T | T |
| 0.1362890032166209 | 0.5197962203508557 | 0.7500002139767918 | T | T | T |
| 0.1125360676008052 | 0.6182470675858657 | 0.7382794117379534 | T | T | T |
| 0.0790556538811352 | 0.5404158504409998 | 0.7478783358636742 | T | T | T |
| 0.1062494057836486 | 0.6282444835949624 | 0.8625529698937258 | T | T | T |

OOH\_B-CNT(8,0) #### KPOINTS: 2x2x2 #### E= -501.49822479 eV

1.0000000000000000

12.9903810600000007 -7.5000000000000000 0.0000000000000000

0.0000000000000000 15.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5305455000000006

C B O H

63 1 2 1

Selective dynamics

Direct

0.0767990119012960 0.1933765622179504 0.0829467112162329 T T T

0.4992326659049269 0.2597587001640276 0.0842504760613336 T T T

0.1356140313552337 0.3772421715750694 0.0828443634047886 T T T

0.5610751362700978 0.4439236720613510 0.0846160762093906 T T T

0.1541508209637058 0.0839708434098139 0.0844432506126937 T T T

0.3275503206260718 0.1086902980411387 0.0841960676351180 T T T

0.3106152520985465 0.5314569020203537 0.0830099617028428 T T T

0.4828367347342968 0.5525250688443939 0.0831156591067207 T T T

0.2336206468490580 0.0779698331344159 0.1678770087225676 T T T

0.0986072025580517 0.1234686656075018 0.1675786689109637 T T T

0.4206971773703142 0.1734066414870059 0.1678294876951670 T T T

0.2146528051758952 0.4667094832928632 0.1656028385157841 T T T

0.5388648122276851 0.5132753664543240 0.1677465371475030 T T T

0.4031431332869738 0.5572613347939391 0.1664501498944050 T T T

0.0914136098425556 0.2818669907172103 0.1662563598213869 T T T

0.5481597393300766 0.3555874495068495 0.1680452847001341 T T T

0.0912777322403796 0.2821015645591059 0.3323563064750960 T T T

0.5483005127534146 0.3555027303203561 0.3343474729326851 T T T

0.2336733025333470 0.0777448331667847 0.3342888525380541 T T T

0.0989858347952322 0.1240912042019473 0.3338439589654527 T T T

0.4208793394958852 0.1731295886773187 0.3348880830072870 T T T

0.2153136683403750 0.4657903511958597 0.3290646457665749 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5383403289720441 | 0.5131535842728445 | 0.3340867045997525 | T | T | T |
| 0.4029759746691369 | 0.5575696036200102 | 0.3325796255581517 | T | T | T |
| 0.1550960630244019 | 0.0851166683866122 | 0.4176121193562585 | T | T | T |
| 0.3276994934566630 | 0.1085015841488370 | 0.4181383017879199 | T | T | T |
| 0.3093945743845547 | 0.5286640272431324 | 0.4132786070016634 | T | T | T |
| 0.4811803312265505 | 0.5512351488968211 | 0.4176152626158291 | T | T | T |
| 0.0785157623521412 | 0.1949514461287572 | 0.4173705646543410 | T | T | T |
| 0.4992751452272151 | 0.2595709780139195 | 0.4182046525719189 | T | T | T |
| 0.1383164929896009 | 0.3778209916349376 | 0.4132281050667659 | T | T | T |
| 0.5598540709475951 | 0.4432004966894448 | 0.4177486868209955 | T | T | T |
| 0.0796077847453438 | 0.1968633114367742 | 0.5845160521450646 | T | T | T |
| 0.4994406916289614 | 0.2593627068919172 | 0.5843015361737747 | T | T | T |
| 0.1376518630355267 | 0.3804947280542987 | 0.5781515574289307 | T | T | T |
| 0.5592236257247484 | 0.4429346553690784 | 0.5848186737777358 | T | T | T |
| 0.1554092805202216 | 0.0857666464910659 | 0.5847026965934756 | T | T | T |
| 0.3278369143601115 | 0.1083286864129091 | 0.5843292129643148 | T | T | T |
| 0.3070144446908197 | 0.5297486277224669 | 0.5782977382090839 | T | T | T |
| 0.4789951112744076 | 0.5501080833283458 | 0.5847853472972939 | T | T | T |
| 0.2341282430715166 | 0.0783936300289644 | 0.6680352708455468 | T | T | T |
| 0.1011579847213386 | 0.1263429329356338 | 0.6680556789656965 | T | T | T |
| 0.4212737674987114 | 0.1725984316958392 | 0.6677572889116881 | T | T | T |
| 0.2117735484817221 | 0.4705244863056653 | 0.6570557256794143 | T | T | T |
| 0.5355505413542788 | 0.5108637401749668 | 0.6682228414442106 | T | T | T |
| 0.3992715255088602 | 0.5556595957399004 | 0.6666450346142840 | T | T | T |
| 0.0929132553056807 | 0.2853074579434393 | 0.6663843999333510 | T | T | T |
| 0.5478514448200137 | 0.3551399136921309 | 0.6681617413256782 | T | T | T |
| 0.0923337183918025 | 0.2847871927522469 | 0.8356235478210678 | T | T | T |
| 0.5483196111436512 | 0.3551955517783794 | 0.8343079435742660 | T | T | T |
| 0.2339701714910437 | 0.0779713903082489 | 0.8342269599337532 | T | T | T |
| 0.1006469376543668 | 0.1255133768291368 | 0.8337719305313871 | T | T | T |
| 0.4212740130574713 | 0.1726107905740894 | 0.8347562173855276 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5364280856665823 | 0.5112150111351945 | 0.8339598345503961 | T | T | T |
| 0.3998426632040122 | 0.5560310950354782 | 0.8359182837516923 | T | T | T |
| 0.1549599418549342 | 0.0846808945543733 | 0.9174111760774791 | T | T | T |
| 0.3278251821516725 | 0.1086011701479597 | 0.9180090811862271 | T | T | T |
| 0.3106111626412225 | 0.5355559417925406 | 0.9193939150768889 | T | T | T |
| 0.4809077267906114 | 0.5506762363644763 | 0.9171012533591113 | T | T | T |
| 0.0784833357192533 | 0.1948630620482208 | 0.9169538318201582 | T | T | T |
| 0.4993227182326193 | 0.2594073554571462 | 0.9181197717219362 | T | T | T |
| 0.1313898411854017 | 0.3777953496501547 | 0.9192862626540056 | T | T | T |
| 0.5602840815281910 | 0.4431236049747487 | 0.9175848592220550 | T | T | T |
| 0.1998801877307323 | 0.4874278129211811 | 0.8354572819490591 | T | T | T |
| 0.2078925877608711 | 0.6525720196502098 | 0.7981736232115498 | T | T | T |
| 0.1441043752494281 | 0.5463504875253791 | 0.8609774902100207 | T | T | T |
| 0.2469619039005835 | 0.6877592377925683 | 0.8915150885780933 | T | T | T |

