Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Band-Structure Engineering in Conjugated 2D Polymers

Rico Gutzler

Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Structure 1

```
  ibrav       = 4,
  celldm(1)   = 14.1474071134,
  celldm(3)   = 1.35,
  ecutwfc     = 200.D0,

ATOMIC_POSITIONS {angstrom}
C        4.978861334   2.885233832   0.000000000
C        4.948052926   1.487704692   0.000000000
C        3.753064280   3.557008238   0.000000000
C        3.753169927   0.762233337   0.000000000
H        5.883037830   0.947938502   0.000000000
C        2.527220564   2.885376892   0.000000000
C        2.558516374   1.487951285   0.000000000
H        1.623380880   0.948533022   0.000000000
C        0.009681156   2.959484517   0.000000000
H        0.010064862   1.879921311   0.000000000
H        3.752689464   4.636571122   0.000000000
C        0.009583976   5.754233737   0.000000000
C       -1.185300639   5.028784987   0.000000000
C        1.204241678   5.028531911   0.000000000
C       -1.216123214   3.631249919   0.000000000
H       -2.120236308   5.568633023   0.000000000
C        1.235533998   3.631102243   0.000000000
H        2.139334482   5.568024165   0.000000000
K_POINTS (automatic)
 15 15 1 0 0 0
```

Structure 2 (0° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C       -4.095178638   8.060383170   0.000000000
C       -2.909076761   6.003248672   0.000000000
C       -2.856665908   7.403898178   0.000000000
H       -4.142810918   9.142436809   0.000000000
H       -1.996945459   5.418244334   0.000000000
C       -1.573089872   8.144547391   0.000000000
C       -0.348781881   7.469862648   0.000000000
C       -1.545646760   9.542387989   0.000000000
C        0.875254780   8.144943412   0.000000000
H       -0.348950683   6.389645827   0.000000000
C       -0.349741022  10.266541103   0.000000000
H       -2.481811131  10.081344270   0.000000000
C        0.846555340   9.542688844   0.000000000
H        1.781997308  10.082556773   0.000000000
C        2.159815768   7.405480818   0.000000000
C        3.398391473   8.062011242   0.000000000
C        2.212299070   6.004832334   0.000000000
C        4.597505074   7.370835018   0.000000000
H        3.446376475   9.144316974   0.000000000
C        3.411283897   5.313693510   0.000000000
H        1.299554885   5.421325592   0.000000000
C        4.649955652   5.969998454   0.000000000
H        5.509857567   7.955095630   0.000000000
H        3.362941908   4.231508698   0.000000000
C        5.934018821   5.229230171   0.000000000
C        7.157916040   5.904272594   0.000000000
C        5.962798934   3.831138856   0.000000000
C        8.382060726   5.229619022   0.000000000
H        7.157780968   6.984443095   0.000000000
C        7.159472844   3.107309417   0.000000000
H        5.027168326   3.291429236   0.000000000
C        8.354886460   3.831838713   0.000000000
H        9.290921326   3.292688039   0.000000000
C        5.972531807   0.879622476   0.000000000
C        8.347326361   0.876724911   0.000000000
C        7.160487469   1.623603969   0.000000000
H        5.012458851   1.381456696   0.000000000
H        9.308762710   1.375235797   0.000000000
C       -0.348349706  11.750036698   0.000000000
C       -1.534686416  12.496848971   0.000000000
C        0.840028237  12.493698480   0.000000000
H       -2.495596604  11.997490986   0.000000000
H        1.800163957  11.991905003   0.000000000
C        9.665516180   5.969979213   0.000000000
C        9.717784274   7.370452910   0.000000000
C       10.903936373   5.313348242   0.000000000
H        8.805483145   7.955113822   0.000000000
H       10.951449245   4.231227571   0.000000000
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (10° dihedral angle)

```
    ibrav = 4
    celldm(1)   = 28.3699954238,
    celldm(3)   = 0.6668661,
    ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -4.08616132    8.04475577    0.20622539
 C                 -2.91808932    6.01886781   -0.20611644
 C                 -2.85666591    7.40389818    0.00000000
 H                 -4.12649666    9.11416351    0.37310577
 H                 -2.01326669    5.44652970   -0.37326515
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.38939544    8.04638374   -0.20610497
 C                  2.22130111    6.02047027    0.20624264
 C                  4.58851496    7.35521781   -0.20596925
 H                  3.43008960    9.11602416   -0.37314271
 C                  3.42029211    5.32934216    0.20638388
 H                  1.31584121    5.44961747    0.37313035
 C                  4.64996894    5.97002154    0.00030453
 H                  5.49357970    7.92681845   -0.37293647
 H                  3.37924151    4.25982363    0.37343435
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  5.99058725    0.87963483   -0.20637463
 C                  8.32930338    0.87671259    0.20600367
 C                  7.16048747    1.62360397    0.00000000
 H                  5.04509473    1.38147902   -0.37302992
 H                  9.27612818    1.37521348    0.37301450
 C                 -0.34834971   11.75003670    0.00000000
 C                 -1.51665267   12.49683206   -0.20612674
 C                  0.82198472   12.49371540    0.20623846
 H                 -2.46297160   11.99746039   -0.37290565
 H                  1.76752668   11.99193561    0.37304593
 C                  9.66551618    5.96997921    0.00000000
 C                  9.72679494    7.35483242    0.20611898
 C                 10.89492117    5.32897659   -0.20622273
 H                  8.82179876    7.92682980    0.37321968
 H                 10.93513825    4.25950358   -0.37311396
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (20° dihedral angle)

