```
&FORCE_EVAL
 METHOD Quickstep

 &DFT
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  CHARGE 2
  MULTIPLICITY 3
  BASIS_SET_FILE_NAME  /home/gkr/softwares/cp2k-6.1/data/BASIS_MOLOPT
  POTENTIAL_FILE_NAME  /home/gkr/softwares/cp2k-6.1/data/GTH_POTENTIALS
  WFN_RESTART_FILE_NAME  RESTART.wfn
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   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
  &END
  &VDW_POTENTIAL
    POTENTIAL_TYPE PAIR_POTENTIAL
    &PAIR_POTENTIAL
      TYPE DFTD2
      REFERENCE_FUNCTIONAL PBE
    &END PAIR_POTENTIAL
  &END
  &END XC

 &PRINT
  &LOWDIN
  &END
 &MULLIKEN
 &END MULLIKEN
 &END
&END DFT

 &SUBSYS
  &CELL
   ABC 12.73 12.73 12.73
   PERIODIC XYZ
  &END CELL
&COORD
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C       1.512430      8.765901      6.891903
C       1.890746      7.335093      6.609513
C       1.414807      6.900164      5.298166
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C	1.151928	9.261353	4.408970
C	1.576360	6.443062	7.776932
C	1.191209	5.505285	5.127116
C	1.193706	4.551841	6.260444
C	1.420530	5.007652	7.576060
C	0.897598	3.194433	5.966729
C	0.639532	2.735718	4.625173
C	0.611899	3.612735	3.512275
C	0.820312	5.022932	3.842180
C	0.579969	5.947371	2.818337
C	0.674666	7.378334	2.954575
C	1.479521	9.232447	8.241567
C	1.391781	8.372469	9.400409
C	1.425939	6.964509	9.045823
C	1.156712	6.026176	10.050475
C	1.061926	4.585285	9.930324
C	1.228330	4.039587	8.659665
C	0.863989	2.303565	7.075348
C	1.036070	2.669617	8.390418
C	0.500060	2.945475	2.121536
C	0.381676	4.051102	1.070466
C	0.760197	0.948879	6.800054
C	0.562193	1.368466	4.398622
C	0.729331	0.510191	5.484066
C	0.913142	1.635256	9.533343
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C	0.666769	3.656551	11.052999
C	0.629372	6.546103	11.232795
C	0.386800	8.020600	11.604003
C	1.082738	8.966096	10.612706
C	1.292693	10.650541	8.460885
C	1.020789	11.431869	7.324388
C	1.090990	10.964702	6.055570
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C	0.602259	9.617006	2.123129
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C	0.832474	11.888336	5.024339
C	0.727676	11.675612	3.676747
C	-0.004413	7.794908	0.524227
C	-0.030463	6.325339	0.620307
C	0.451704	1.505656	2.122934
C	0.566787	0.597741	3.154902
C	0.823565	0.008132	7.798153
C	0.935474	0.159937	9.171403
C	0.442294	4.215892	12.356597
C	0.257415	5.643097	12.191072
C	0.917486	10.521514	10.794486
C	1.178744	11.404878	9.713988
C	0.214203	5.389571	1.609247
N	3.426906	7.474614	6.605038
C	4.535390	6.637462	6.364197
C	4.502343	5.251719	6.392179
C	5.768331	7.317132	6.015160
C	5.683550	4.583053	6.163950
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C	6.860034	6.561180	5.804834
H	5.860813	8.393003	5.911374
H	5.627635	3.501531	6.071458
N	6.847191	5.195803	5.896981
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C	8.529446	8.426921	5.807252
N	9.169519	6.128846	5.500540
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O	10.265977	3.491322	5.500856
O	8.257155	4.215267	3.650274

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H	7.161781	2.383296	4.941915
H	8.704396	3.347981	3.347236
H	7.251405	4.143096	3.371707
H	9.583316	4.243771	7.871379
H	7.815289	3.759036	8.136874
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H	11.831157	8.127020	5.246331
Co	8.466334	4.328080	5.691466
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H	11.269433	6.893382	9.576385
H	10.805401	12.195208	5.739795
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H	8.968001	5.514729	10.474093
H	7.410246	5.362667	9.944148
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H	10.527409	4.914907	11.573855
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H	3.241490	3.119753	5.331633
H	4.688752	6.098692	3.157048
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H	7.200211	10.291184	9.865758
H	7.303514	11.662718	10.747802
O	11.686345	8.117149	11.110869
H	12.806440	9.986127	11.607265
H	11.445365	9.077517	11.148952
O	7.104657	2.933511	8.733033
H	6.746959	3.086625	9.646274
H	7.605890	2.108115	8.661942
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H	4.776537	1.031217	0.223357
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H	11.218659	11.114172	6.957370
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H	8.146660	4.181247	10.873126
H	8.519496	2.256748	11.857455
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H	11.509089	12.048338	10.173888
H	13.635022	10.595582	13.036298
O	10.016574	2.371620	3.201635

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H	10.480770	6.281837	2.473875
H	9.379848	5.271522	3.023415
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H	4.133895	11.861765	11.570325
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O	6.496258	9.232074	3.632157
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H	6.218156	9.261213	2.654743
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H	5.137366	5.338428	11.026422
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H       3.704189      10.662058       9.504138
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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
   &COLVAR
      &COORDINATION
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        ATOMS_TO  136
        R_0 [angstrom] 2.00
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        ND 18
     &END COORDINATION
  &END COLVAR
  &COLVAR
    &COORDINATION
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       ATOMS_TO 263
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       NN 6
       ND 18
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  &END COLVAR
 &END SUBSYS
&END FORCE_EVAL

&GLOBAL
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  PRINT_LEVEL LOW
&END GLOBAL

&MOTION
&CONSTRAINT
&FIXED_ATOMS
LIST 136
&END
&END
  &MD
    ENSEMBLE NVT
    STEPS 8000
    TIMESTEP 0.5
    TEMPERATURE 300
    TEMP_TOL 5
    &THERMOSTAT
      &NOSE
        LENGTH 3
        YOSHIDA 3
        TIMECON 30.0
        MTS 2
      &END NOSE
    &END
  &END MD
  &FREE_ENERGY
    &METADYN
      DO_HILLS T
      NT_HILLS 5
      WW 5.0e-3
      WELL_TEMPERED
      WTGAMMA 25
      &METAVAR
        SCALE 0.1
        COLVAR 1
        MASS 10
      &END METAVAR
      &METAVAR
        SCALE 0.1
        COLVAR 2
        MASS 10
      &END METAVAR
      &PRINT
      &COLVAR  SILENT
       COMMON_ITERATION_LEVELS            3
      &END COLVAR
      &HILLS  SILENT
       COMMON_ITERATION_LEVELS            3
      &END HILLS
#     &FREE_ENERGY_INFO   SILENT
#      COMMON_ITERATION_LEVELS            3
#    &END FREE_ENERGY_INFO
      &END PRINT
    &END METADYN
  &END
  &PRINT
    &TRAJECTORY  SILENT
     COMMON_ITERATION_LEVELS            3
    &END TRAJECTORY
    &CELL  SILENT
     COMMON_ITERATION_LEVELS            3
    &END CELL
    &VELOCITIES  SILENT
     COMMON_ITERATION_LEVELS            3
    &END VELOCITIES
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    &RESTART  SILENT
      COMMON_ITERATION_LEVELS            3
    &END RESTART
  &END PRINT
&END MOTION
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