OOH\_B-CNT(9,0) #### KPOINTS: 2x2x2 #### E= -565.71187144 eV

1.0000000000000000

13.8564064600000005 -8.0000000000000000 0.0000000000000000

0.0000000000000000 16.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5367054200000005

C B O H

71 1 2 1

Selective dynamics

Direct

0.1986818755191209 0.0684746743939714 0.0823364197166137 T T T

0.0887949820718638 0.1328199006251846 0.0821925080012271 T T T

0.3711387614200046 0.1234417501532535 0.0819853666091848 T T T

0.0852441331717674 0.2846811817291482 0.0835523410333248 T T T

0.5253127388076853 0.2741761058348703 0.0818450532216560 T T T

0.1902839510380010 0.4610003895392618 0.0920635833265389 T T T

0.5824935392879959 0.4469300428099225 0.0820701998482486 T T T

0.3670244945087580 0.5622564418198552 0.0832346258793877 T T T

0.5178993730792292 0.5567102737645512 0.0818844481752873 T T T

0.1318391165277793 0.0864394049183339 0.1658168065189282 T T T

0.2815146011529118 0.0807360667272585 0.1658662446494507 T T T

0.4557823663719444 0.1906696539003105 0.1654105789714884 T T T

0.0733931996298184 0.2019833319428402 0.1654485301552040 T T T

0.5697883240386691 0.3639041741704898 0.1657752071612807 T T T

0.1263082478730985 0.3742874087771926 0.1712041338763138 T T T

0.5641254180156976 0.5135376993229186 0.1654771917396164 T T T

0.2776291331506296 0.5233928337339986 0.1710924911371303 T T T

0.4493525647161465 0.5730927196037968 0.1651411506929658 T T T

0.1314132420974695 0.0855525320114833 0.3324831196437695 T T T

0.2813446280413114 0.0805168951237869 0.3319489600154553 T T T

0.4555429244481915 0.1908434240731997 0.3321601171042150 T T T

0.0726161083827769 0.2001411802414705 0.3328487482608290 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5697774783944547 | 0.3640452832072663 | 0.3316949941183001 | T | T | T |
| 0.1273547879944918 | 0.3718416739203193 | 0.3362102912945252 | T | T | T |
| 0.5650547105694212 | 0.5141090554811293 | 0.3322436990293497 | T | T | T |
| 0.2802369348602381 | 0.5225708931987378 | 0.3361704772105392 | T | T | T |
| 0.4514393828897040 | 0.5742980205401155 | 0.3325185130078392 | T | T | T |
| 0.1980899502892392 | 0.0674897544561796 | 0.4155479025197919 | T | T | T |
| 0.0873161596466221 | 0.1310891738836756 | 0.4163153101684305 | T | T | T |
| 0.3709068160797541 | 0.1234348626238202 | 0.4156574646424686 | T | T | T |
| 0.0858649733326123 | 0.2823980561431100 | 0.4177493952545199 | T | T | T |
| 0.5251000269797954 | 0.2744045570988679 | 0.4156290806358948 | T | T | T |
| 0.1949876484624009 | 0.4563997198902012 | 0.4207364399888915 | T | T | T |
| 0.5832564218161350 | 0.4475096929279549 | 0.4153098904254066 | T | T | T |
| 0.3696930791838456 | 0.5625032046976624 | 0.4174742278235781 | T | T | T |
| 0.5199132016366047 | 0.5586294673086677 | 0.4159372762753535 | T | T | T |
| 0.1981441238298109 | 0.0676042666664567 | 0.5823720915564108 | T | T | T |
| 0.0870052709033042 | 0.1307110498894477 | 0.5826976870770053 | T | T | T |
| 0.3709212223742293 | 0.1235944818006409 | 0.5819673943074726 | T | T | T |
| 0.0859082707378487 | 0.2824830027796827 | 0.5835956905128571 | T | T | T |
| 0.5250256295666704 | 0.2744254141074102 | 0.5817650469339978 | T | T | T |
| 0.1939167642971888 | 0.4574714940155961 | 0.5842379759104307 | T | T | T |
| 0.5832530585725179 | 0.4474502379322412 | 0.5821114926064425 | T | T | T |
| 0.3695925280643739 | 0.5622765545091475 | 0.5832710014976432 | T | T | T |
| 0.5202639670427740 | 0.5588489785225800 | 0.5824164724091555 | T | T | T |
| 0.1309109617141214 | 0.0849653122956890 | 0.6660240119374965 | T | T | T |
| 0.2812941631705645 | 0.0806597684125339 | 0.6657985384916318 | T | T | T |
| 0.4555123981955805 | 0.1909706158035754 | 0.6652596928848625 | T | T | T |
| 0.0719507366823898 | 0.1995513733938369 | 0.6670662516192769 | T | T | T |
| 0.5699505022114739 | 0.3641550718825770 | 0.6656949054996909 | T | T | T |
| 0.1241592378557246 | 0.3715417863517319 | 0.6674675899537837 | T | T | T |
| 0.5657036385965801 | 0.5145534297901935 | 0.6656485247783307 | T | T | T |
| 0.2807419252069252 | 0.5252452723288535 | 0.6672373731629645 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4520082092496998 | 0.5746984983144717 | 0.6667324315287304 | T | T | T |
| 0.1314747472147197 | 0.0856368037345297 | 0.8324966454619086 | T | T | T |
| 0.2813755952577037 | 0.0807501840833198 | 0.8319864734763879 | T | T | T |
| 0.4555397705460948 | 0.1909704309083837 | 0.8321011763067846 | T | T | T |
| 0.0733744089872417 | 0.2010830693047807 | 0.8334168269053827 | T | T | T |
| 0.5700323512081480 | 0.3640631936146397 | 0.8317632943182580 | T | T | T |
| 0.1186309313698328 | 0.3722827995001244 | 0.8308446909037693 | T | T | T |
| 0.5651006652975987 | 0.5139372270367207 | 0.8322190641910384 | T | T | T |
| 0.2799729157312113 | 0.5299613859169615 | 0.8306020752841140 | T | T | T |
| 0.4503545834844051 | 0.5729302185586556 | 0.8330665800487314 | T | T | T |
| 0.1984602837905926 | 0.0680473439173582 | 0.9157395515650215 | T | T | T |
| 0.0887774406937483 | 0.1324805344592548 | 0.9163952145543716 | T | T | T |
| 0.3710092834424862 | 0.1235418306581136 | 0.9156078962565032 | T | T | T |
| 0.0852696159990248 | 0.2848706447254247 | 0.9149135137224458 | T | T | T |
| 0.5253343487957348 | 0.2743105665201040 | 0.9156166814469823 | T | T | T |
| 0.5830275014944439 | 0.4471643073652896 | 0.9154841104641176 | T | T | T |
| 0.3669895625465919 | 0.5619133633168806 | 0.9145749686892739 | T | T | T |
| 0.5183865193667611 | 0.5567348011863984 | 0.9160263782536548 | T | T | T |
| 0.1763939859342746 | 0.4759290494482408 | 0.9146558999319346 | T | T | T |
| 0.1750223758115978 | 0.6263264657358627 | 0.9472194030280471 | T | T | T |
| 0.1168816858396464 | 0.5243160058986576 | 0.8915559885766026 | T | T | T |
| 0.1328935234302406 | 0.6248116647188836 | 0.0304666058135147 | T | T | T |