```
    ibrav = 4
    celldm(1)   = 28.3699954238,
    celldm(3)   = 0.6668661,
    ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
  C                 -4.05938334    7.99834841    0.40618472
   C                 -2.94485315    6.06525065   -0.40597013
   C                 -2.85666591    7.40389818    0.00000000
   H                 -4.07804958    9.03020269    0.73487491
   H                 -2.06173447    5.53052639   -0.73518883
   C                 -1.57308987    8.14454739    0.00000000
   C                 -0.34878188    7.46986265    0.00000000
   C                 -1.54564676    9.54238799    0.00000000
   C                  0.87525478    8.14494341    0.00000000
   H                 -0.34895068    6.38964583    0.00000000
   C                 -0.34974102   10.26654110    0.00000000
   H                 -2.48181113   10.08134427    0.00000000
   C                  0.84655534    9.54268884    0.00000000
   H                  1.78199731   10.08255677    0.00000000
   C                  2.15981577    7.40548082    0.00000000
   C                  3.36268068    7.99997606   -0.40594754
   C                  2.24803372    6.06690895    0.40621871
   C                  4.56181779    7.30884069   -0.40568023
   H                  3.38172386    9.03200538   -0.73494766
   C                  3.44704303    5.37581264    0.40649689
   H                  1.36420535    5.53363346    0.73492333
   C                  4.65000841    5.97009011    0.00059981
   H                  5.44524069    7.84284611   -0.73454146
   H                  3.42764505    4.34390807    0.73552209
   C                  5.93401882    5.22923017    0.00000000
   C                  7.15791604    5.90427259    0.00000000
   C                  5.96279893    3.83113886    0.00000000
   C                  8.38206073    5.22961902    0.00000000
   H                  7.15778097    6.98444309    0.00000000
   C                  7.15947284    3.10730942    0.00000000
   H                  5.02716833    3.29142924    0.00000000
   C                  8.35488646    3.83183871    0.00000000
   H                  9.29092133    3.29268804    0.00000000
   C                  6.04420496    0.87967150   -0.40647868
   C                  8.27578205    0.87667599    0.40574803
   C                  7.16048747    1.62360397    0.00000000
   H                  5.14201075    1.38154530   -0.73472552
   H                  9.17921616    1.37514721    0.73469515
   C                 -0.34834971   11.75003670    0.00000000
   C                 -1.46309938   12.49678183   -0.40599042
   C                  0.76840240   12.49376565    0.40621047
   H                 -2.36608789   11.99736953   -0.73448075
   H                  1.67060652   11.99202651    0.73475705
   C                  9.66551618    5.96997921    0.00000000
   C                  9.75355315    7.30844557    0.40597515
   C                 10.86814949    5.37538678   -0.40617949
   H                  8.87024986    7.84283713    0.73509928
   H                 10.88670087    4.34347246   -0.73489104
  K_POINTS (automatic)
   12 12 1 0 0 0
```

Structure 2 (30° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -4.01565834    7.92257115    0.59380234
 C                 -2.98855505    6.14098787   -0.59348863
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.99894171    8.89310545    1.07431526
 H                 -2.14087613    5.66768220   -1.07477417
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.31905890    7.92419828   -0.59345560
 C                  2.29168464    6.14273735    0.59385203
 C                  4.51822474    7.23311281   -0.59306482
 H                  3.30274882    8.89481351   -1.07442160
 C                  3.49072384    5.45169297    0.59425870
 H                  1.44317778    5.67082079    1.07438604
 C                  4.65007286    5.97020208    0.00087686
 H                  5.36630930    7.70573006   -1.07382779
 H                  3.50668182    4.48120717    1.07526137
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.13175578    0.87973137   -0.59423207
 C                  8.18838860    0.87661623    0.59316393
 C                  7.16048747    1.62360397    0.00000000
 H                  5.30026216    1.38165352   -1.07409685
 H                  9.02097129    1.37503899    1.07405244
 C                 -0.34834971   11.75003670    0.00000000
 C                 -1.37565374   12.49669982   -0.59351829
 C                  0.68090936   12.49384771    0.59383998
 H                 -2.20788923   11.99722116   -1.07373903
 H                  1.51234834   11.99217493    1.07414295
 C                  9.66551618    5.96997921    0.00000000
 C                  9.79724587    7.23270181    0.59349596
 C                 10.82443477    5.45116867   -0.59379468
 H                  8.94936428    7.70568789    1.07464325
 H                 10.80760886    4.48058285   -1.07433882
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (40° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.95631488    7.81972645    0.76337758
 C                 -3.04786716    6.24377824   -0.76297428
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.89157671    8.70703742    1.38111308
 H                 -2.24828699    5.85382971   -1.38170304
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.25985553    7.82135287   -0.76293181
 C                  2.35092756    6.24565147    0.76344146
 C                  4.45906036    7.13033512   -0.76242944
 H                  3.19556409    8.70861705   -1.38124979
 C                  3.55000732    5.55467756    0.76396426
 H                  1.55035896    5.85701109    1.38120407
 C                  4.65016034    5.97035404    0.00112727
 H                  5.25918381    7.51963650   -1.38048640
 H                  3.61395032    4.66754917    1.38232938
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.25057954    0.87981263   -0.76393003
 C                  8.06977843    0.87653512    0.76255685
 C                  7.16048747    1.62360397    0.00000000
 H                  5.51504059    1.38180040   -1.38083230
 H                  8.80620175    1.37489212    1.38077521
 C                 -0.34834971   11.75003670    0.00000000
 C                 -1.25697273   12.49658851   -0.76301241
 C                  0.56216403   12.49395908    0.76342597
 H                 -1.99318240   11.99701980   -1.38037229
 H                  1.29756074   11.99237637    1.38089156
 C                  9.66551618    5.96997921    0.00000000
 C                  9.85654553    7.12990257    0.76298370
 C                 10.76510527    5.55401965   -0.76336773
 H                  9.05673818    7.51954928    1.38153473
 H                 10.70026538    4.66666873   -1.38114337
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (50° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.88315608    7.69293920    0.90975796
 C                 -3.12098731    6.37049851   -0.90927733
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.75921682    8.47765220    1.64594646
 H                 -2.38070342    6.08331291   -1.64664954
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.18686944    7.69456473   -0.90922673
 C                  2.42396241    6.37252431    0.90983411
 C                  4.38612233    7.00363046   -0.90862803
 H                  3.06342643    8.47907348   -1.64610941
 C                  3.62309218    5.68163728    0.91045716
 H                  1.68249225    6.08654707    1.64605492
 C                  4.65026818    5.97054138    0.00134343
 H                  5.12711918    7.29021979   -1.64519964
 H                  3.74619126    4.89727216    1.64739601
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.39706583    0.87991280   -0.91041636
 C                  7.92355545    0.87643513    0.90877987
 C                  7.16048747    1.62360397    0.00000000
 H                  5.77982008    1.38198147   -1.64561185
 H                  8.54143320    1.37471106    1.64554382
 C                 -0.34834971   11.75003670    0.00000000
 C                 -1.11066242   12.49645129   -0.90932278
 C                  0.41577442   12.49409637    0.90981564
 H                 -1.72849117   11.99677156   -1.64506363
 H                  1.03276994   11.99262471    1.64568247
 C                  9.66551618    5.96997921    0.00000000
 C                  9.92965033    7.00317135    0.90928857
 C                 10.69196368    5.68081466   -0.90974623
 H                  9.18910905    7.29007703    1.64644898
 H                 10.56793201    4.89607597   -1.64598257
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (60° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.79840483    7.54606175    1.02849582
 C                 -3.20569378    6.51729837   -1.02795246
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.60588371    8.21191952    1.86076860
 H                 -2.53410202    6.34915910   -1.86156345
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.10231827    7.54768626   -1.02789525
 C                  2.50857006    6.51950090    1.02858190
 C                  4.30162683    6.85684870   -1.02721842
 H                  2.91035077    8.21315736   -1.86095283
 C                  3.70775777    5.82871452    1.02928628
 H                  1.83556284    6.35245438    1.86089122
 C                  4.65039311    5.97075840    0.00151877
 H                  4.97412812    7.02445064   -1.85992432
 H                  3.89938656    5.16339612    1.86240735
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.56676374    0.88002885   -1.02924015
 C                  7.75416257    0.87631929    1.02739007
 C                  7.16048747    1.62360397    0.00000000
 H                  6.08655545    1.38219123   -1.86039032
 H                  8.23471051    1.37450131    1.86031341
 C                 -0.34834971   11.75003670    0.00000000
 C                 -0.94116838   12.49629233   -1.02800384
 C                  0.24618851   12.49425542    1.02856102
 H                 -1.42185805   11.99648398   -1.85977054
 H                  0.72602147   11.99291240    1.86047015
 C                  9.66551618    5.96997921    0.00000000
 C                 10.01433902    6.85635882    1.02796516
 C                 10.60723237    5.82770109   -1.02848255
 H                  9.34245487    7.02424355    1.86133671
 H                 10.41462963    5.16183414   -1.86080942
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (70° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.70463626    7.38355690    1.11598335
 C                 -3.29941281    6.67971737   -1.11539377
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.43623634    7.91791354    2.01905223
 H                 -2.70382185    6.64329067   -2.01991469
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  3.00877106    7.38518028   -1.11533170
 C                  2.60217976    6.68211544    1.11607676
 C                  4.20814122    6.69444972   -1.11459730
 H                  2.74098824    7.91894842   -2.01925214
 C                  3.80143157    5.99144042    1.11684106
 H                  2.00491977    6.64665358    2.01918529
 C                  4.65053133    5.97099851    0.00164796
 H                  4.80485919    6.73040430   -2.01813614
 H                  4.06888147    5.45783501    2.02083038
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.75451709    0.88015724   -1.11679100
 C                  7.56674671    0.87619113    1.11478354
 C                  7.16048747    1.62360397    0.00000000
 H                  6.42592670    1.38242331   -2.01864177
 H                  7.89535329    1.37426924    2.01855832
 C                 -0.34834971   11.75003670    0.00000000
 C                 -0.75364059   12.49611646   -1.11544952
 C                  0.05855908   12.49443139    1.11605410
 H                 -1.08259992   11.99616580   -2.01796927
 H                  0.38663572   11.99323070    2.01872839
 C                  9.66551618    5.96997921    0.00000000
 C                 10.10803837    6.69392580    1.11540755
 C                 10.51348586    5.99021587   -1.11596895
 H                  9.51211630    6.73012604    2.01966867
 H                 10.24501626    5.45586833   -2.01909652
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (80° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.60469948    7.21036229    1.16956229
 C                 -3.39929679    6.85282049   -1.16894441
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.25542936    7.60456749    2.11598798
 H                 -2.88470606    6.95677057   -2.11689185
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  2.90907020    7.21198446   -1.16887936
 C                  2.70194722    6.85542696    1.16966019
 C                  4.10850601    6.52136794   -1.16810970
 H                  2.56048483    7.60538606   -2.11619749
 C                  3.90126735    6.16487063    1.17046118
 H                  2.18541720    6.96020556    2.11612743
 C                  4.65067864    5.97125442    0.00172708
 H                  4.62445554    6.41701524   -2.11502791
 H                  4.24952596    5.77164245    2.11785150
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  6.95462110    0.88029408   -1.17040872
 C                  7.36700239    0.87605454    1.16830488
 C                  7.16048747    1.62360397    0.00000000
 H                  6.78762223    1.38267066   -2.11555782
 H                  7.53367272    1.37402191    2.11547036
 C                 -0.34834971   11.75003670    0.00000000
 C                 -0.55377700   12.49592902   -1.16900283
 C                 -0.14141284   12.49461894    1.16963644
 H                 -0.72102499   11.99582669   -2.11485302
 H                  0.02492477   11.99356993    2.11564859
 C                  9.66551618    5.96997921    0.00000000
 C                 10.20790138    6.52080773    1.16895885
 C                 10.41357259    6.16342107   -1.16954720
 H                  9.69293828    6.41666112    2.11663402
 H                 10.06424551    5.76924445   -2.11603440
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 2 (90° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 28.3699954238,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
 C                 -3.50163102    7.03174033    1.18760467
 C                 -3.50231080    7.03134808   -1.18697726
 C                 -2.85666591    7.40389818    0.00000000
 H                 -3.06895649    7.28140222    2.14863050
 H                 -3.07125858    7.28007389   -2.14954832
 C                 -1.57308987    8.14454739    0.00000000
 C                 -0.34878188    7.46986265    0.00000000
 C                 -1.54564676    9.54238799    0.00000000
 C                  0.87525478    8.14494341    0.00000000
 H                 -0.34895068    6.38964583    0.00000000
 C                 -0.34974102   10.26654110    0.00000000
 H                 -2.48181113   10.08134427    0.00000000
 C                  0.84655534    9.54268884    0.00000000
 H                  1.78199731   10.08255677    0.00000000
 C                  2.15981577    7.40548082    0.00000000
 C                  2.80624506    7.03336127   -1.18691121
 C                  2.80484105    7.03416948    1.18770408
 C                  4.00574857    6.34286236   -1.18612968
 H                  2.37432506    7.28199772   -2.14884325
 C                  4.00423165    6.34373555    1.18851743
 H                  2.37157081    7.28358319    2.14877211
 C                  4.65083057    5.97151835    0.00175372
 H                  4.43839866    6.09380563   -2.14765563
 H                  4.43583123    6.09528355    2.15052277
 C                  5.93401882    5.22923017    0.00000000
 C                  7.15791604    5.90427259    0.00000000
 C                  5.96279893    3.83113886    0.00000000
 C                  8.38206073    5.22961902    0.00000000
 H                  7.15778097    6.98444309    0.00000000
 C                  7.15947284    3.10730942    0.00000000
 H                  5.02716833    3.29142924    0.00000000
 C                  8.35488646    3.83183871    0.00000000
 H                  9.29092133    3.29268804    0.00000000
 C                  7.16099568    0.88043521   -1.18846416
 C                  7.16099878    0.87591366    1.18632786
 C                  7.16048747    1.62360397    0.00000000
 H                  7.16065205    1.38292576   -2.14819371
 H                  7.16065833    1.37376682    2.14810490
 C                 -0.34834971   11.75003670    0.00000000
 C                 -0.34765035   12.49573570   -1.18703658
 C                 -0.34765121   12.49481236    1.18767997
 H                 -0.34811950   11.99547696   -2.14747803
 H                 -0.34812100   11.99391979    2.14828588
 C                  9.66551618    5.96997921    0.00000000
 C                 10.31089376    6.34226472    1.18699192
 C                 10.31052837    6.34205394   -1.18758935
 H                  9.87942661    6.09337326    2.14928651
 H                  9.87781001    6.09244073   -2.14867764
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 3 (0° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 42.6216488226,
  celldm(3)   = 0.9,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C        4.442436436  -3.944251153   0.000000000
C        4.414217213  -2.546168006   0.000000000
C        5.639274783  -1.872041563   0.000000000
C        6.863844973  -2.547123529   0.000000000
C        6.835682758  -3.945062216   0.000000000
C        5.638864567  -4.668114718   0.000000000
H        3.506855313  -4.484335443   0.000000000
H        5.640351292  -0.791723841   0.000000000
H        7.771365553  -4.485090781   0.000000000
C        8.147820494  -1.805971069   0.000000000
C        9.387177692  -2.461774378   0.000000000
C        8.198924922  -0.404432841   0.000000000
C       10.585824410  -1.770092089   0.000000000
H        9.434233277  -3.544053741   0.000000000
C        9.397161342   0.288416418   0.000000000
H        7.284095634   0.176066779   0.000000000
C       10.637008779  -0.368456837   0.000000000
H       11.501506380  -2.348589764   0.000000000
C        3.130163383  -1.804825556   0.000000000
C        3.078021716  -0.403351272   0.000000000
C        1.890942819  -2.461363523   0.000000000
C        1.879264080   0.288704556   0.000000000
H        3.991901224   0.178632189   0.000000000
C        0.691697938  -1.770421419   0.000000000
H        1.844741592  -3.543756665   0.000000000
C        0.639816553  -0.368583597   0.000000000
H        1.923191893   1.371222326   0.000000000
H       -0.223276637  -2.350559464   0.000000000
C        5.638520771  -6.150687638   0.000000000
C        6.826113123  -6.896499260   0.000000000
C        4.450521672  -6.896180076   0.000000000
C        6.826303641  -8.281046975   0.000000000
H        7.786895769  -6.395400748   0.000000000
C        4.450018379  -8.280775192   0.000000000
H        3.489799582  -6.394774684   0.000000000
C        5.638169834  -9.027647906   0.000000000
H        7.786123727  -8.783388874   0.000000000
H        3.489578705  -8.782601152   0.000000000
C       -0.639698124   0.368865384   0.000000000
C       -1.879133897  -0.288444808   0.000000000
C       -0.691619637   1.770705160   0.000000000
C       -3.077902876   0.403576770   0.000000000
H       -1.923081958  -1.370960794   0.000000000
C       -1.890886782   2.461615032   0.000000000
H        0.223324431   2.350892906   0.000000000
C       -3.130089590   1.805045913   0.000000000
H       -3.991749675  -0.178453342   0.000000000
H       -1.844708047   3.544009212   0.000000000
C       -4.414178912   2.546317083   0.000000000
C       -4.442510160   3.944394392   0.000000000
C       -5.639177406   1.872094947   0.000000000
C       -5.639003576   4.668159884   0.000000000
H       -3.506959348   4.484532950   0.000000000
C       -6.863802409   2.547058087   0.000000000
H       -5.640168187   0.791780964   0.000000000
```

```
C       -6.835767854   3.945007805   0.000000000
H       -7.771494432   4.484967030   0.000000000
C       -5.638753701   6.150736478   0.000000000
C       -6.826373075   6.896512315   0.000000000
C       -4.450782115   6.896269384   0.000000000
C       -6.826608259   8.281066960   0.000000000
H       -7.787135324   6.395371741   0.000000000
C       -4.450323723   8.280859099   0.000000000
H       -3.490038043   6.394909329   0.000000000
C       -5.638492209   9.027700244   0.000000000
H       -7.786437797   8.783394385   0.000000000
H       -3.489893877   8.782700727   0.000000000
C       -8.147683278   1.805741308   0.000000000
C       -8.198670428   0.404188459   0.000000000
C       -9.387086658   2.461434705   0.000000000
C       -9.396849040  -0.288784831   0.000000000
H       -7.283782065  -0.176218767   0.000000000
C      -10.585655181   1.769640456   0.000000000
H       -9.434252849   3.543708527   0.000000000
C      -10.636744560   0.368005510   0.000000000
H       -9.351427878  -1.371393953   0.000000000
H      -11.501368583   2.348075418   0.000000000
H        9.351811495   1.371021607   0.000000000
K_POINTS { automatic}
 8 8 1 0 0 0
```

