&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

&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

C 1.160546 9.353213 5.371613

C 1.324170 8.505898 6.530995

C 1.953744 7.112737 6.254045

C 1.372554 6.651041 4.926012

C 1.187254 7.592546 3.850465

C 1.216491 9.021275 4.006654

C 1.736850 6.209560 7.461468

C 1.405978 5.226120 4.768989

C 1.352027 4.338665 5.921669

C 1.642265 4.707699 7.200697

C 1.076776 2.956856 5.654847

C 0.897321 2.457032 4.305866

C 0.957998 3.341896 3.189810

C 1.032896 4.727115 3.521995

C 0.677948 5.671436 2.496174

C 0.915703 7.075999 2.608086

C 1.190589 8.964607 7.862969

C 1.313087 8.101510 9.009796

C 1.466506 6.709324 8.709363

C 1.048528 5.725872 9.682728

C 1.141167 4.345119 9.538034

C 1.314006 3.778322 8.289798

C 1.059715 1.982188 6.679267

C 1.113144 2.322878 8.063836

C 0.780283 2.730700 1.875221

C 0.556601 3.756356 0.778030

C 0.914980 0.644473 6.373044

C 0.959360 1.133267 4.062901

C 0.892901 0.283998 5.089631

C 1.152949 1.352255 9.125617

C 0.937595 1.944688 10.510672

C 0.837230 3.436960 10.720276

C 0.660810 6.292472 10.823940

C 0.422698 7.716880 11.245183

C 1.075748 8.754872 10.247314

C 0.990399 10.325196 8.091377

C 0.893335 11.132207 6.968788

C 0.782453 10.636828 5.678818

C 1.093400 10.004527 2.932047

C 0.964094 9.357644 1.705360

C 0.770416 8.022366 1.513656

C 0.747519 11.614961 4.647823

C 0.891620 11.395251 3.309911

C 0.123177 7.576733 0.195900

C 0.120133 6.114604 0.243920

C 0.730751 1.201194 1.854510

C 0.879846 0.343849 2.842999

C 0.983933 -0.271866 7.425473

C 1.106640 -0.091360 8.824082

C 0.571743 4.010707 11.980573

C 0.291740 5.429399 11.831637

C 0.967821 10.190632 10.272889

C 1.105572 11.101778 9.260490

C 0.369736 5.138941 1.272208

N 3.414337 7.331741 6.153456

C 4.453390 6.440907 6.110343

C 4.460197 5.029667 6.154690

C 5.703723 7.115432 5.962767

C 5.665274 4.416094 5.966585

H 3.569495 4.440015 6.093763

C 6.900640 6.432732 5.837856

H 5.825530 8.158790 6.117792

H 5.710501 3.352141 5.764939

N 6.843682 5.039752 5.833621

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C 8.495999 8.443100 5.776100

N 9.266346 6.163847 5.537775

O 8.073179 2.553463 5.888252

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O 8.968756 4.618174 7.672766

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H 7.694004 9.172077 5.993472

C 10.534965 6.601218 5.262304

H 8.897843 2.097636 5.779857

H 9.320695 3.480817 3.616221

H 7.848097 4.406188 3.316852

H 9.972022 4.873806 7.790112

H 8.698655 3.865714 8.239867

C 10.825416 7.947205 5.183948

H 10.016137 9.870893 5.442700

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H 11.793391 8.395885 5.039369

Co 8.755121 4.345615 5.795444

O 11.158037 8.066751 8.225367

H 11.287082 8.041759 9.190322

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H 8.634106 6.039676 11.339479

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H 10.956012 5.295788 10.796071

H 11.179359 3.777426 10.560032

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H 3.638554 3.815300 3.666487

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H 8.232370 10.910603 0.908420

&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 264

ATOMS\_TO 68

R\_0 [angstrom] 2.10

NN 6

ND 18

&END COORDINATION

&END COLVAR

&COLVAR

&COORDINATION

ATOMS\_FROM 262

ATOMS\_TO 69

R\_0 [angstrom] 2.20

NN 8

ND 24

&END COORDINATION

&END COLVAR

&END SUBSYS

&END FORCE\_EVAL

&GLOBAL

PROJECT co-grap-step1

RUN\_TYPE MD

PRINT\_LEVEL LOW

&END GLOBAL

&MOTION

&MD

ENSEMBLE NVT

STEPS 12000

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

&WALL

TYPE QUADRATIC

POSITION [angstrom] 2.80

&QUADRATIC

DIRECTION WALL\_MINUS

K [kcalmol] 5.0

&END

&END

&END METAVAR

&METAVAR

SCALE 0.1

COLVAR 2

MASS 10

&WALL

TYPE QUADRATIC

POSITION [angstrom] 3.00

&QUADRATIC

DIRECTION WALL\_MINUS

K [kcalmol] 5.0

&END

&END

&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