&FORCE\_EVAL

METHOD Quickstep

&DFT

LSD

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

&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

&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

C 1.154629 7.836567 4.220885

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

C 0.675763 2.267656 10.738759

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

C 0.796047 10.247252 3.350371

C 0.602259 9.617006 2.123129

C 0.543486 8.313978 1.873531

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

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C 0.823565 0.008132 7.798153

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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

H 3.697183 4.613246 6.731235

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 8.257155 4.215267 3.650274

O 8.640236 4.437449 7.627783

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C 10.464417 6.493339 5.335218

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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

C 10.818289 7.818561 5.437760

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H 11.159387 5.708351 5.098722

H 11.831157 8.127020 5.246331

Co 8.466334 4.328080 5.691466

O 11.160275 6.929748 8.570827

H 11.269433 6.893382 9.576385

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O 8.094541 5.190529 10.748919

H 8.968001 5.514729 10.474093

H 7.410246 5.362667 9.944148

O 10.610281 5.460627 10.726241

H 10.527409 4.914907 11.573855

H 10.997878 4.693872 10.216729

O 3.726624 6.379367 3.144712

H 3.241490 3.119753 5.331633

H 4.688752 6.098692 3.157048

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&END COORD

&KIND H

BASIS\_SET DZVP-MOLOPT-SR-GTH-q1

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

ATOMS\_FROM 263

ATOMS\_TO 136

R\_0 [angstrom] 2.00

NN 6

ND 18

&END COORDINATION

&END COLVAR

&COLVAR

&COORDINATION

ATOMS\_FROM 262

ATOMS\_TO 263

R\_0 [angstrom] 2.10

NN 6

ND 18

&END COORDINATION

&END COLVAR

&END SUBSYS

&END FORCE\_EVAL

&GLOBAL

PROJECT co-grap-step2

RUN\_TYPE MD

PRINT\_LEVEL LOW

&END GLOBAL

&MOTION

&CONSTRAINT

&FIXED\_ATOMS

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&END

&MD

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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

&RESTART SILENT

COMMON\_ITERATION\_LEVELS 3

&END RESTART

&END PRINT

&END MOTION