Structure 3 (60° dihedral angle)

```
  ibrav = 4
  celldm(1)   = 42.232651351,
  celldm(3)   = 0.9,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C        2.164638422  -1.944479939  -1.035369263
C        3.089324824  -1.777933532  -0.000073177
C        2.769976849  -0.894418851   1.035361589
C        1.557829510  -0.217272367   1.046032621
C        0.641027187  -0.368651737   0.000954826
C        4.371326540  -2.517762215  -0.000243626
C        4.384130106  -3.914795139  -0.000071603
H        2.396041510  -2.622964260  -1.850685551
H        3.473599824  -0.753599662   1.850070887
H        1.324349626   0.456445478   1.864768839
H        3.443244068  -4.457176629   0.000469079
C        0.970317179  -1.236525723  -1.044972423
H        0.270075779  -1.372461213  -1.863437279
C       -9.616431620   0.217261840  -1.047042475
H       -9.849902046  -0.456452516  -1.865785018
C       -8.404284563   0.894407574  -1.036354231
C       -8.084949348   1.777926682  -0.000921998
C       -9.009638236   1.944451208   1.034382796
C      -10.203960073   1.236497527   1.043968531
C      -10.533248196   0.368644505  -0.001980852
C       -6.802951205   2.517760108  -0.000722925
C       -5.587120555   1.830323269  -0.000449284
H       -7.700659121   0.753592277  -1.851062607
H       -8.778240984   2.622923687   1.849710296
H      -10.904209360   1.372417838   1.862429022
H       -5.587107871   0.744227907  -0.000554585
C       -2.164630652   1.944577133  -1.035215620
C       -3.089292017   1.777972483   0.000094705
C       -2.769915265   0.894406085   1.035475553
C       -1.557764272   0.217265274   1.046082069
C       -0.640987543   0.368702570   0.000990224
C       -4.371304295   2.517782476  -0.000024154
C       -4.384132155   3.914815105   0.000175170
H       -2.396057415   2.623101689  -1.850491615
H       -3.473518250   0.753540080   1.850194083
H       -1.324261365  -0.456494053   1.864777648
H       -3.443255580   4.457213039   0.000719756
C        8.404356136  -0.894420142  -1.036470203
C        8.084982355  -1.777967177  -0.001074688
C        9.009636728  -1.944527157   1.034256258
C       10.203963109  -1.236581369   1.043901035
C       10.533289768  -0.368700062  -0.002012946
C        6.802973442  -2.517782244  -0.000929253
C        5.587154353  -1.830324145  -0.000650312
H        7.700757264  -0.753575996  -1.851196537
H        8.778208496  -2.623020801   1.849557333
H       10.904184845  -1.372529152   1.862380533
H        5.587160362  -0.744228797  -0.000720746
C        6.185473028  -6.826639582  -1.038732173
C        5.587115212  -6.106785808  -0.000319372
C        4.988752912  -6.826501210   1.038189878
C        5.006406279  -8.215146190   1.048255776
C        5.587117324  -8.936721779  -0.000129661
C        5.587128214  -4.625277258  -0.000431265
C        6.790140425  -3.914816062  -0.000894004
```

```
H        6.652546413  -6.286920966  -1.856689083
H        4.521629874  -6.286675945   1.856048179
H        4.543549242  -8.750597165   1.871512630
H        7.731016691  -4.457215468  -0.001326710
C       -0.970305761   1.236629757  -1.044884193
H       -0.270084719   1.372610916  -1.863358827
C       -6.185484000   6.826580991  -1.038594206
C       -5.587153079   6.106785282  -0.000125135
C       -4.988829156   6.826558636   1.038365127
C       -5.006490390   8.215204291   1.048355456
C       -5.587169552   8.936721293  -0.000087789
C       -5.587142649   4.625276262  -0.000188107
C       -6.790142380   3.914794506  -0.000663560
H       -6.652529373   6.286814398  -1.856535310
H       -4.521728819   6.286781351   1.856268200
H       -4.543662121   8.750702439   1.871598129
H       -7.731027967   4.457177675  -0.001107515
C        6.167825333  -8.215280439  -1.048607785
H        6.630651143  -8.750839994  -1.871812070
C        9.616507691  -0.217282043  -1.047099586
H        9.850008620   0.456454908  -1.865814825
C       -6.167843397   8.215221270  -1.048544461
H       -6.630646605   8.750733530  -1.871791896
K_POINTS { automatic}
 8 8 1 0 0 0
```

Structure 4 (monolayer)

```
  ibrav = 4
  celldm(1)   = 27.4182837709,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C       -3.965993269   7.851973866   0.000000000
C       -2.761215825   5.762367843   0.000000000
C       -2.748008429   7.162118101   0.000000000
H       -3.955958891   8.934879727   0.000000000
H       -1.819330505   5.227978774   0.000000000
C       -1.469582763   7.899973293   0.000000000
N       -0.335927979   7.187507615   0.000000000
N       -1.519996772   9.238034823   0.000000000
C        0.797718098   7.900184080   0.000000000
C       -0.336178207   9.863844130   0.000000000
N        0.847785100   9.238233824   0.000000000
C        2.077016153   7.162349828   0.000000000
C        3.295277303   7.852126567   0.000000000
C        2.090344821   5.762508432   0.000000000
C        4.493524918   7.161144628   0.000000000
H        3.284422413   8.935223095   0.000000000
C        3.288611787   5.071554346   0.000000000
H        1.147448028   5.229421635   0.000000000
C        4.506935954   5.761240161   0.000000000
H        5.436282573   7.694404042   0.000000000
H        3.299375329   3.988488962   0.000000000
C        5.786302517   5.023302078   0.000000000
N        6.919935062   5.736161229   0.000000000
N        5.736546437   3.685185364   0.000000000
C        8.053675144   5.023770605   0.000000000
C        6.920677854   3.059753608   0.000000000
N        8.104436829   3.685684996   0.000000000
C        5.714258990   0.871553629   0.000000000
C        8.126554300   0.870181564   0.000000000
C        6.920799197   1.582070368   0.000000000
H        4.782099229   1.423504980   0.000000000
H        9.059819209   1.420393945   0.000000000
C       -0.335765076  11.341528195   0.000000000
C       -1.541427135  12.053408155   0.000000000
C        0.870846620  12.051988096   0.000000000
H       -2.474553567  11.502954629   0.000000000
H        1.802992594  11.500003525   0.000000000
C        9.331973017   5.761600705   0.000000000
C        9.345129160   7.161291533   0.000000000
C       10.549910568   5.071724347   0.000000000
H        8.403087761   7.695427688   0.000000000
H       10.539595070   3.988814846   0.000000000
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 4 (bilayer)

```
  ibrav = 14
  celldm(1)   = 27.3594907,
  celldm(2)   = 0.9999996,
  celldm(3)   = 1.3392088,
  celldm(4)   = 0.3738145,
  celldm(5)   = 0.0,
  celldm(6)   = -0.5000002,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {crystal}
C     0.0255900      0.5980400      0.0368624
C     0.0248900      0.4305500      0.0378117
C     0.0817900      0.5426100      0.0371751
H     0.0700100      0.6841100      0.0372830
H     0.0689500      0.3884100      0.0373314
C     0.1990700      0.6012100      0.0375771
N     0.2493700      0.5452800      0.0363486
N     0.2483500      0.7067600      0.0391891
C     0.3555600      0.6011900      0.0376144
C     0.3549700      0.7565200      0.0393045
N     0.4118100      0.7066900      0.0392672
C     0.4142800      0.5425900      0.0372049
C     0.5259200      0.5980700      0.0368438
C     0.3591300      0.4305400      0.0378489
C     0.5809700      0.5427300      0.0373538
H     0.5675900      0.6841400      0.0372346
C     0.4142000      0.3752300      0.0383589
H     0.2729100      0.3884200      0.0373873
C     0.5258300      0.4307000      0.0380052
H     0.6672100      0.5849000      0.0378005
H     0.3725400      0.2891600      0.0379420
C     0.5846000      0.3721600      0.0375883
N     0.6908000      0.4281000      0.0388280
N     0.5283500      0.2666300      0.0359652
C     0.7410600      0.3721100      0.0376293
C     0.5851700      0.2168000      0.0359168
N     0.6917800      0.2665700      0.0360285
C     0.4145000      0.0422100      0.0369033
C     0.5811700      0.0422100      0.0369480
C     0.5262900      0.0991200      0.0362109
H     0.3727700      0.0870300      0.0363524
H     0.6677000      0.0870000      0.0364343
C     0.4138100      0.8741700      0.0390104
C     0.3589300      0.9311000      0.0382733
C     0.5256200      0.9310800      0.0383068
H     0.2724100      0.8863300      0.0387647
H     0.5673700      0.8863200      0.0388391
C     0.8583500      0.4307000      0.0380239
C     0.9152400      0.5427400      0.0373873
C     0.9145000      0.3752400      0.0383440
H     0.8711700      0.5849000      0.0378861
H     0.8700900      0.2891800      0.0379122
C     0.0255900      0.5980400      0.2229984
C     0.0248900      0.4305500      0.2239476
C     0.0817800      0.5426100      0.2233111
H     0.0700100      0.6841100      0.2234227
H     0.0689500      0.3884100      0.2234674
C     0.1990600      0.6012100      0.2237131
N     0.2493700      0.5452800      0.2224846
N     0.2483500      0.7067600      0.2253251
C     0.3555600      0.6011900      0.2237541
```

```
C     0.3549700      0.7565200      0.2254405
N     0.4118100      0.7066900      0.2254070
C     0.4142800      0.5426000      0.2233408
C     0.5259200      0.5980700      0.2229760
C     0.3591300      0.4305400      0.2239886
C     0.5809700      0.5427400      0.2234860
H     0.5675900      0.6841400      0.2233706
C     0.4142000      0.3752300      0.2244949
H     0.2729100      0.3884200      0.2235233
C     0.5258200      0.4307000      0.2241412
H     0.6672100      0.5848900      0.2239365
H     0.3725400      0.2891500      0.2240779
C     0.5845900      0.3721500      0.2237243
N     0.6908000      0.4281000      0.2249639
N     0.5283500      0.2666300      0.2221012
C     0.7410600      0.3721200      0.2237578
C     0.5851700      0.2168000      0.2220491
N     0.6917800      0.2665600      0.2221645
C     0.4145000      0.0422100      0.2230393
C     0.5811700      0.0422000      0.2230840
C     0.5262900      0.0991300      0.2223469
H     0.3727700      0.0870300      0.2224883
H     0.6677000      0.0870000      0.2225628
C     0.4138100      0.8741700      0.2251464
C     0.3589300      0.9311100      0.2244093
C     0.5256200      0.9310800      0.2244465
H     0.2724100      0.8863300      0.2249007
H     0.5673700      0.8863200      0.2249751
C     0.8583500      0.4307000      0.2241598
C     0.9152400      0.5427400      0.2235195
C     0.9145000      0.3752400      0.2244800
H     0.8711700      0.5849000      0.2240221
H     0.8701100      0.2891800      0.2240519
K_POINTS (automatic)
 6 6 1 0 0 0
```

Structure 4 (3 layers)