OOH\_B-CNT(10,0) #### KPOINTS: 2x2x2 #### E= -630.01108046 eV

1.0000000000000000

14.7224318600000004 -8.500000000000000 0.0000000000000000

0.0000000000000000 17.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5393644000000002

C B O H

79 1 2 1

Selective dynamics

Direct

0.2420448003483710 0.0620364048528663 0.0847209888142536 T T T

0.1111205368860700 0.0851314628296117 0.0845674562042767 T T T

0.4079489881274296 0.1404479049727285 0.0847417009308494 T T T

0.5447453778663226 0.2908545622437623 0.0847649918682189 T T T

0.1083274964301178 0.3591205655489167 0.0829235605281177 T T T

0.2487704177684424 0.5124777371519873 0.0830995860688662 T T T

0.5470331288416638 0.5649745268566949 0.0847114552294613 T T T

0.4142720725550487 0.5854392556759936 0.0834311496560997 T T T

0.0616236212592430 0.1979341570751419 0.0832059237524539 T T T

0.5980943398371110 0.4536390753621040 0.0848046429407927 T T T

0.1685442111346661 0.0607398985191372 0.1679330194562935 T T T

0.4837812826165477 0.2100831307702372 0.1682407406445902 T T T

0.1706140416794198 0.4418695522136783 0.1654543060458380 T T T

0.4883309018204426 0.5877108457684593 0.1677639945799181 T T T

0.3247057692729671 0.0895076519065683 0.1679481786182012 T T T

0.0742477998065697 0.1320776171025514 0.1675892508767865 T T T

0.0744131920835089 0.2757457213964263 0.1664452780247621 T T T

0.5840903514802021 0.3747326597829263 0.1680104411606455 T T T

0.5851043499612906 0.5191425667600088 0.1680441191561718 T T T

0.3324189652899752 0.5587553545254039 0.1666760240498510 T T T

0.3247634801519287 0.0894660033919400 0.3347685998369088 T T T

0.0744892595138972 0.1324128297848516 0.3343018611590030 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0745346374191714 | 0.2757196520066172 | 0.3325095221466121 | T | T | T |
| 0.5841663817624101 | 0.3746812171720424 | 0.3348059279989484 | T | T | T |
| 0.5848933383188535 | 0.5189988373083129 | 0.3348208945155371 | T | T | T |
| 0.3323745734869925 | 0.5586171747724413 | 0.3327343715333509 | T | T | T |
| 0.1686166509162377 | 0.0608828938677582 | 0.3347143949245647 | T | T | T |
| 0.4839398764504519 | 0.2099533780599916 | 0.3346627897362893 | T | T | T |
| 0.1718528672141136 | 0.4409080389935531 | 0.3293228615198750 | T | T | T |
| 0.4879782824756226 | 0.5874108090188815 | 0.3344964974117390 | T | T | T |
| 0.0625085693212844 | 0.1985742110234994 | 0.4173907649006443 | T | T | T |
| 0.5979248820466985 | 0.4534052615749291 | 0.4183457099870110 | T | T | T |
| 0.2422467941283357 | 0.0621719532202195 | 0.4182552180506758 | T | T | T |
| 0.1117107073291627 | 0.0857278330186382 | 0.4177663359776557 | T | T | T |
| 0.4080510221971840 | 0.1404915635141839 | 0.4179637235245495 | T | T | T |
| 0.5447506891553285 | 0.2907472986595649 | 0.4179830285994759 | T | T | T |
| 0.1118922488226023 | 0.3595558660405918 | 0.4134265213749053 | T | T | T |
| 0.2487459166700735 | 0.5093336682116698 | 0.4134694226630089 | T | T | T |
| 0.5464010369306722 | 0.5642444694312693 | 0.4179210466330965 | T | T | T |
| 0.4136384971615151 | 0.5844087897903164 | 0.4176008066254768 | T | T | T |
| 0.2422861051443780 | 0.0622081538410338 | 0.5846811906670761 | T | T | T |
| 0.1120120398872383 | 0.0863500617882770 | 0.5847412576451736 | T | T | T |
| 0.4081074992465699 | 0.1403933639398100 | 0.5847609324817344 | T | T | T |
| 0.5448932757345536 | 0.2907277010009061 | 0.5848014833228967 | T | T | T |
| 0.1106871518038298 | 0.3616416416308556 | 0.5787135282211634 | T | T | T |
| 0.2462163640717131 | 0.5099002463769765 | 0.5788173416964916 | T | T | T |
| 0.5458241296948759 | 0.5638516747900826 | 0.5848653747623543 | T | T | T |
| 0.4119018467415212 | 0.5832923267348640 | 0.5849661457132370 | T | T | T |
| 0.0632096411094900 | 0.2002332038987943 | 0.5847452815706122 | T | T | T |
| 0.5979578174875585 | 0.4533760099246095 | 0.5847667008122207 | T | T | T |
| 0.1690104930179346 | 0.0614071706528082 | 0.6680289523024038 | T | T | T |
| 0.4840168775704059 | 0.2099257216860648 | 0.6681780346909872 | T | T | T |
| 0.1671450000316297 | 0.4444101814803254 | 0.6571051395311415 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4864103432166247 | 0.5854570171153731 | 0.6682583080424823 | T | T | T |
| 0.3248550244884668 | 0.0896166667727339 | 0.6679761138219205 | T | T | T |
| 0.0761868379854942 | 0.1341493585432946 | 0.6680779668875986 | T | T | T |
| 0.0742467082950334 | 0.2779420999776369 | 0.6663093664643367 | T | T | T |
| 0.5840910399183745 | 0.3745911307209883 | 0.6680509885859264 | T | T | T |
| 0.5845131758610330 | 0.5185992319391166 | 0.6681354625516095 | T | T | T |
| 0.3297999669804342 | 0.5579872390879813 | 0.6665404615391716 | T | T | T |
| 0.3248045913877434 | 0.0896292727673995 | 0.8348008579979240 | T | T | T |
| 0.0761004719545344 | 0.1338182867208215 | 0.8341987912965988 | T | T | T |
| 0.0733695111520458 | 0.2776078029569796 | 0.8354707175396132 | T | T | T |
| 0.5840721428666854 | 0.3746273927655235 | 0.8348525808074654 | T | T | T |
| 0.5847393139582839 | 0.5187749895620539 | 0.8347462405161662 | T | T | T |
| 0.3301626758535547 | 0.5588239103991496 | 0.8357332863527439 | T | T | T |
| 0.1688637349743695 | 0.0611853720054800 | 0.8346256904256750 | T | T | T |
| 0.4840288310514690 | 0.2099054178544886 | 0.8346739433011904 | T | T | T |
| 0.4869006631325531 | 0.5857431195630098 | 0.8343730932448469 | T | T | T |
| 0.0628716052235748 | 0.1991475175021949 | 0.9169451473897804 | T | T | T |
| 0.5978812751051475 | 0.4533636347104290 | 0.9183247768668746 | T | T | T |
| 0.2422967881870772 | 0.0623100451261799 | 0.9182307166795404 | T | T | T |
| 0.1118170366134458 | 0.0858243427282829 | 0.9176018369810915 | T | T | T |
| 0.4080802294475623 | 0.1405456512333795 | 0.9179831033701050 | T | T | T |
| 0.5447037781026799 | 0.2907211766073342 | 0.9180011597385401 | T | T | T |
| 0.1031366288169112 | 0.3590857478676937 | 0.9192460502868032 | T | T | T |
| 0.2477279490254009 | 0.5163835675152257 | 0.9193681471446870 | T | T | T |
| 0.5464437003456136 | 0.5641981760378144 | 0.9177689940810929 | T | T | T |
| 0.4132176727930615 | 0.5840124216150082 | 0.9171399343187279 | T | T | T |
| 0.1517387277767184 | 0.4561560447348518 | 0.8342195086862229 | T | T | T |
| 0.1320885914925040 | 0.5866562449901902 | 0.7837835756219140 | T | T | T |
| 0.0875955757895023 | 0.4931064947761802 | 0.8516502433452797 | T | T | T |
| 0.1452158101244353 | 0.6214307678813253 | 0.8801244649708064 | T | T | T |

OOH\_B-CNT(11,0) #### KPOINTS: 2x2x2 #### E= -693.92518969 eV

1.0000000000000000

15.5884572699999993 -9.0000000000000000 0.0000000000000000

0.0000000000000000 18.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.5415445000000005

