```
&FORCE_EVAL
 METHOD Quickstep
 &DFT
  LSD
  CHARGE 2
  MULTIPLICITY 3
  BASIS_SET_FILE_NAME  /home/softwares/cp2k-6.1/data/BASIS_MOLOPT
  POTENTIAL_FILE_NAME  /home/softwares/cp2k-6.1/data/GTH_POTENTIALS
  WFN_RESTART_FILE_NAME  RESTART.wfn
  &MGRID
   CUTOFF 400
   REL_CUTOFF 40
   NGRIDS    5
  &END MGRID
  &QS
   METHOD            GPW
   EPS_DEFAULT       1.0E-12
   EXTRAPOLATION     ASPC
   EXTRAPOLATION_ORDER  3
  &END QS
  &SCF
   MAX_SCF           40
   EPS_SCF           1.0E-7
   SCF_GUESS         RESTART
  &OUTER_SCF
   EPS_SCF           1.0E-7
   MAX_SCF           10
  &END OUTER_SCF
  &OT
   PRECONDITIONER      FULL_ALL
   MINIMIZER           DIIS
   N_DIIS              7
  &END OT
  &END SCF

 &XC
  &XC_FUNCTIONAL PBE                    ! PBE functional + ...
  &END
  &VDW_POTENTIAL                        ! ... dispersion interactions
    POTENTIAL_TYPE PAIR_POTENTIAL
    &PAIR_POTENTIAL
      TYPE DFTD2                        ! computed with the DFTD2 method
      REFERENCE_FUNCTIONAL PBE
    &END PAIR_POTENTIAL
  &END
  &END XC
&END DFT

&SUBSYS
 &CELL
  ABC 12.73 12.73 12.73
  PERIODIC XYZ
  &END CELL

&COORD
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C       1.190000      9.000000      6.580000
C       1.690000      7.530000      6.250000
C       1.120000      7.030000      4.870000
C       0.820000      8.000000      3.820000
C       0.740000      9.430000      4.110000
C       1.330000      6.540000      7.420000
C       0.950000      5.610000      4.650000
C       1.000000      4.660000      5.760000
C       1.140000      5.130000      7.140000
C       0.880000      3.230000      5.500000
```

C	0.730000	2.750000	4.130000
C	0.650000	3.710000	3.020000
C	0.720000	5.130000	3.290000
C	0.570000	6.090000	2.190000
C	0.590000	7.530000	2.460000
C	1.070000	9.450000	7.960000
C	1.120000	8.480000	9.060000
C	1.200000	7.040000	8.790000
C	1.130000	6.100000	9.900000
C	1.100000	4.660000	9.630000
C	1.070000	4.190000	8.250000
C	0.900000	2.280000	6.600000
C	0.990000	2.760000	7.990000
C	0.490000	3.240000	1.650000
C	0.400000	4.280000	0.830000
C	0.830000	0.850000	6.320000
C	0.670000	1.320000	3.870000
C	0.740000	0.650000	5.020000
C	0.990000	1.820000	9.100000
C	1.040000	2.480000	10.250000
C	1.070000	3.710000	10.730000
C	1.100000	6.600000	11.280001
C	1.080000	7.920000	11.280001
C	1.050000	8.950000	10.450000
C	0.890000	10.880001	8.230000
C	0.760000	11.540001	7.100000
C	0.700000	11.350000	5.790000
C	0.500000	10.380000	3.020000
C	0.390000	9.720000	1.880000
C	0.390000	8.500000	1.380000
C	0.520000	12.030000	4.670000
C	0.440000	11.619999	3.490000
C	0.270000	7.850000	0.230000
C	0.260000	6.620000	0.000000
C	0.480000	1.910000	1.630000
C	0.560000	1.100000	2.570000
C	0.870000	0.170000	7.460000
C	0.940000	0.570000	8.640000
C	1.090000	4.350000	11.890000
C	1.100000	5.580000	12.120000
C	0.960000	10.270000	10.480000
C	0.890000	11.090000	9.540000
C	0.390000	5.600000	0.830000
N	3.180000	7.650000	6.080000
C	4.280000	6.810000	6.040000
C	4.400000	5.370000	6.060000
C	5.470000	7.500000	5.920000
C	5.680000	4.780000	5.920000
H	3.550000	4.740000	6.190000
C	6.600000	6.850000	5.830000
H	5.480000	8.550000	5.920000
H	5.800000	3.700000	5.900000
N	6.770000	5.580000	5.820000
C	7.870000	7.450000	5.720000
C	8.090000	8.770000	5.690000
N	8.750000	6.520000	5.650000
O	8.230000	2.960000	5.670000
O	10.050000	4.130000	5.850000
O	9.180000	4.460000	3.660000
O	9.180000	4.630000	7.440000
C	9.400000	9.190001	5.620000
H	7.280000	9.450000	5.730000
C	10.039999	6.850000	5.570000
H	8.809999	2.200000	5.770000
H	10.080000	4.490000	3.350000
H	8.750000	3.650000	3.380000