```
  ibrav = 14
  celldm(1)   = 27.3594907,
  celldm(2)   = 0.9999996,
  celldm(3)   = 1.5884837,
  celldm(4)   = 0.3738145,
  celldm(5)   = 0.0,
  celldm(6)   = -0.5000002,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {crystal}
C     0.0255900      0.5980400      0.0310761
C     0.0248900      0.4305500      0.0318764
C     0.0817900      0.5426100      0.0313398
H     0.0700100      0.6841100      0.0314339
H     0.0689500      0.3884100      0.0314716
C     0.1990700      0.6012100      0.0316787
N     0.2493700      0.5452800      0.0306430
N     0.2483500      0.7067600      0.0330393
C     0.3555600      0.6011900      0.0317117
C     0.3549700      0.7565200      0.0331334
N     0.4118100      0.7066900      0.0331052
C     0.4142800      0.5425900      0.0313680
C     0.5259200      0.5980700      0.0310620
C     0.3591300      0.4305400      0.0319094
C     0.5809700      0.5427300      0.0314904
H     0.5675900      0.6841400      0.0313915
C     0.4142000      0.3752300      0.0323378
H     0.2729100      0.3884200      0.0315187
C     0.5258300      0.4307000      0.0320412
H     0.6672100      0.5849000      0.0318670
H     0.3725400      0.2891600      0.0319894
C     0.5846000      0.3721600      0.0316881
N     0.6908000      0.4281000      0.0327333
N     0.5283500      0.2666300      0.0303182
C     0.7410600      0.3721100      0.0317211
C     0.5851700      0.2168000      0.0302805
N     0.6917800      0.2665700      0.0303747
C     0.4145000      0.0422100      0.0311091
C     0.5811700      0.0422100      0.0311514
C     0.5262900      0.0991200      0.0305253
H     0.3727700      0.0870300      0.0306477
H     0.6677000      0.0870000      0.0307136
C     0.4138100      0.8741700      0.0328886
C     0.3589300      0.9311000      0.0322672
C     0.5256200      0.9310800      0.0322954
H     0.2724100      0.8863300      0.0326815
H     0.5673700      0.8863200      0.0327427
C     0.8583500      0.4307000      0.0320553
C     0.9152400      0.5427400      0.0315187
C     0.9145000      0.3752400      0.0323237
H     0.8711700      0.5849000      0.0319376
H     0.8700900      0.2891800      0.0319659
C     0.0255900      0.5980400      0.1880056
C     0.0248900      0.4305500      0.1888059
C     0.0817800      0.5426100      0.1882692
H     0.0700100      0.6841100      0.1883587
H     0.0689500      0.3884100      0.1884011
C     0.1990600      0.6012100      0.1886082
N     0.2493700      0.5452800      0.1875725
N     0.2483500      0.7067600      0.1899640
C     0.3555600      0.6011900      0.1886412
```

C	0.3549700	0.7565200	0.1900629
N	0.4118100	0.7066900	0.1900347
C	0.4142800	0.5426000	0.1882928
C	0.5259200	0.5980700	0.1879868
C	0.3591300	0.4305400	0.1888389
C	0.5809700	0.5427400	0.1884152
H	0.5675900	0.6841400	0.1883163
C	0.4142000	0.3752300	0.1892673
H	0.2729100	0.3884200	0.1884481
C	0.5258200	0.4307000	0.1889660
H	0.6672100	0.5848900	0.1887965
H	0.3725400	0.2891500	0.1889142
C	0.5845900	0.3721500	0.1886176
N	0.6908000	0.4281000	0.1896627
N	0.5283500	0.2666300	0.1872476
C	0.7410600	0.3721200	0.1886459
C	0.5851700	0.2168000	0.1872053
N	0.6917800	0.2665600	0.1872994
C	0.4145000	0.0422100	0.1880386
C	0.5811700	0.0422000	0.1880762
C	0.5262900	0.0991300	0.1874548
H	0.3727700	0.0870300	0.1875772
H	0.6677000	0.0870000	0.1876384
C	0.4138100	0.8741700	0.1898181
C	0.3589300	0.9311100	0.1891967
C	0.5256200	0.9310800	0.1892249
H	0.2724100	0.8863300	0.1896110
H	0.5673700	0.8863200	0.1896722
C	0.8583500	0.4307000	0.1889848
C	0.9152400	0.5427400	0.1884434
C	0.9145000	0.3752400	0.1892532
H	0.8711700	0.5849000	0.1888671
H	0.8701100	0.2891800	0.1888907
C	0.0255900	0.5980400	0.3449304
C	0.0248900	0.4305500	0.3457307
C	0.0817800	0.5426100	0.3451940
H	0.0700100	0.6841100	0.3452882
H	0.0689500	0.3884000	0.3453258
C	0.1990600	0.6012100	0.3455330
N	0.2493700	0.5452800	0.3444973
N	0.2483500	0.7067600	0.3468935
C	0.3555600	0.6011900	0.3455659
C	0.3549700	0.7565200	0.3469877
N	0.4118100	0.7066900	0.3469594
C	0.4142800	0.5426000	0.3452223
C	0.5259200	0.5980700	0.3449115
C	0.3591300	0.4305400	0.3457636
C	0.5809700	0.5427400	0.3453399
H	0.5675900	0.6841400	0.3452458
C	0.4142000	0.3752300	0.3461921
H	0.2729100	0.3884200	0.3453729
C	0.5258200	0.4307000	0.3458955
H	0.6672100	0.5848900	0.3457213
H	0.3725400	0.2891500	0.3458437
C	0.5845900	0.3721500	0.3455424
N	0.6908000	0.4281000	0.3465875
N	0.5283500	0.2666300	0.3441724
C	0.7410600	0.3721200	0.3455706
C	0.5851700	0.2168000	0.3441300
N	0.6917800	0.2665600	0.3442289
C	0.4145000	0.0422100	0.3449633
C	0.5811700	0.0422000	0.3450057
C	0.5262900	0.0991300	0.3443796

```
H     0.3727700      0.0870300      0.3445020
H     0.6677000      0.0870000      0.3445632
C     0.4138100      0.8741700      0.3467429
C     0.3589300      0.9311100      0.3461214
C     0.5256200      0.9310800      0.3461497
H     0.2724100      0.8863300      0.3465357
H     0.5673700      0.8863200      0.3465969
C     0.8583500      0.4307000      0.3459096
C     0.9152400      0.5427500      0.3453682
C     0.9145000      0.3752400      0.3461779
H     0.8711700      0.5849000      0.3457919
H     0.8701000      0.2891800      0.3458201
K_POINTS (automatic)
 6 6 1 0 0 0
```

Structure 4 (4 layers)

```
  ibrav = 14
  celldm(1)   = 27.3594907,
  celldm(2)   = 0.9999996,
  celldm(3)   = 1.8377586,
  celldm(4)   = 0.3738145,
  celldm(5)   = 0.0,
  celldm(6)   = -0.5000002,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {crystal}
C     0.0255900      0.5980400      0.0268623
C     0.0248900      0.4305500      0.0275513
C     0.0817900      0.5426100      0.0270902
H     0.0700100      0.6841100      0.0271716
H     0.0689500      0.3884100      0.0272041
C     0.1990700      0.6012100      0.0273832
N     0.2493700      0.5452800      0.0264879
N     0.2483500      0.7067600      0.0285551
C     0.3555600      0.6011900      0.0274103
C     0.3549700      0.7565200      0.0286419
N     0.4118100      0.7066900      0.0286148
C     0.4142800      0.5425900      0.0271119
C     0.5259200      0.5980700      0.0268514
C     0.3591300      0.4305400      0.0275839
C     0.5809700      0.5427300      0.0272204
H     0.5675900      0.6841400      0.0271336
C     0.4142000      0.3752300      0.0279528
H     0.2729100      0.3884200      0.0272475
C     0.5258300      0.4307000      0.0276924
H     0.6672100      0.5849000      0.0275459
H     0.3725400      0.2891600      0.0276490
C     0.5846000      0.3721600      0.0273886
N     0.6908000      0.4281000      0.0282947
N     0.5283500      0.2666300      0.0262058
C     0.7410600      0.3721100      0.0274211
C     0.5851700      0.2168000      0.0261732
N     0.6917800      0.2665700      0.0262546
C     0.4145000      0.0422100      0.0268894
C     0.5811700      0.0422100      0.0269220
C     0.5262900      0.0991200      0.0263848
H     0.3727700      0.0870300      0.0264933
H     0.6677000      0.0870000      0.0265476
C     0.4138100      0.8741700      0.0284303
C     0.3589300      0.9311000      0.0278932
C     0.5256200      0.9310800      0.0279149
H     0.2724100      0.8863300      0.0282513
H     0.5673700      0.8863200      0.0283055
C     0.8583500      0.4307000      0.0277087
C     0.9152400      0.5427400      0.0272475
C     0.9145000      0.3752400      0.0279420
H     0.8711700      0.5849000      0.0276056
H     0.8700900      0.2891800      0.0276273
C     0.0255900      0.5980400      0.1625030
C     0.0248900      0.4305500      0.1631921
C     0.0817800      0.5426100      0.1627309
H     0.0700100      0.6841100      0.1628123
H     0.0689500      0.3884100      0.1628448
C     0.1990600      0.6012100      0.1630239
N     0.2493700      0.5452800      0.1621287
N     0.2483500      0.7067600      0.1642012
C     0.3555600      0.6011900      0.1630510
```

C	0.3549700	0.7565200	0.1642826
N	0.4118100	0.7066900	0.1642555
C	0.4142800	0.5426000	0.1627526
C	0.5259200	0.5980700	0.1624867
C	0.3591300	0.4305400	0.1632246
C	0.5809700	0.5427400	0.1628557
H	0.5675900	0.6841400	0.1627743
C	0.4142000	0.3752300	0.1635936
H	0.2729100	0.3884200	0.1628882
C	0.5258200	0.4307000	0.1633386
H	0.6672100	0.5848900	0.1631867
H	0.3725400	0.2891500	0.1632897
C	0.5845900	0.3721500	0.1630347
N	0.6908000	0.4281000	0.1639354
N	0.5283500	0.2666300	0.1618465
C	0.7410600	0.3721200	0.1630564
C	0.5851700	0.2168000	0.1618140
N	0.6917800	0.2665600	0.1618954
C	0.4145000	0.0422100	0.1625302
C	0.5811700	0.0422000	0.1625681
C	0.5262900	0.0991300	0.1620256
H	0.3727700	0.0870300	0.1621341
H	0.6677000	0.0870000	0.1621883
C	0.4138100	0.8741700	0.1640710
C	0.3589300	0.9311100	0.1635339
C	0.5256200	0.9310800	0.1635556
H	0.2724100	0.8863300	0.1638920
H	0.5673700	0.8863200	0.1639462
C	0.8583500	0.4307000	0.1633494
C	0.9152400	0.5427400	0.1628828
C	0.9145000	0.3752400	0.1635827
H	0.8711700	0.5849000	0.1632463
H	0.8701100	0.2891800	0.1632680
C	0.0255900	0.5980400	0.2981438
C	0.0248900	0.4305500	0.2988382
C	0.0817800	0.5426100	0.2983716
H	0.0700100	0.6841100	0.2984530
H	0.0689500	0.3884000	0.2984856
C	0.1990600	0.6012100	0.2986646
N	0.2493700	0.5452800	0.2977694
N	0.2483500	0.7067600	0.2998420
C	0.3555600	0.6011800	0.2986917
C	0.3549700	0.7565200	0.2999234
N	0.4118100	0.7066900	0.2998962
C	0.4142800	0.5426000	0.2983933
C	0.5259200	0.5980700	0.2981275
C	0.3591300	0.4305400	0.2988654
C	0.5809700	0.5427400	0.2984964
H	0.5675900	0.6841400	0.2984150
C	0.4142000	0.3752300	0.2992343
H	0.2729100	0.3884200	0.2985290
C	0.5258200	0.4307000	0.2989793
H	0.6672100	0.5848900	0.2988274
H	0.3725400	0.2891500	0.2989305
C	0.5845900	0.3721500	0.2986755
N	0.6908000	0.4281000	0.2995761
N	0.5283500	0.2666300	0.2974927
C	0.7410600	0.3721200	0.2986972
C	0.5851700	0.2168000	0.2974547
N	0.6917800	0.2665600	0.2975361
C	0.4145000	0.0422100	0.2981709
C	0.5811700	0.0422000	0.2982089
C	0.5262900	0.0991300	0.2976717

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H     0.3727700      0.0870300      0.2977748
H     0.6677000      0.0870000      0.2978291
C     0.4138100      0.8741700      0.2997118
C     0.3589300      0.9311100      0.2991746
C     0.5256200      0.9310800      0.2991963
H     0.2724100      0.8863300      0.2995327
H     0.5673700      0.8863200      0.2995870
C     0.8583500      0.4307000      0.2989902
C     0.9152400      0.5427500      0.2985235
C     0.9145000      0.3752400      0.2992235
H     0.8711700      0.5849000      0.2988925
H     0.8701000      0.2891800      0.2989088
C     0.0255900      0.5980400      0.4337791
C     0.0248900      0.4305500      0.4344790
C     0.0817800      0.5426100      0.4340124
H     0.0700100      0.6841100      0.4340937
H     0.0689600      0.3884200      0.4341209
C     0.1990600      0.6012100      0.4343053
N     0.2493700      0.5452800      0.4334101
N     0.2483500      0.7067600      0.4354827
C     0.3555600      0.6011900      0.4343379
C     0.3549700      0.7565200      0.4355641
N     0.4118100      0.7066900      0.4355424
C     0.4142800      0.5426000      0.4340341
C     0.5259200      0.5980700      0.4337682
C     0.3591300      0.4305400      0.4345061
C     0.5809700      0.5427400      0.4341372
H     0.5675900      0.6841400      0.4340558
C     0.4142000      0.3752300      0.4348750
H     0.2729100      0.3884200      0.4341697
C     0.5258200      0.4307000      0.4346200
H     0.6672100      0.5848900      0.4344681
H     0.3725400      0.2891500      0.4345712
C     0.5845900      0.3721500      0.4343162
N     0.6908000      0.4281000      0.4352169
N     0.5283500      0.2666300      0.4331280
C     0.7410600      0.3721200      0.4343379
C     0.5851700      0.2168000      0.4330954
N     0.6917800      0.2665600      0.4331768
C     0.4145000      0.0422100      0.4338170
C     0.5811700      0.0422000      0.4338496
C     0.5262900      0.0991300      0.4333070
H     0.3727700      0.0870300      0.4334155
H     0.6677000      0.0870000      0.4334698
C     0.4138100      0.8741700      0.4353525
C     0.3589300      0.9311100      0.4348099
C     0.5256200      0.9310800      0.4348425
H     0.2724100      0.8863300      0.4351680
H     0.5673700      0.8863200      0.4352277
C     0.8583500      0.4307000      0.4346309
C     0.9152400      0.5427400      0.4341643
C     0.9145000      0.3752400      0.4348642
H     0.8711700      0.5849000      0.4345278
H     0.8701000      0.2891800      0.4345549
K_POINTS (automatic)
 6 6 1 0 0 0
```