C B O H

87 1 2 1

Selective dynamics

Direct

0.1511185306944404 0.0532465469466382 0.0844443685768331 T T T

0.2962320601130873 0.0736129537677837 0.0847234043975885 T T T

0.0651799356903439 0.1242429128979516 0.0842285546108547 T T T

0.4506686516585412 0.1762284788197317 0.0850697110503740 T T T

0.0617742922011031 0.2587258517245499 0.0827719301839000 T T T

0.5677792054623216 0.3256068308029492 0.0847463377576711 T T T

0.1371347099060138 0.4159059058359917 0.0824862773538381 T T T

0.6096715147144610 0.4777416304932555 0.0845583421737477 T T T

0.2818468182019078 0.5485050367987655 0.0826724588511072 T T T

0.5595467764064532 0.5816484493594275 0.0843873301412788 T T T

0.4372078939994911 0.6058992703151772 0.0829535012672120 T T T

0.2194662129251699 0.0523442817901151 0.1680067217855792 T T T

0.0985148808741394 0.0785876952245046 0.1677474507512175 T T T

0.3756554636702508 0.1164685905298647 0.1682953477667766 T T T

0.0525780795814790 0.1857821769476229 0.1671927658006108 T T T

0.5165479532131159 0.2473517160266042 0.1683060455336990 T T T

0.0916727362284552 0.3368562896043429 0.1659587766072210 T T T

0.5992722418214179 0.4043329214849950 0.1680550795070688 T T T

0.2042728254526432 0.4890036302652815 0.1650486260264787 T T T

0.5954516125703422 0.5383727671946281 0.1678825910964030 T T T

0.3610660707598425 0.5855910484399960 0.1661708342612691 T T T

0.5053964480138784 0.6047823837415289 0.1673994646634914 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2195406450144176 | 0.0524191854227933 | 0.3349156680475602 | T | T | T |
| 0.0987862325982714 | 0.0788519533651634 | 0.3344162813596941 | T | T | T |
| 0.3757097267863562 | 0.1163191763140621 | 0.3346901535743722 | T | T | T |
| 0.0530112073649796 | 0.1862054390242145 | 0.3337039146681883 | T | T | T |
| 0.5166865089306847 | 0.2472299421170036 | 0.3347330254052844 | T | T | T |
| 0.0920894961266110 | 0.3369966119700764 | 0.3319935176657411 | T | T | T |
| 0.5991691105159018 | 0.4042307067991308 | 0.3349743909335867 | T | T | T |
| 0.2052550648804453 | 0.4878724940569781 | 0.3290518282994181 | T | T | T |
| 0.5950928555216087 | 0.5380521924343165 | 0.3345080277675996 | T | T | T |
| 0.3608273181511105 | 0.5853386980490546 | 0.3321819595902993 | T | T | T |
| 0.5048818258632940 | 0.6043587936840299 | 0.3338885574204218 | T | T | T |
| 0.1516165047167462 | 0.0537906018188672 | 0.4181342792718717 | T | T | T |
| 0.2963359794777394 | 0.0736120881785896 | 0.4181628919862237 | T | T | T |
| 0.0662767055436717 | 0.1250880420281968 | 0.4175255769911666 | T | T | T |
| 0.4507530525234810 | 0.1760881844696641 | 0.4180642794795498 | T | T | T |
| 0.0631031207076606 | 0.2595154030237545 | 0.4169474927318432 | T | T | T |
| 0.5677782872017535 | 0.3254532045143892 | 0.4182088473499327 | T | T | T |
| 0.1403106430454359 | 0.4157315394474653 | 0.4130711145225679 | T | T | T |
| 0.6090422705390580 | 0.4772325498544790 | 0.4181984064661239 | T | T | T |
| 0.2813639799932654 | 0.5457732332121739 | 0.4130190093512874 | T | T | T |
| 0.5583950587786429 | 0.5803996309472620 | 0.4176562308450025 | T | T | T |
| 0.4362036228744439 | 0.6046580222511170 | 0.4171521382708271 | T | T | T |
| 0.1514778515536008 | 0.0536049651568629 | 0.5844161765304983 | T | T | T |
| 0.2962666176320641 | 0.0734129019469909 | 0.5846809710196185 | T | T | T |
| 0.0667274451134041 | 0.1256952368232318 | 0.5846487831547630 | T | T | T |