H	10.130000	4.640000	7.620000
H	8.809999	3.810000	7.780000
C	10.369999	8.230000	5.570000
H	9.639999	10.240001	5.620000
H	10.809999	6.090000	5.510000
H	11.400000	8.530000	5.530000
Co	8.430000	4.710000	5.530000
O	12.404098	9.332770	9.447946
H	11.923949	8.499675	9.068308
H	12.162019	9.897792	9.097250
O	8.286545	5.348079	10.851565
H	9.069373	5.949940	10.693591
H	7.726088	5.415790	10.071713
O	11.281870	5.050102	10.869153
H	10.737642	4.765806	11.633730
H	11.177316	4.574296	10.044624
O	3.588240	5.606637	3.146801
H	3.263690	5.362759	4.040280
H	4.579387	5.412274	3.117908
O	5.857522	10.711571	10.624726
H	6.402214	10.239841	9.914412
H	6.409789	10.675488	11.467713
O	12.366385	12.058693	12.824754
H	13.399948	11.925178	12.969203
H	11.961684	11.114391	12.716013
O	6.707994	3.479222	8.839972
H	6.611348	3.347001	9.798984
H	7.432682	2.887933	8.484090
O	5.471995	2.373734	1.772371
H	4.753633	3.026297	1.507735
H	5.392340	1.633820	1.098818
O	3.955551	3.816030	8.363642
H	3.819342	4.751440	8.633911
H	4.933250	3.770520	8.372482
O	10.544162	11.751232	7.400161
H	10.724796	12.192279	6.516649
H	10.781874	10.732900	7.532798
O	9.669894	2.602030	10.525193
H	9.044835	3.305825	10.868420
H	10.166478	2.294454	11.349806
O	7.034010	8.274551	10.885018
H	6.980515	7.518046	10.249358
H	7.440249	7.949741	11.706105
O	4.284448	9.162192	8.663743
H	3.657076	8.697364	8.058378
H	4.145706	10.070763	8.498639
O	5.972058	0.614543	9.218296
H	5.314219	1.223690	9.647124
H	6.198081	-0.058803	9.860693
O	7.355778	2.533702	3.268481
H	7.611379	2.362614	4.261191
H	6.473466	2.227802	2.962226
O	10.331949	12.387435	4.762896
H	9.362175	12.118032	4.981767
H	10.530723	12.037282	3.828362
O	10.845941	10.062298	12.029486
H	10.890564	9.158543	11.706609
H	10.132658	10.404480	11.395255
O	10.289761	1.998159	2.897460
H	9.851845	1.556696	3.663063
H	11.180053	1.633564	2.941514
O	10.764009	2.039192	0.068647
H	10.109786	1.762525	0.759856
H	11.495730	1.355284	-0.003068
O	10.418432	6.562651	2.649082
H	10.891055	7.340462	2.259623