Structure 4 (5 layers)

```
  ibrav = 14
  celldm(1)   = 27.3594907,
  celldm(2)   = 0.9999996,
  celldm(3)   = 2.0870335,
  celldm(4)   = 0.3738145,
  celldm(5)   = 0.0,
  celldm(6)   = -0.5000002,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {crystal}
C     0.0255900      0.5980400      0.0236551
C     0.0248900      0.4305500      0.0242642
C     0.0817900      0.5426100      0.0238521
H     0.0700100      0.6841100      0.0239238
H     0.0689500      0.3884100      0.0239537
C     0.1990700      0.6012100      0.0241089
N     0.2493700      0.5452800      0.0233206
N     0.2483500      0.7067600      0.0251481
C     0.3555600      0.6011900      0.0241388
C     0.3549700      0.7565200      0.0252197
N     0.4118100      0.7066900      0.0251958
C     0.4142800      0.5425900      0.0238760
C     0.5259200      0.5980700      0.0236431
C     0.3591300      0.4305400      0.0242881
C     0.5809700      0.5427300      0.0239716
H     0.5675900      0.6841400      0.0238939
C     0.4142000      0.3752300      0.0246165
H     0.2729100      0.3884200      0.0239895
C     0.5258300      0.4307000      0.0243896
H     0.6672100      0.5849000      0.0242523
H     0.3725400      0.2891600      0.0243478
C     0.5846000      0.3721600      0.0241209
N     0.6908000      0.4281000      0.0249151
N     0.5283500      0.2666300      0.0230758
C     0.7410600      0.3721100      0.0241448
C     0.5851700      0.2168000      0.0230459
N     0.6917800      0.2665700      0.0231176
C     0.4145000      0.0422100      0.0236789
C     0.5811700      0.0422100      0.0237088
C     0.5262900      0.0991200      0.0232370
H     0.3727700      0.0870300      0.0233266
H     0.6677000      0.0870000      0.0233803
C     0.4138100      0.8741700      0.0250346
C     0.3589300      0.9311000      0.0245568
C     0.5256200      0.9310800      0.0245807
H     0.2724100      0.8863300      0.0248733
H     0.5673700      0.8863200      0.0249211
C     0.8583500      0.4307000      0.0243956
C     0.9152400      0.5427400      0.0239895
C     0.9145000      0.3752400      0.0246046
H     0.8711700      0.5849000      0.0243120
H     0.8700900      0.2891800      0.0243299
C     0.0255900      0.5980400      0.1430949
C     0.0248900      0.4305500      0.1437040
C     0.0817800      0.5426100      0.1432979
H     0.0700100      0.6841100      0.1433636
H     0.0689500      0.3884100      0.1433935
C     0.1990600      0.6012100      0.1435547
N     0.2493700      0.5452800      0.1427664
N     0.2483500      0.7067600      0.1445879
C     0.3555600      0.6011900      0.1435786
```

C	0.3549700	0.7565200	0.1446595
N	0.4118100	0.7066900	0.1446357
C	0.4142800	0.5426000	0.1433158
C	0.5259200	0.5980700	0.1430770
C	0.3591300	0.4305400	0.1437279
C	0.5809700	0.5427400	0.1434054
H	0.5675900	0.6841400	0.1433338
C	0.4142000	0.3752300	0.1440564
H	0.2729100	0.3884200	0.1434293
C	0.5258200	0.4307000	0.1438294
H	0.6672100	0.5848900	0.1436981
H	0.3725400	0.2891500	0.1437876
C	0.5845900	0.3721500	0.1435607
N	0.6908000	0.4281000	0.1443550
N	0.5283500	0.2666300	0.1425156
C	0.7410600	0.3721200	0.1435846
C	0.5851700	0.2168000	0.1424857
N	0.6917800	0.2665600	0.1425574
C	0.4145000	0.0422100	0.1431188
C	0.5811700	0.0422000	0.1431486
C	0.5262900	0.0991300	0.1426768
H	0.3727700	0.0870300	0.1427664
H	0.6677000	0.0870000	0.1428142
C	0.4138100	0.8741700	0.1444744
C	0.3589300	0.9311100	0.1440026
C	0.5256200	0.9310800	0.1440205
H	0.2724100	0.8863300	0.1443132
H	0.5673700	0.8863200	0.1443609
C	0.8583500	0.4307000	0.1438414
C	0.9152400	0.5427400	0.1434293
C	0.9145000	0.3752400	0.1440444
H	0.8711700	0.5849000	0.1437518
H	0.8701100	0.2891800	0.1437697
C	0.0255900	0.5980400	0.2625347
C	0.0248900	0.4305500	0.2631439
C	0.0817800	0.5426100	0.2627378
H	0.0700100	0.6841100	0.2628034
H	0.0689500	0.3884000	0.2628333
C	0.1990600	0.6012100	0.2629946
N	0.2493700	0.5452800	0.2622062
N	0.2483500	0.7067600	0.2640277
C	0.3555600	0.6011800	0.2630184
C	0.3549700	0.7565200	0.2640994
N	0.4118100	0.7066900	0.2640815
C	0.4142800	0.5426000	0.2627557
C	0.5259200	0.5980700	0.2625168
C	0.3591300	0.4305400	0.2631677
C	0.5809700	0.5427400	0.2628453
H	0.5675900	0.6841400	0.2627736
C	0.4142000	0.3752300	0.2634962
H	0.2729100	0.3884200	0.2628691
C	0.5258200	0.4307000	0.2632693
H	0.6672100	0.5848900	0.2631379
H	0.3725400	0.2891500	0.2632275
C	0.5845900	0.3721500	0.2630005
N	0.6908000	0.4281000	0.2637948
N	0.5283500	0.2666300	0.2619554
C	0.7410600	0.3721200	0.2630244
C	0.5851700	0.2168000	0.2619256
N	0.6917800	0.2665600	0.2619972
C	0.4145000	0.0422100	0.2625586
C	0.5811700	0.0422000	0.2625885
C	0.5262900	0.0991300	0.2621167

H	0.3727700	0.0870300	0.2622062
H	0.6677000	0.0870000	0.2622540
C	0.4138100	0.8741700	0.2639142
C	0.3589300	0.9311100	0.2634425
C	0.5256200	0.9310800	0.2634604
H	0.2724100	0.8863300	0.2637530
H	0.5673700	0.8863200	0.2638008
C	0.8583500	0.4307000	0.2632812
C	0.9152400	0.5427500	0.2628691
C	0.9145000	0.3752400	0.2634843
H	0.8711700	0.5849000	0.2631916
H	0.8701000	0.2891800	0.2632095
C	0.0255900	0.5980400	0.3819686
C	0.0248900	0.4305500	0.3825837
C	0.0817800	0.5426100	0.3821776
H	0.0700100	0.6841100	0.3822433
H	0.0689600	0.3884200	0.3822731
C	0.1990600	0.6012100	0.3824344
N	0.2493700	0.5452800	0.3816461
N	0.2483500	0.7067600	0.3834675
C	0.3555600	0.6011900	0.3824583
C	0.3549700	0.7565200	0.3835392
N	0.4118100	0.7066900	0.3835213
C	0.4142800	0.5426000	0.3821955
C	0.5259200	0.5980700	0.3819626
C	0.3591300	0.4305400	0.3826076
C	0.5809700	0.5427400	0.3822851
H	0.5675900	0.6841400	0.3822134
C	0.4142000	0.3752300	0.3829301
H	0.2729100	0.3884200	0.3823090
C	0.5258200	0.4307000	0.3827091
H	0.6672100	0.5848900	0.3825777
H	0.3725400	0.2891500	0.3826673
C	0.5845900	0.3721500	0.3824403
N	0.6908000	0.4281000	0.3832346
N	0.5283500	0.2666300	0.3813953
C	0.7410600	0.3721200	0.3824642
C	0.5851700	0.2168000	0.3813654
N	0.6917800	0.2665600	0.3814371
C	0.4145000	0.0422100	0.3819984
C	0.5811700	0.0422000	0.3820283
C	0.5262900	0.0991300	0.3815505
H	0.3727700	0.0870300	0.3816461
H	0.6677000	0.0870000	0.3816939
C	0.4138100	0.8741700	0.3833541
C	0.3589300	0.9311100	0.3828763
C	0.5256200	0.9310800	0.3829002
H	0.2724100	0.8863300	0.3831928
H	0.5673700	0.8863200	0.3832466
C	0.8583500	0.4307000	0.3827210
C	0.9152400	0.5427400	0.3823090
C	0.9145000	0.3752400	0.3829241
H	0.8711700	0.5849000	0.3826255
H	0.8701000	0.2891800	0.3826494
C	0.0255900	0.5980400	0.5014084
C	0.0248900	0.4305500	0.5020235
C	0.0817800	0.5426100	0.5016174
H	0.0700100	0.6841100	0.5016891
H	0.0689600	0.3884100	0.5017130
C	0.1990600	0.6012100	0.5018742
N	0.2493700	0.5452800	0.5010799
N	0.2483500	0.7067600	0.5029074
C	0.3555600	0.6011900	0.5018981

```
C     0.3549700      0.7565200      0.5029790
N     0.4118100      0.7066900      0.5029611
C     0.4142800      0.5426000      0.5016294
C     0.5259200      0.5980700      0.5014024
C     0.3591300      0.4305400      0.5020474
C     0.5809700      0.5427400      0.5017249
H     0.5675900      0.6841400      0.5016532
C     0.4142000      0.3752300      0.5023699
H     0.2729100      0.3884200      0.5017548
C     0.5258200      0.4307100      0.5021429
H     0.6672100      0.5848900      0.5020175
H     0.3725400      0.2891500      0.5021071
C     0.5845900      0.3721500      0.5018802
N     0.6908000      0.4281000      0.5026744
N     0.5283500      0.2666300      0.5008351
C     0.7410600      0.3721200      0.5019041
C     0.5851700      0.2168000      0.5008052
N     0.6917800      0.2665600      0.5008769
C     0.4145000      0.0422100      0.5014382
C     0.5811700      0.0422000      0.5014681
C     0.5262900      0.0991300      0.5009903
H     0.3727700      0.0870300      0.5010859
H     0.6677000      0.0870000      0.5011337
C     0.4138100      0.8741700      0.5027939
C     0.3589300      0.9311100      0.5023161
C     0.5256200      0.9310800      0.5023400
H     0.2724100      0.8863300      0.5026326
H     0.5673700      0.8863200      0.5026864
C     0.8583500      0.4307000      0.5021609
C     0.9152400      0.5427400      0.5017488
C     0.9145000      0.3752400      0.5023639
H     0.8711700      0.5849000      0.5020653
H     0.8701000      0.2891800      0.5020892
K_POINTS (automatic)
 6 6 1 0 0 0
```