| 0.4507066422519724 | 0.1761648499086411 | 0.5850090139806101 | T | T | T |
| 0.0639291916192801 | 0.2609305961257240 | 0.5843299119606130 | T | T | T |
| 0.5679834075825899 | 0.3255273975510052 | 0.5847180244772047 | T | T | T |
| 0.1393442036922773 | 0.4181482237666192 | 0.5782227020529025 | T | T | T |
| 0.6092997041736677 | 0.4773930201978321 | 0.5845038339297652 | T | T | T |
| 0.2792097610974114 | 0.5470246254657413 | 0.5782537454114242 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5577999297591094 | 0.5800117167051148 | 0.5847384244232787 | T | T | T |
| 0.4346516036066665 | 0.6037149033597842 | 0.5844444975376710 | T | T | T |
| 0.2193619389195000 | 0.0518089175131346 | 0.6679569605743129 | T | T | T |
| 0.0992666071106847 | 0.0793068454601466 | 0.6679132942358278 | T | T | T |
| 0.3756360510983031 | 0.1164912367725972 | 0.6682520055804680 | T | T | T |
| 0.0547316672028191 | 0.1874980907504999 | 0.6677202770905183 | T | T | T |
| 0.5165229047606046 | 0.2473879816053235 | 0.6682622039610172 | T | T | T |
| 0.0919948280159125 | 0.3392681894965339 | 0.6660111324290575 | T | T | T |
| 0.5998376383086086 | 0.4043773680783255 | 0.6680110937551523 | T | T | T |
| 0.2013453721843276 | 0.4927460497318032 | 0.6567104319897740 | T | T | T |
| 0.5947171571739538 | 0.5376829510120266 | 0.6680239037520237 | T | T | T |
| 0.3585390007615297 | 0.5851001034902619 | 0.6661245807965895 | T | T | T |
| 0.5033094749482792 | 0.6024699121224426 | 0.6678488633435954 | T | T | T |
| 0.2191535227618630 | 0.0514959590503745 | 0.8348778895938856 | T | T | T |
| 0.0989073460370168 | 0.0788331185250546 | 0.8343398724083962 | T | T | T |
| 0.3755273195801880 | 0.1165023272615781 | 0.8346971071542785 | T | T | T |
| 0.0544097879925221 | 0.1870469717077786 | 0.8337447624918615 | T | T | T |
| 0.5165691539704891 | 0.2475456468365588 | 0.8347295076206571 | T | T | T |
| 0.0910858521583495 | 0.3389166865323269 | 0.8352473209468292 | T | T | T |
| 0.6001349326694716 | 0.4045811736947613 | 0.8349456694667075 | T | T | T |
| 0.5952766928040106 | 0.5380510392777591 | 0.8344370348409583 | T | T | T |
| 0.3591847137033627 | 0.5856206551620332 | 0.8354140079420210 | T | T | T |
| 0.5040140931083317 | 0.6029437174836024 | 0.8338624146809837 | T | T | T |
| 0.1512030672113106 | 0.0530948859684933 | 0.9180960781570140 | T | T | T |
| 0.2961384056681218 | 0.0733970404752391 | 0.9182036319056833 | T | T | T |
| 0.0659726890468482 | 0.1247722858933798 | 0.9172816699443341 | T | T | T |
| 0.4505316412318423 | 0.1764441223695259 | 0.9180720166773839 | T | T | T |
| 0.0629487546069333 | 0.2595748605802984 | 0.9165857833209504 | T | T | T |
| 0.5680227226787969 | 0.3257147054865616 | 0.9182415336823258 | T | T | T |
| 0.1326174961630296 | 0.4167157192892026 | 0.9189126015030764 | T | T | T |
| 0.6098292075804798 | 0.4776483799501062 | 0.9181866046683856 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2817631884354374 | 0.5523084057749590 | 0.9189978959288806 | T | T | T |
| 0.5589942686230146 | 0.5808781282685166 | 0.9174457711407632 | T | T | T |
| 0.4363082562800581 | 0.6046360963342658 | 0.9168015145663522 | T | T | T |
| 0.1905577256264475 | 0.5068150518119240 | 0.8341462678592061 | T | T | T |
| 0.1970623829135675 | 0.6445951165417660 | 0.7898054957180023 | T | T | T |
| 0.1433563831512250 | 0.5565294556151610 | 0.8544866497302318 | T | T | T |
| 0.2229472661161887 | 0.6759873050736076 | 0.8858365539013673 | T | T | T |