H	9.472508	6.845689	2.818567
O	8.904014	10.187630	10.391479
H	8.540599	10.805346	9.657059
H	8.116128	9.522020	10.577090
O	3.191913	1.662600	12.914807
H	3.191911	2.428343	13.515638
H	4.304636	1.502898	12.819210
O	5.988401	12.901939	4.207874
H	5.852409	12.472088	3.338287
H	5.114140	13.014837	4.627586
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H	3.519938	8.804147	1.318326
H	3.234285	9.752371	3.501006
O	3.650465	1.823495	6.530085
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H	3.579216	2.663052	7.078559
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H	10.302110	9.597089	9.235606
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H	4.405170	11.616640	10.667486
H	3.422035	12.801785	10.347300
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H	2.826215	10.342841	1.171566
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O	11.086710	12.944433	9.897257
H	11.102164	12.625845	8.957537
H	11.130258	12.162741	10.490171
O	8.115506	10.487190	3.276587
H	7.231500	10.028698	3.326102
H	8.302737	10.951592	4.129316
O	5.860290	8.471178	0.589910
H	6.477704	9.222869	0.625578
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O	4.138031	5.365257	11.739085
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H	4.011102	5.652783	10.809882
O	7.985861	0.986660	11.054819
H	8.376000	0.131301	10.926792
H	8.539503	1.688649	10.642510
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H	3.120881	6.403535	1.475402
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H	9.579092	8.522217	0.958306
H	8.445730	7.474398	1.111896
O	3.975399	2.142374	10.325369
H	3.857405	3.055978	9.848350
H	3.647168	2.176110	11.312949
O	3.692770	2.918682	3.989937
H	3.707637	2.459240	4.846477
H	4.427780	2.551426	3.467799
O	3.969370	6.547176	9.249332
H	3.875604	7.491505	9.610918
H	4.923296	6.492752	9.026237
O	11.151983	6.841617	8.101723
H	11.465461	6.076881	8.670675
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H	3.469419	1.174743	2.391759
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H	9.082364	11.683496	8.030562
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O	8.693889	7.526555	8.778485
H	9.219491	7.844552	9.580883

H	8.163457	8.292822	8.490111
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O	6.166491	1.418694	6.774884
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O	8.706095	1.661384	8.202447
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H	7.310173	6.286022	2.752607
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H	3.319571	9.328631	11.641226
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H	9.374416	9.579218	2.642653
H	10.603825	9.888906	1.776797
O	6.360941	3.438975	11.367216
H	7.014350	3.335550	12.077885
H	5.595289	2.811101	11.344168
O	3.543402	12.340779	5.118610
H	3.101452	12.935148	5.752086
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H	10.469232	2.793992	6.108580
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H	7.736375	11.987056	6.627651
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O	3.956469	11.810072	7.914109
H	4.787072	12.419822	8.110357

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 H       7.192448       5.945185      -0.418825
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 O       5.354506      11.481859       1.859102
 H       4.745312      10.713911       1.583958
 H       5.671007      12.070744       1.115976
 O       6.577593       6.163820       8.799687
 H       7.483995       6.539760       8.545852
 H       6.560746       5.291751       8.417702
 O       7.550302      10.463799       0.236409
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 H       7.842514      11.005569       1.022850
  &END COORD

    &KIND H
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      POTENTIAL GTH-PBE-q1
    &END KIND
    &KIND C
      BASIS_SET DZVP-MOLOPT-SR-GTH-q4
      POTENTIAL GTH-PBE-q4
    &END KIND
    &KIND N
      BASIS_SET DZVP-MOLOPT-SR-GTH-q5
      POTENTIAL GTH-PBE-q5
    &END KIND
    &KIND O
      BASIS_SET DZVP-MOLOPT-SR-GTH-q6
      POTENTIAL GTH-PBE-q6
    &END KIND
    &KIND Co
      BASIS_SET DZVP-MOLOPT-SR-GTH-q17
      POTENTIAL GTH-PBE-q17
    &END KIND
  &END SUBSYS
&END FORCE_EVAL

&GLOBAL
  PROJECT co-graphene-oh-oxo-nve
  RUN_TYPE MD
  PRINT_LEVEL LOW
&END GLOBAL

&MOTION
&CONSTRAINT
 &FIXED_ATOMS
  COMPONENTS_TO_FIX  XYZ
  LIST 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49
50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84
 &END FIXED_ATOMS
 &END CONSTRAINT
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    ENSEMBLE NVE
    STEPS 10000
    TIMESTEP 0.5
    TEMPERATURE 300
    TEMP_TOL 05
  &END MD

  &PRINT
     &TRAJECTORY  SILENT
      COMMON_ITERATION_LEVELS            3
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    &CELL  SILENT
      COMMON_ITERATION_LEVELS            3
    &END CELL
    &VELOCITIES  SILENT
      COMMON_ITERATION_LEVELS            3
    &END VELOCITIES
    &RESTART  SILENT
      COMMON_ITERATION_LEVELS            3
    &END RESTART
  &END PRINT
&END MOTION
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