Structure 4 (3D)

```
  ibrav = 14
  celldm(1)   = 27.3594548,
  celldm(2)   = 1.00,
  celldm(3)   = 0.24927476,
  celldm(4)   = 0.373813518,
  celldm(5)   = 0.0,
  celldm(6)   = -0.5,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C       -3.958646505   7.806890921   0.644683561
C       -2.756419154   5.714777507   0.661320895
C       -2.743927523   7.114552652   0.650241879
H       -3.938596205   8.889591289   0.652136400
H       -1.813361423   5.182402478   0.652889575
C       -1.470108261   7.852665870   0.657235840
N       -0.336900571   7.141124308   0.635709415
N       -1.520620369   9.189577215   0.685444366
C        0.795816818   7.852669860   0.657912481
C       -0.337181111   9.814393606   0.687441819
N        0.846398292   9.189379219   0.686834171
C        2.070077652   7.114622088   0.650713931
C        3.284866702   7.807096012   0.644362015
C        2.082768024   5.715008940   0.662007141
C        4.482383867   7.117604824   0.653255612
H        3.265130241   8.889599319   0.651223017
C        3.280487824   5.025795687   0.670901354
H        1.139360254   5.183071226   0.653933024
C        4.495064645   5.718254180   0.664690902
H        5.425810163   7.649946253   0.661112325
H        3.300408103   3.943054637   0.663647630
C        5.769748999   4.980757851   0.657444579
N        6.902377321   5.692601684   0.679106372
N        5.719275305   3.644052890   0.628990356
C        8.035315627   4.980625891   0.658060793
C        6.902657038   3.018884151   0.628156904
N        8.085972976   3.643783982   0.630104402
C        5.695564708   0.838088016   0.645436007
C        8.108679188   0.838357546   0.646216344
C        6.902063620   1.545925356   0.633282984
H        4.766956497   1.395493032   0.635794131
H        9.037164751   1.395702081   0.637161679
C       -0.336980923  11.287084239   0.682312479
C       -1.543673359  11.994801255   0.669378399
C        0.869872047  11.994803595   0.670035721
H       -2.472201203  11.437525783   0.677974638
H        1.798337951  11.437978897   0.679316732
C        9.309315693   5.718441157   0.665037724
C        9.321943534   7.117871622   0.653877679
C       10.523777852   5.025800038   0.670599224
H        8.378680734   7.650671659   0.662600545
H       10.503930297   3.943111223   0.663137737
K_POINTS (automatic)
 6 6 15 0 0 0
```

Structure 5 (monolayer)

```
  ibrav = 4
  celldm(1)   = 28.4980265149,
  celldm(3)   = 0.6668661,
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS {angstrom}
C       -4.119236241   8.104577390   0.000000000
C       -2.917396407   6.019013352   0.000000000
C       -2.894222597   7.421449082   0.000000000
H       -4.119831029   9.190037950   0.000000000
H       -1.978768337   5.473712997   0.000000000
B       -1.550734729   8.196875155   0.000000000
O       -0.349075858   7.516111049   0.000000000
O       -1.540269612   9.578109121   0.000000000
B        0.852326935   8.197475213   0.000000000
B       -0.349633154  10.278077567   0.000000000
O        0.841174761   9.578547222   0.000000000
C        2.197025470   7.422462599   0.000000000
C        3.422557467   8.105246782   0.000000000
C        2.220015933   6.019883421   0.000000000
C        4.623872377   7.412783739   0.000000000
H        3.422744200   9.190916794   0.000000000
C        3.421266622   5.327437636   0.000000000
H        1.280398920   5.475918057   0.000000000
C        4.646782392   6.010172423   0.000000000
H        5.563416121   7.956873958   0.000000000
H        3.421026220   4.241771109   0.000000000
B        5.991306020   5.234906167   0.000000000
O        7.192303288   5.916917889   0.000000000
O        6.002705430   3.853798345   0.000000000
B        8.393760774   5.235765307   0.000000000
B        7.193602508   3.153941866   0.000000000
O        8.383613811   3.854714949   0.000000000
C        5.989747574   0.880527623   0.000000000
C        8.397183625   0.878730444   0.000000000
C        7.193967354   1.600716794   0.000000000
H        5.049865625   1.424297177   0.000000000
H        9.338384890   1.420427279   0.000000000
C       -0.348657573  11.830994019   0.000000000
C       -1.551694411  12.552782012   0.000000000
C        0.855694822  12.550952078   0.000000000
H       -2.492589053  12.010626329   0.000000000
H        1.795566219  12.007009490   0.000000000
C        9.737199612   6.010682063   0.000000000
C        9.760227110   7.412974246   0.000000000
C       10.962102487   5.327387603   0.000000000
H        8.821428344   7.957920170   0.000000000
H       10.962577777   4.241863644   0.000000000
K_POINTS (automatic)
 12 12 1 0 0 0
```

Structure 5 (bilayer)

```
  ibrav = 14
  celldm(1) = 28.3988042
  celldm(2) =  1.0
  celldm(3) =  1.038993792
  celldm(4) =  0.3948001
  celldm(5) =  0.0
  celldm(6) =  -0.5
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS (crystal)
C     0.036930000    0.620810000    0.000379593
C     0.037990000    0.462220000    -0.002504386
C     0.092690000    0.569620000    -0.001985918
H     0.078240000    0.702910000    0.002573823
H     0.080840000    0.422400000    -0.005152276
B     0.211560000    0.629440000    -0.002365510
O     0.266920000    0.580090000    -0.007656662
O     0.263770000    0.732510000    0.002800653
B     0.371620000    0.629440000    -0.002365510
B     0.370060000    0.786340000    0.001999805
O     0.422510000    0.732500000    0.002791395
C     0.430710000    0.569650000    -0.001962772
C     0.537660000    0.620870000    0.000425884
C     0.378030000    0.462250000    -0.002467352
C     0.590090000    0.566330000    0.002527532
H     0.578400000    0.702990000    0.002610857
C     0.430470000    0.407730000    -0.000365705
H     0.295360000    0.422450000    -0.005110613
C     0.537410000    0.458920000    0.002013693
H     0.672780000    0.606170000    0.005152276
H     0.389730000    0.325620000    -0.002559936
B     0.596410000    0.399040000    0.002374769
O     0.701040000    0.448280000    0.007827941
O     0.545580000    0.296070000    -0.002962674
B     0.756430000    0.399010000    0.002374769
B     0.598010000    0.242180000    -0.002115535
O     0.704290000    0.296020000    -0.002897866
C     0.430890000    0.068170000    -0.001425787
C     0.591240000    0.068130000    -0.001388754
C     0.538920000    0.123870000    -0.002870091
H     0.389800000    0.110680000    -0.002189602
H     0.674840000    0.110560000    -0.002138681
C     0.429240000    0.904580000    0.002851574
C     0.376920000    0.960290000    0.001398012
C     0.537270000    0.960240000    0.001430416
H     0.293330000    0.917810000    0.002157197
H     0.578350000    0.917720000    0.002208118
C     0.875280000    0.458850000    0.001972030
C     0.929960000    0.566230000    0.002490498
C     0.931030000    0.407660000    -0.000411997
H     0.887080000    0.606020000    0.005143018
H     0.889700000    0.325550000    -0.002610857
C     0.036930000    0.620810000    0.231838531
C     0.037990000    0.462220000    0.228954553
C     0.092700000    0.569610000    0.229473021
H     0.078240000    0.702910000    0.234032762
H     0.080850000    0.422400000    0.226306662
B     0.211560000    0.629440000    0.229088799
O     0.266920000    0.580080000    0.223802277
O     0.263780000    0.732510000    0.234254962
B     0.371620000    0.629440000    0.229088799
```

```
B     0.370060000    0.786350000    0.233458744
O     0.422510000    0.732500000    0.234250333
C     0.430710000    0.569650000    0.229491537
C     0.537660000    0.620870000    0.231880194
C     0.378030000    0.462250000    0.228996215
C     0.590100000    0.566340000    0.233981841
H     0.578400000    0.702990000    0.234069795
C     0.430470000    0.407730000    0.231097862
H     0.295360000    0.422450000    0.226348325
C     0.537410000    0.458920000    0.233472631
H     0.672780000    0.606180000    0.236615844
H     0.389730000    0.325620000    0.228894373
B     0.596410000    0.399040000    0.233833707
O     0.701050000    0.448280000    0.239286880
O     0.545580000    0.296070000    0.228500893
B     0.756430000    0.399010000    0.233838336
B     0.598020000    0.242180000    0.229348033
O     0.704290000    0.296020000    0.228556443
C     0.430890000    0.068180000    0.230033151
C     0.591240000    0.068130000    0.230070185
C     0.538920000    0.123870000    0.228584218
H     0.389800000    0.110680000    0.229269337
H     0.674830000    0.110560000    0.229329516
C     0.429240000    0.904580000    0.234305883
C     0.376920000    0.960300000    0.232852321
C     0.537270000    0.960250000    0.232889355
H     0.293330000    0.917810000    0.233616136
H     0.578350000    0.917710000    0.233671686
C     0.875280000    0.458850000    0.233430969
C     0.929970000    0.566230000    0.233944807
C     0.931030000    0.407660000    0.231046941
H     0.887080000    0.606020000    0.236601956
H     0.889700000    0.325550000    0.228843452
K_POINTS (automatic)
 8 8 1 0 0 0
```