OOH\_B-CNT(12,0) #### KPOINTS: 1x1x2 #### E= -757.26485827 eV

1.0000000000000000

15.588499999999998 -9.000000000000000 0.000000000000000

0.0000000000000000 18.000000000000000 0.000000000000000

0.0000000000000000 0.000000000000000 8.457919999999997

C B O H

95 1 2 1

Selective dynamics

Direct

0.6519102796258209 0.5339930727860323 0.4188199432699873 T T T

0.6516578999474406 0.5337818880853302 0.9188102177525498 T T T

0.4630049594262352 0.6474150013704261 0.4181697647645926 T T T

0.4625048540986501 0.6472966850571900 0.9175287315410487 T T T

0.3927274142847882 0.1071444292320844 0.4188799668337877 T T T

0.3928279470746848 0.1069656498468281 0.9188476460063485 T T T

0.1123050287363585 0.0683231050740966 0.4186765801206594 T T T

0.1124337412975783 0.0684203927698154 0.9186488724466869 T T T

0.6330769792378999 0.3891596464178838 0.4186859818230886 T T T

0.6330052227400794 0.3889926749923382 0.9187151699699856 T T T

0.5879673532493583 0.6265892385961529 0.4184356535186750 T T T

0.5877598728126849 0.6263949665879792 0.9182958741036440 T T T

0.1637868860781035 0.4679337879104148 0.4147148189453826 T T T

0.1552637675814844 0.4707488420334471 0.9192918165515267 T T T

0.0741161540837776 0.3118468320149854 0.4179005670855710 T T T

0.0742882897150075 0.3125143664464345 0.9172475485739787 T T T

0.2364744827619391 0.0464213673544293 0.4185867895792441 T T T

0.2365308703713440 0.0463770991131596 0.9186159509464359 T T T

0.5377858449361479 0.2328191442783655 0.4189261511948948 T T T

0.5380615463050734 0.2325490229446397 0.9188929765571227 T T T

0.3084594443786671 0.5926516415891246 0.4147737788850230 T T T

0.3085105935742428 0.6019846258003825 0.9193841636626903 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0551014063925533 | 0.1667653984576447 | 0.4182224523535673 | T | T | T |
| 0.0553984918368899 | 0.1670231950399227 | 0.9181139876131832 | T | T | T |
| 0.5883716993296774 | 0.6270705455831876 | 0.0853915850779286 | T | T | T |
| 0.5872374190729762 | 0.6261492170070904 | 0.5856159531575659 | T | T | T |
| 0.0546697531765356 | 0.1665181082075872 | 0.0852061475896099 | T | T | T |
| 0.0556510667870032 | 0.1674465046899763 | 0.5853918049544701 | T | T | T |
| 0.3088315199753105 | 0.5964117054874313 | 0.0834294578252354 | T | T | T |
| 0.3063798841726760 | 0.5942835384959245 | 0.5804546228309400 | T | T | T |
| 0.1122453111586306 | 0.0683102442753175 | 0.0853040373119964 | T | T | T |
| 0.1124455164054276 | 0.0685146496445738 | 0.5853029982524766 | T | T | T |
| 0.6518658677707372 | 0.5339936003686928 | 0.0854581141874283 | T | T | T |
| 0.6517439826121328 | 0.5338863146765154 | 0.5854295669797844 | T | T | T |
| 0.2364460889532053 | 0.0463288342783781 | 0.0857266714359951 | T | T | T |
| 0.2364965089009207 | 0.0463983090346175 | 0.5856830165060853 | T | T | T |
| 0.1604394083886262 | 0.4688179405097492 | 0.0832341924989080 | T | T | T |
| 0.1628826056096450 | 0.4706926981337733 | 0.5803656805421716 | T | T | T |
| 0.3927949551951723 | 0.1070024937062183 | 0.0857439893447485 | T | T | T |
| 0.3927710184525120 | 0.1070135791798441 | 0.5857355172388919 | T | T | T |
| 0.4635315287509926 | 0.6482005789282274 | 0.0843434504736638 | T | T | T |
| 0.4615320603137953 | 0.6469010429080547 | 0.5858588709242624 | T | T | T |
| 0.5380444825002219 | 0.2326380051323354 | 0.0857628350206023 | T | T | T |
| 0.5379037481699360 | 0.2327257232561395 | 0.5857555992985722 | T | T | T |
| 0.0733623368594341 | 0.3115852572251168 | 0.0840786923811664 | T | T | T |
| 0.0747532274707889 | 0.3133075074522149 | 0.5856380575214514 | T | T | T |
| 0.6330722387431539 | 0.3891026641498243 | 0.0858246533532714 | T | T | T |
| 0.6330641673816153 | 0.3891084158087216 | 0.5857929932376851 | T | T | T |
| 0.2302425616423987 | 0.5395528343202182 | 0.1659523665442459 | T | T | T |
| 0.2273936317845267 | 0.5439173835953289 | 0.6589016330727844 | T | T | T |
| 0.0543329865040037 | 0.2352363287081827 | 0.1679949873660573 | T | T | T |