Structure 5 (3 layers)

```
  ibrav = 14
  celldm(1) = 28.3988042
  celldm(2) =  1.0
  celldm(3) =  1.279478192
  celldm(4) =  0.3948001
  celldm(5) =  0.0
  celldm(6) =  -0.5
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS (crystal)
C     0.036930000    0.620810000    0.000310126
C     0.037990000    0.462220000    -0.002035553
C     0.092690000    0.569620000    -0.001612654
H     0.078240000    0.702910000    0.002091940
H     0.080840000    0.422400000    -0.004183880
B     0.211560000    0.629440000    -0.001922780
O     0.266920000    0.580090000    -0.006219433
O     0.263770000    0.732510000    0.002272377
B     0.371620000    0.629440000    -0.001922780
B     0.370060000    0.786340000    0.001623932
O     0.422510000    0.732500000    0.002266738
C     0.430710000    0.569650000    -0.001595738
C     0.537660000    0.620870000    0.000343958
C     0.378030000    0.462250000    -0.002001721
C     0.590090000    0.566330000    0.002052469
H     0.578400000    0.702990000    0.002120133
C     0.430470000    0.407730000    -0.000298849
H     0.295360000    0.422450000    -0.004150048
C     0.537410000    0.458920000    0.001635209
H     0.672780000    0.606170000    0.004183880
H     0.389730000    0.325620000    -0.002080663
B     0.596410000    0.399040000    0.001928419
O     0.701040000    0.448280000    0.006354761
O     0.545590000    0.296070000    -0.002407704
B     0.756430000    0.399010000    0.001928419
B     0.598010000    0.242180000    -0.001719789
O     0.704290000    0.296020000    -0.002356956
C     0.430890000    0.068170000    -0.001155924
C     0.591240000    0.068130000    -0.001127730
C     0.538920000    0.123870000    -0.002328763
H     0.389800000    0.110680000    -0.001776175
H     0.674840000    0.110560000    -0.001736705
C     0.429240000    0.904580000    0.002311847
C     0.376920000    0.960290000    0.001133369
C     0.537270000    0.960240000    0.001161562
H     0.293330000    0.917810000    0.001753621
H     0.578350000    0.917720000    0.001793091
C     0.875280000    0.458850000    0.001601377
C     0.929960000    0.566230000    0.002024276
C     0.931030000    0.407660000    -0.000332680
H     0.887080000    0.606020000    0.004178241
H     0.889700000    0.325550000    -0.002120133
C     0.036930000    0.620810000    0.188263306
C     0.037990000    0.462220000    0.185917627
C     0.092700000    0.569610000    0.186340526
H     0.078240000    0.702910000    0.190045120
H     0.080850000    0.422400000    0.183769301
B     0.211560000    0.629440000    0.186030400
```

O	0.266920000	0.580080000	0.181733747
O	0.263780000	0.732510000	0.190225557
B	0.371620000	0.629440000	0.186030400
B	0.370060000	0.786350000	0.189577112
O	0.422510000	0.732500000	0.190219918
C	0.430710000	0.569650000	0.186357442
C	0.537660000	0.620870000	0.188297138
C	0.378030000	0.462250000	0.185957098
C	0.590100000	0.566340000	0.190005649
H	0.578400000	0.702990000	0.190073313
C	0.430470000	0.407730000	0.187659970
H	0.295360000	0.422450000	0.183803133
C	0.537410000	0.458920000	0.189588389
H	0.672780000	0.606180000	0.192142699
H	0.389730000	0.325620000	0.185872518
B	0.596410000	0.399040000	0.189881599
O	0.701050000	0.448280000	0.194313579
O	0.545580000	0.296070000	0.185551115
B	0.756430000	0.399010000	0.189887238
B	0.598020000	0.242180000	0.186239030
O	0.704290000	0.296020000	0.185596224
C	0.430890000	0.068180000	0.186797257
C	0.591240000	0.068130000	0.186825450
C	0.538920000	0.123870000	0.185624417
H	0.389800000	0.110680000	0.186177005
H	0.674830000	0.110560000	0.186222114
C	0.429240000	0.904580000	0.190265027
C	0.376920000	0.960300000	0.189086549
C	0.537270000	0.960250000	0.189114743
H	0.293330000	0.917810000	0.189706801
H	0.578350000	0.917710000	0.189751910
C	0.875280000	0.458850000	0.189554557
C	0.929970000	0.566230000	0.189977456
C	0.931030000	0.407660000	0.187620500
H	0.887080000	0.606020000	0.192131421
H	0.889700000	0.325550000	0.185833047
C	0.036930000	0.620810000	0.376222125
C	0.037990000	0.462220000	0.373876446
C	0.092700000	0.569610000	0.374293706
H	0.078240000	0.702910000	0.377998300
H	0.080850000	0.422400000	0.371722481
B	0.211560000	0.629440000	0.373989219
O	0.266920000	0.580080000	0.369692566
O	0.263780000	0.732510000	0.378184376
B	0.371620000	0.629440000	0.373989219
B	0.370060000	0.786350000	0.377535931
O	0.422510000	0.732500000	0.378173099
C	0.430710000	0.569650000	0.374316261
C	0.537660000	0.620870000	0.376250318
C	0.378030000	0.462250000	0.373910278
C	0.590100000	0.566340000	0.377964468
H	0.578400000	0.702980000	0.378032132
C	0.430470000	0.407730000	0.375613151
H	0.295360000	0.422450000	0.371761951
C	0.537410000	0.458920000	0.377541570
H	0.672780000	0.606180000	0.380095879
H	0.389730000	0.325620000	0.373825698
B	0.596410000	0.399040000	0.377834779
O	0.701050000	0.448280000	0.382266760
O	0.545580000	0.296070000	0.373504295
B	0.756430000	0.399010000	0.377840418
B	0.598020000	0.242180000	0.374197849
O	0.704290000	0.296020000	0.373555043

```
C     0.430890000    0.068180000    0.374750437
C     0.591240000    0.068130000    0.374778630
C     0.538920000    0.123870000    0.373577597
H     0.389800000    0.110680000    0.374130185
H     0.674840000    0.110560000    0.374175294
C     0.429240000    0.904580000    0.378223846
C     0.376920000    0.960300000    0.377039729
C     0.537270000    0.960250000    0.377067923
H     0.293330000    0.917810000    0.377659981
H     0.578350000    0.917710000    0.377705090
C     0.875280000    0.458850000    0.377507738
C     0.929970000    0.566230000    0.377930636
C     0.931030000    0.407660000    0.375573680
H     0.887080000    0.606020000    0.380084601
H     0.889700000    0.325550000    0.373791866
K_POINTS (automatic)
 8 8 1 0 0 0
```

Structure 5 (4 layers)

```
  ibrav = 14
  celldm(1) = 28.3988042
  celldm(2) =  1.0
  celldm(3) =  1.519962592
  celldm(4) =  0.3948001
  celldm(5) =  0.0
  celldm(6) =  -0.5
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS (crystal)
C     0.036930000    0.620810000    0.000259476
C     0.037990000    0.462220000    -0.001708747
C     0.092690000    0.569620000    -0.001360669
H     0.078240000    0.702910000    0.001759377
H     0.080840000    0.422400000    -0.003518753
B     0.211560000    0.629440000    -0.001620145
O     0.266920000    0.580090000    -0.005233829
O     0.263770000    0.732510000    0.001911265
B     0.371620000    0.629440000    -0.001620145
B     0.370060000    0.786340000    0.001366998
O     0.422510000    0.732500000    0.001911265
C     0.430710000    0.569650000    -0.001341683
C     0.537660000    0.620870000    0.000291120
C     0.378030000    0.462250000    -0.001689761
C     0.590090000    0.566330000    0.001727733
H     0.578400000    0.702990000    0.001784691
C     0.430470000    0.407730000    -0.000253148
H     0.295360000    0.422450000    -0.003493438
C     0.537410000    0.458920000    0.001379655
H     0.672780000    0.606170000    0.003518753
H     0.389730000    0.325620000    -0.001753048
B     0.596410000    0.399040000    0.001620145
O     0.701040000    0.448280000    0.005354074
O     0.545580000    0.296070000    -0.002025182
B     0.756430000    0.399010000    0.001620145
B     0.598010000    0.242180000    -0.001449271
O     0.704290000    0.296020000    -0.001980881
C     0.430890000    0.068170000    -0.000974619
C     0.591240000    0.068130000    -0.000949304
C     0.538920000    0.123870000    -0.001961895
H     0.389800000    0.110680000    -0.001493571
H     0.674840000    0.110560000    -0.001461928
C     0.429240000    0.904580000    0.001949237
C     0.376920000    0.960290000    0.000955633
C     0.537270000    0.960240000    0.000980947
H     0.293330000    0.917810000    0.001474585
H     0.578350000    0.917720000    0.001512558
C     0.875280000    0.458850000    0.001348012
C     0.929960000    0.566230000    0.001702418
C     0.931030000    0.407660000    -0.000278462
H     0.887080000    0.606020000    0.003518753
H     0.889700000    0.325550000    -0.001784691
C     0.036930000    0.620810000    0.158476791
C     0.037990000    0.462220000    0.156502239
C     0.092700000    0.569610000    0.156856646
H     0.078240000    0.702910000    0.159976691
H     0.080850000    0.422400000    0.154692233
B     0.211560000    0.629440000    0.156597170
O     0.266920000    0.580080000    0.152983486
O     0.263780000    0.732510000    0.160128580
B     0.371620000    0.629440000    0.156597170
```

```
B     0.370060000    0.786350000    0.159584313
O     0.422510000    0.732500000    0.160122251
C     0.430710000    0.569650000    0.156875632
C     0.537660000    0.620870000    0.158508435
C     0.378030000    0.462250000    0.156533883
C     0.590100000    0.566340000    0.159945048
H     0.578400000    0.702990000    0.160002006
C     0.430470000    0.407730000    0.157970496
H     0.295360000    0.422450000    0.154723877
C     0.537410000    0.458920000    0.159590641
H     0.672780000    0.606180000    0.161742397
H     0.389730000    0.325620000    0.156464267
B     0.596410000    0.399040000    0.159837460
O     0.701050000    0.448280000    0.163565060
O     0.545580000    0.296070000    0.156192133
B     0.756430000    0.399010000    0.159843789
B     0.598020000    0.242180000    0.156774373
O     0.704290000    0.296020000    0.156236434
C     0.430890000    0.068180000    0.157242696
C     0.591240000    0.068130000    0.157268011
C     0.538920000    0.123870000    0.156255420
H     0.389800000    0.110680000    0.156723743
H     0.674830000    0.110560000    0.156761716
C     0.429240000    0.904580000    0.160166552
C     0.376920000    0.960300000    0.159172947
C     0.537270000    0.960250000    0.159191934
H     0.293330000    0.917810000    0.159691900
H     0.578350000    0.917710000    0.159729872
C     0.875280000    0.458850000    0.159565326
C     0.929970000    0.566230000    0.159919733
C     0.931030000    0.407660000    0.157938852
H     0.887080000    0.606020000    0.161736068
H     0.889700000    0.325550000    0.156432624
C     0.036930000    0.620810000    0.316700435
C     0.037990000    0.462220000    0.314719554
C     0.092700000    0.569610000    0.315073961
H     0.078240000    0.702910000    0.318194006
H     0.080850000    0.422400000    0.312909548
B     0.211560000    0.629440000    0.314820813
O     0.266920000    0.580080000    0.311200801
O     0.263780000    0.732510000    0.318352224
B     0.371620000    0.629440000    0.314820813
B     0.370060000    0.786350000    0.317801627
O     0.422510000    0.732500000    0.318339566
C     0.430710000    0.569650000    0.315092947
C     0.537660000    0.620870000    0.316725750
C     0.378030000    0.462250000    0.314751198
C     0.590100000    0.566340000    0.318162363
H     0.578400000    0.702980000    0.318225650
C     0.430470000    0.407730000    0.316187811
H     0.295360000    0.422450000    0.312947520
C     0.537410000    0.458920000    0.317807956
H     0.672780000    0.606180000    0.319959712
H     0.389730000    0.325620000    0.314681582
B     0.596410000    0.399040000    0.318054775
O     0.701050000    0.448280000    0.321782375
O     0.545580000    0.296070000    0.314409448
B     0.756430000    0.399010000    0.318061104
B     0.598020000    0.242180000    0.314991688
O     0.704290000    0.296020000    0.314447420
C     0.430890000    0.068180000    0.315460011
C     0.591240000    0.068130000    0.315485326
C     0.538920000    0.123870000    0.314472735
```

```
H     0.389800000   0.110680000   0.314934730
H     0.674840000   0.110560000   0.314979031
C     0.429240000   0.904580000   0.318377538
C     0.376920000   0.960300000   0.317383934
C     0.537270000   0.960250000   0.317409248
H     0.293330000   0.917810000   0.317909215
H     0.578350000   0.917710000   0.317947187
C     0.875280000   0.458850000   0.317782641
C     0.929970000   0.566230000   0.318137048
C     0.931030000   0.407660000   0.316149839
H     0.887080000   0.606020000   0.319947054
H     0.889700000   0.325550000   0.314649939
C     0.036930000   0.620810000   0.474911421
C     0.037990000   0.462220000   0.472936869
C     0.092700000   0.569610000   0.473297605
H     0.078240000   0.702910000   0.476411321
H     0.080850000   0.422400000   0.471126863
B     0.211560000   0.629440000   0.473038128
O     0.266920000   0.580080000   0.469418116
O     0.263780000   0.732510000   0.476569539
B     0.371620000   0.629440000   0.473038128
B     0.370060000   0.786350000   0.476018942
O     0.422510000   0.732500000   0.476556881
C     0.430710000   0.569650000   0.473310262
C     0.537660000   0.620870000   0.474943065
C     0.378030000   0.462250000   0.472968512
C     0.590100000   0.566340000   0.476379678
H     0.578400000   0.702980000   0.476436636
C     0.430470000   0.407730000   0.474405126
H     0.295360000   0.422450000   0.471158506
C     0.537410000   0.458920000   0.476031600
H     0.672780000   0.606180000   0.478177027
H     0.389730000   0.325620000   0.472898897
B     0.596410000   0.399040000   0.476278419
O     0.701050000   0.448280000   0.479999690
O     0.545580000   0.296070000   0.472626763
B     0.756430000   0.399010000   0.476278419
B     0.598020000   0.242180000   0.473209003
O     0.704290000   0.296020000   0.472664735
C     0.430890000   0.068180000   0.473677326
C     0.591240000   0.068130000   0.473702641
C     0.538920000   0.123870000   0.472683721
H     0.389800000   0.110680000   0.473152045
H     0.674840000   0.110560000   0.473190017
C     0.429240000   0.904580000   0.476594853
C     0.376920000   0.960300000   0.475607577
C     0.537270000   0.960250000   0.475626563
H     0.293330000   0.917810000   0.476126530
H     0.578350000   0.917710000   0.476164502
C     0.875280000   0.458850000   0.475993628
C     0.929970000   0.566230000   0.476348034
C     0.931030000   0.407660000   0.474367154
H     0.887080000   0.606020000   0.478164369
H     0.889700000   0.325550000   0.472867253
K_POINTS (automatic)
 8 8 1 0 0 0
```

Structure 5 (5 layers)

```
  ibrav = 14
  celldm(1) = 28.3988042
  celldm(2) =  1.0
  celldm(3) =  1.76044699
  celldm(4) =  0.3948001
  celldm(5) =  0.0
  celldm(6) =  -0.5
  ecutwfc     = 100.D0,

ATOMIC_POSITIONS (crystal)
C     0.036930       0.620810       0.000225
C     0.037990       0.462220       -0.001475
C     0.092690       0.569620       -0.001175
H     0.078240       0.702910       0.001523
H     0.080840       0.422400       -0.003039
B     0.211560       0.629440       -0.001400
O     0.266920       0.580090       -0.004522
O     0.263770       0.732510       0.001653
B     0.371620       0.629440       -0.001400
B     0.370060       0.786340       0.001182
O     0.422510       0.732500       0.001646
C     0.430710       0.569650       -0.001161
C     0.537660       0.620870       0.000253
C     0.378030       0.462250       -0.001455
C     0.590090       0.566330       0.001489
H     0.578400       0.702990       0.001544
C     0.430470       0.407730       -0.000219
H     0.295360       0.422450       -0.003012
C     0.537410       0.458920       0.001188
H     0.672780       0.606170       0.003039
H     0.389730       0.325620       -0.001509
B     0.596410       0.399040       0.001400
O     0.701040       0.448280       0.004617
O     0.545580       0.296070       -0.001749
B     0.756430       0.399010       0.001400
B     0.598010       0.242180       -0.001250
O     0.704290       0.296020       -0.001714
C     0.430890       0.068170       -0.000840
C     0.591240       0.068130       -0.000820
C     0.538920       0.123870       -0.001694
H     0.389800       0.110680       -0.001291
H     0.674840       0.110560       -0.001264
C     0.429240       0.904580       0.001680
C     0.376920       0.960290       0.000826
C     0.537270       0.960240       0.000847
H     0.293330       0.917810       0.001277
H     0.578350       0.917720       0.001305
C     0.875280       0.458850       0.001161
C     0.929960       0.566230       0.001468
C     0.931030       0.407660       -0.000239
H     0.887080       0.606020       0.003039
H     0.889700       0.325550       -0.001544
C     0.036930       0.620810       0.136830
C     0.037990       0.462220       0.135122
C     0.092700       0.569610       0.135430
H     0.078240       0.702910       0.138121
H     0.080850       0.422400       0.133565
B     0.211560       0.629440       0.135204
O     0.266920       0.580080       0.132083
O     0.263780       0.732510       0.138257
B     0.371620       0.629440       0.135204
```

B	0.370060	0.786350	0.137786
O	0.422510	0.732500	0.138250
C	0.430710	0.569650	0.135443
C	0.537660	0.620870	0.136857
C	0.378030	0.462250	0.135150
C	0.590100	0.566340	0.138093
H	0.578400	0.702990	0.138148
C	0.430470	0.407730	0.136393
H	0.295360	0.422450	0.133585
C	0.537410	0.458920	0.137793
H	0.672780	0.606180	0.139651
H	0.389730	0.325620	0.135095
B	0.596410	0.399040	0.138005
O	0.701050	0.448280	0.141222
O	0.545580	0.296070	0.134856
B	0.756430	0.399010	0.138011
B	0.598020	0.242180	0.135361
O	0.704290	0.296020	0.134890
C	0.430890	0.068180	0.135764
C	0.591240	0.068130	0.135785
C	0.538920	0.123870	0.134910
H	0.389800	0.110680	0.135313
H	0.674830	0.110560	0.135348
C	0.429240	0.904580	0.138285
C	0.376920	0.960300	0.137424
C	0.537270	0.960250	0.137451
H	0.293330	0.917810	0.137875
H	0.578350	0.917710	0.137909
C	0.875280	0.458850	0.137766
C	0.929970	0.566230	0.138073
C	0.931030	0.407660	0.136358
H	0.887080	0.606020	0.139637
H	0.889700	0.325550	0.135061
C	0.036930	0.620810	0.273434
C	0.037990	0.462220	0.271727
C	0.092700	0.569610	0.272034
H	0.078240	0.702910	0.274725
H	0.080850	0.422400	0.270169
B	0.211560	0.629440	0.271815
O	0.266920	0.580080	0.268687
O	0.263780	0.732510	0.274862
B	0.371620	0.629440	0.271815
B	0.370060	0.786350	0.274390
O	0.422510	0.732500	0.274855
C	0.430710	0.569650	0.272054
C	0.537660	0.620870	0.273455
C	0.378030	0.462250	0.271754
C	0.590100	0.566340	0.274705
H	0.578400	0.702980	0.274752
C	0.430470	0.407730	0.272997
H	0.295360	0.422450	0.270197
C	0.537410	0.458920	0.274397
H	0.672780	0.606180	0.276255
H	0.389730	0.325620	0.271692
B	0.596410	0.399040	0.274609
O	0.701050	0.448280	0.277826
O	0.545580	0.296070	0.271460
B	0.756430	0.399010	0.274616
B	0.598020	0.242180	0.271966
O	0.704290	0.296020	0.271494
C	0.430890	0.068180	0.272369
C	0.591240	0.068130	0.272389
C	0.538920	0.123870	0.271515

H	0.389800	0.110680	0.271918
H	0.674840	0.110560	0.271952
C	0.429240	0.904580	0.274889
C	0.376920	0.960300	0.274028
C	0.537270	0.960250	0.274049
H	0.293330	0.917810	0.274479
H	0.578350	0.917710	0.274513
C	0.875280	0.458850	0.274370
C	0.929970	0.566230	0.274677
C	0.931030	0.407660	0.272963
H	0.887080	0.606020	0.276241
H	0.889700	0.325550	0.271672
C	0.036930	0.620810	0.410039
C	0.037990	0.462220	0.408331
C	0.092700	0.569610	0.408645
H	0.078240	0.702910	0.411329
H	0.080850	0.422400	0.406767
B	0.211560	0.629440	0.408420
O	0.266920	0.580080	0.405292
O	0.263780	0.732510	0.411466
B	0.371620	0.629440	0.408420
B	0.370060	0.786350	0.410995
O	0.422510	0.732500	0.411459
C	0.430710	0.569650	0.408652
C	0.537660	0.620870	0.410066
C	0.378030	0.462250	0.408358
C	0.590100	0.566340	0.411302
H	0.578400	0.702980	0.411357
C	0.430470	0.407730	0.409595
H	0.295360	0.422450	0.406801
C	0.537410	0.458920	0.411002
H	0.672780	0.606180	0.412853
H	0.389730	0.325620	0.408297
B	0.596410	0.399040	0.411213
O	0.701050	0.448280	0.414430
O	0.545580	0.296070	0.408065
B	0.756430	0.399010	0.411213
B	0.598020	0.242180	0.408563
O	0.704290	0.296020	0.408099
C	0.430890	0.068180	0.408966
C	0.591240	0.068130	0.408994
C	0.538920	0.123870	0.408119
H	0.389800	0.110680	0.408522
H	0.674840	0.110560	0.408556
C	0.429240	0.904580	0.411493
C	0.376920	0.960300	0.410640
C	0.537270	0.960250	0.410653
H	0.293330	0.917810	0.411084
H	0.578350	0.917710	0.411118
C	0.875280	0.458850	0.410974
C	0.929970	0.566230	0.411282
C	0.931030	0.407660	0.409567
H	0.887080	0.606020	0.412846
H	0.889700	0.325550	0.408276
C	0.036930	0.620810	0.546643
C	0.037990	0.462220	0.544942
C	0.092700	0.569610	0.545243
H	0.078240	0.702910	0.547941
H	0.080850	0.422400	0.543378
B	0.211560	0.629440	0.545024
O	0.266920	0.580070	0.541903
O	0.263780	0.732510	0.548070
B	0.371620	0.629440	0.545024

```
B     0.370060       0.786350       0.547599
O     0.422510       0.732500       0.548064
C     0.430710       0.569650       0.545256
C     0.537660       0.620870       0.546670
C     0.378030       0.462250       0.544963
C     0.590100       0.566340       0.547907
H     0.578400       0.702980       0.547961
C     0.430470       0.407730       0.546199
H     0.295360       0.422450       0.543405
C     0.537410       0.458920       0.547606
H     0.672780       0.606180       0.549457
H     0.389730       0.325620       0.544901
B     0.596410       0.399040       0.547818
O     0.701050       0.448280       0.551035
O     0.545580       0.296070       0.544669
B     0.756430       0.399010       0.547818
B     0.598020       0.242180       0.545168
O     0.704290       0.296020       0.544703
C     0.430890       0.068180       0.545571
C     0.591240       0.068130       0.545598
C     0.538920       0.123870       0.544717
H     0.389800       0.110680       0.545127
H     0.674840       0.110560       0.545154
C     0.429240       0.904580       0.548098
C     0.376920       0.960300       0.547244
C     0.537270       0.960250       0.547264
H     0.293330       0.917810       0.547688
H     0.578350       0.917710       0.547722
C     0.875280       0.458850       0.547579
C     0.929970       0.566230       0.547886
C     0.931030       0.407660       0.546178
H     0.887080       0.606020       0.549457
H     0.889700       0.325550       0.544874
K_POINTS (automatic)
 8 8 1 0 0 0
```