| 0.0559825393066495 | 0.2364692041980716 | 0.6683953206284527 | T | T | T |
| 0.3131934643418172 | 0.0668842622335907 | 0.1688551695701164 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3131753128449516 | 0.0668073583683774 | 0.6688831756711072 | T | T | T |
| 0.3878254271967979 | 0.6297017133214807 | 0.1673050197870203 | T | T | T |
| 0.3860806314417630 | 0.6308533795701756 | 0.6673363889627120 | T | T | T |
| 0.6295065990262093 | 0.5888375822709865 | 0.1684821473032861 | T | T | T |
| 0.6288265929316512 | 0.5883056740001761 | 0.6685753612819121 | T | T | T |
| 0.4693598444065312 | 0.1637388635982389 | 0.1688461244662015 | T | T | T |
| 0.4693771509266360 | 0.1636648663540280 | 0.6687669666853998 | T | T | T |
| 0.0739727935973948 | 0.1094800212955796 | 0.1682922808768325 | T | T | T |
| 0.0746182975576434 | 0.1101105357188316 | 0.6683827615869515 | T | T | T |
| 0.1104580021963705 | 0.3904570904084619 | 0.1670122926370214 | T | T | T |
| 0.1094954035526105 | 0.3926107459728339 | 0.6670938220080389 | T | T | T |
| 0.5939118579971594 | 0.3096500265964635 | 0.1689269662663031 | T | T | T |
| 0.5939457871923692 | 0.3096621783274091 | 0.6689570775659693 | T | T | T |
| 0.5319132869279097 | 0.6473914541358690 | 0.1681997296521948 | T | T | T |
| 0.5303087209707406 | 0.6457212125942945 | 0.6686230709959122 | T | T | T |
| 0.1678671532034500 | 0.0467128764595260 | 0.1685789322940713 | T | T | T |
| 0.1679707649403444 | 0.0468588680417946 | 0.6685926285244082 | T | T | T |
| 0.6529752991776175 | 0.4655921803557274 | 0.1686854049722401 | T | T | T |
| 0.6528719851264597 | 0.4655470250805472 | 0.6687285484349288 | T | T | T |
| 0.0739616108976270 | 0.1095273883946177 | 0.3354982163927725 | T | T | T |
| 0.0745573866739192 | 0.1099628519975711 | 0.8353634549923372 | T | T | T |
| 0.5316342660899162 | 0.6471331250330451 | 0.3351245224105147 | T | T | T |
| 0.5305507107117401 | 0.6457370626685756 | 0.8350286524710951 | T | T | T |
| 0.6294523941955048 | 0.5888503603198744 | 0.3356899746322424 | T | T | T |
| 0.6289396569483752 | 0.5883339421680940 | 0.8355277544231299 | T | T | T |
| 0.4693145032554573 | 0.1637670081269528 | 0.3359949090504786 | T | T | T |
| 0.4694344629082929 | 0.1635877788039830 | 0.8359107054184055 | T | T | T |
| 0.0546032855982559 | 0.2354316480036500 | 0.3348953689014271 | T | T | T |
| 0.0560250301199843 | 0.2363324999573020 | 0.8348105356029768 | T | T | T |
| 0.1678218911138648 | 0.0467247529160072 | 0.3355319157679457 | T | T | T |
| 0.1678996541923503 | 0.0467237925514538 | 0.8355119852695208 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3878420467118910 | 0.6294119254558752 | 0.3336330051248867 | T | T | T |
| 0.3862540379157268 | 0.6314927916641427 | 0.8363535506345681 | T | T | T |
| 0.5938007350959434 | 0.3097134126984677 | 0.3356368059357399 | T | T | T |
| 0.5940316327896040 | 0.3095646101817111 | 0.8356677642653374 | T | T | T |
| 0.1106778218441539 | 0.3902722786246871 | 0.3333715260766797 | T | T | T |
| 0.1088361095625417 | 0.3927523604462519 | 0.8360552932186933 | T | T | T |
| 0.2313376339149065 | 0.5378505036371568 | 0.3303855898151675 | T | T | T |
| 0.3131773937945078 | 0.0669740261657843 | 0.3355530182955609 | T | T | T |
| 0.3132035294301230 | 0.0667618420954297 | 0.8355867942014960 | T | T | T |
| 0.6530703613213591 | 0.4657234636164964 | 0.3356274830826699 | T | T | T |
| 0.6528999609836941 | 0.4655216139448836 | 0.8356523711099044 | T | T | T |
| 0.2168750564597307 | 0.5607097691678186 | 0.8355569934056692 | T | T | T |
| 0.2293185963300563 | 0.7012677570615503 | 0.7903969628500785 | T | T | T |
| 0.1724732003827940 | 0.6130545577493697 | 0.8551439880530988 | T | T | T |
| 0.2479852092657901 | 0.7330036590844832 | 0.8890587693988439 | T | T | T |

OOH\_B-CNT(13,0) #### KPOINTS: 1x1x2 #### E= -1228.65854291 eV

1.0000000000000000

24.248699999999995 -14.000000000000000 0.0000000000000000

0.0000000000000000 28.000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 12.838699999999993

C B O H

155 1 2 1

Selective dynamics

Direct

0.4415702106709197 0.4067747983986031 0.0281967741295687 T T T

0.4529923884080361 0.3694749990218935 0.1950094133838137 T T T

0.4530061864847820 0.3694221610744921 0.3058806441543102 T T T

0.3838022923273028 0.4496526956803598 0.0279808147097514 T T T

0.4410798038181634 0.4064994839551533 0.1393255380550644 T T T

0.4169162016344518 0.4331683758624507 0.1948653092892191 T T T

0.4162348115497730 0.4326572553968550 0.3060150867859767 T T T

0.2937769277395613 0.4441719054563605 0.0263813913769264 T T T

0.3831540315787851 0.4492876024825925 0.1390504076988245 T T T

0.3406085689162347 0.4525699055498515 0.1941600278898030 T T T

0.3395035151745585 0.4521217183578530 0.3058804588096413 T T T

0.1926071709839577 0.3932598424073203 0.0257880430613472 T T T

0.2934515691751471 0.4442019745103649 0.1371206844523540 T T T

0.2428915315473254 0.4245241462607252 0.1915541284768559 T T T

0.2417726951914515 0.4261348452920527 0.3020975161127788 T T T

0.1027430717378067 0.3081183000032470 0.0263140762333865 T T T

0.1924418483406246 0.3936997334598342 0.1359719670459872 T T T

0.1446241853966438 0.3546755319124565 0.1914817411258364 T T T

0.1442749732241700 0.3570043724119870 0.3020082419330899 T T T

0.0443252239216927 0.2076557414041068 0.0278731641537096 T T T

0.1028790668854629 0.3084956464206381 0.1370309153199047 T T T

0.0692887866953922 0.2592699241608817 0.1940757784784350 T T T

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.0700839333061480 | 0.2603316845493243 | 0.3057966878660502 | T | T | T |
| 0.0317913738621718 | 0.1145503063680427 | 0.0280837001932174 | T | T | T |
| 0.0449167653940333 | 0.2081619711476876 | 0.1389473167982325 | T | T | T |
| 0.0328418260569822 | 0.1592976804400280 | 0.1947682296869381 | T | T | T |
| 0.0336221323357782 | 0.1598545905490962 | 0.3059347596595554 | T | T | T |
| 0.0683780253411224 | 0.0511271537182931 | 0.0281638761186944 | T | T | T |
| 0.0322510295692440 | 0.1149510913302187 | 0.1392234506827191 | T | T | T |
| 0.0447786844137493 | 0.0783570630493404 | 0.1949111547150578 | T | T | T |
| 0.0448858393059296 | 0.0783928903537422 | 0.3057842211199512 | T | T | T |
| 0.1444689979792003 | 0.0313832091922344 | 0.0283822396297878 | T | T | T |
| 0.0685127741385540 | 0.0512172518637254 | 0.1392530808980228 | T | T | T |
| 0.1024285629747137 | 0.0352483682641907 | 0.1949025924541752 | T | T | T |
| 0.1023876587576480 | 0.0351710637261651 | 0.3059195202674233 | T | T | T |
| 0.2426493448922229 | 0.0593503682316042 | 0.0283682217686963 | T | T | T |
| 0.1444282547614501 | 0.0312485767351647 | 0.1393187819983328 | T | T | T |
| 0.1920811520546409 | 0.0394145542119416 | 0.1949878210182429 | T | T | T |
| 0.1920835942602565 | 0.0394485689210332 | 0.3060577652211396 | T | T | T |
| 0.3409095460811788 | 0.1293985246393808 | 0.0283873722625304 | T | T | T |
| 0.2426435940412729 | 0.0593425774670080 | 0.1394140883067526 | T | T | T |
| 0.2932438321535635 | 0.0899936697124487 | 0.1951103904814248 | T | T | T |
| 0.2932323818026379 | 0.0900022056356206 | 0.3060600234165199 | T | T | T |
| 0.4164722182139535 | 0.2254252930032800 | 0.0284254469483543 | T | T | T |
| 0.3409317895600704 | 0.1294259873369535 | 0.1394334402126593 | T | T | T |
| 0.3828283275704471 | 0.1754597885037249 | 0.1950349296555141 | T | T | T |
| 0.3828018831732075 | 0.1754813143198439 | 0.3061036820744090 | T | T | T |
| 0.4529427105516797 | 0.3254111041716938 | 0.0282403954185546 | T | T | T |
| 0.4165927587573598 | 0.2253964461726599 | 0.1393695147916221 | T | T | T |
| 0.4404158897738824 | 0.2763218544892904 | 0.1949712114749232 | T | T | T |
| 0.4405293461583605 | 0.2763460036386350 | 0.3059966606336851 | T | T | T |
| 0.4528363956419397 | 0.3253174394298726 | 0.1393264795982458 | T | T | T |
| 0.4404794460731574 | 0.4059127722231459 | 0.3615365527433964 | T | T | T |

|                    |                    |                    |   |   |   |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4533393465505684 | 0.3695398706002924 | 0.5282147959996213 | T | T | T |
| 0.4535273018244910 | 0.3696939000171877 | 0.6391563310408962 | T | T | T |
| 0.3818667832866056 | 0.4480455770994942 | 0.3615517484686099 | T | T | T |
| 0.4408567267521458 | 0.4061114150752046 | 0.4724249190497289 | T | T | T |
| 0.4169108941450972 | 0.4329935835744631 | 0.5278539202484641 | T | T | T |
| 0.4175255502096403 | 0.4335372074174539 | 0.6389479083757703 | T | T | T |
| 0.2922979424207947 | 0.4452451141069068 | 0.3606170308723421 | T | T | T |
| 0.3823088512120361 | 0.4482096826332468 | 0.4723610708155851 | T | T | T |
| 0.3405451379233104 | 0.4524827302868973 | 0.5279594755868889 | T | T | T |
| 0.3411613262089987 | 0.4529537921151148 | 0.6387773468114539 | T | T | T |
| 0.1906021799747784 | 0.3989940873403375 | 0.3544053289434515 | T | T | T |
| 0.2928408808143969 | 0.4457278156989155 | 0.4736048235317138 | T | T | T |
| 0.2440413745116376 | 0.4301843865403695 | 0.5299228436201420 | T | T | T |
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