&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 1.473338 9.042006 6.872808

C 1.871920 7.594796 6.585205

C 1.361210 7.185406 5.198626

C 1.130568 8.155428 4.179097

C 1.162789 9.566407 4.447065

C 1.479944 6.717242 7.737480

C 1.274587 5.785113 5.050220

C 1.263703 4.862930 6.192904

C 1.321144 5.301508 7.551966

C 1.007277 3.497416 5.942383

C 0.818149 3.010180 4.555513

C 0.621888 3.855013 3.501387

C 0.788368 5.305673 3.791470

C 0.544227 6.254681 2.816025

C 0.743846 7.666261 2.896974

C 1.417575 9.502350 8.220738

C 1.224159 8.614226 9.327566

C 1.250211 7.181982 9.019809

C 0.978739 6.281020 10.029866

C 0.794097 4.873604 9.917070

C 0.971962 4.343790 8.611820

C 0.882080 2.601656 7.042028

C 0.945462 2.928225 8.393734

C 0.475976 3.304384 2.142936

C 0.295634 4.322230 1.066471

C 0.707004 1.248603 6.763621

C 0.656204 1.626663 4.364342

C 0.659192 0.818226 5.466466

C 0.791161 1.975931 9.504293

C 0.520784 2.580906 10.715963

C 0.497719 3.936709 11.020539

C 0.565595 6.822560 11.208206

C 0.199952 8.267625 11.558542

C 0.891194 9.204770 10.541804

C 1.181914 10.892880 8.461343

C 0.958509 11.693470 7.318765

C 0.963175 11.303180 6.032446

C 0.887687 10.575111 3.347942

C 0.667479 9.950805 2.142375

C 0.623690 8.597779 1.797059

C 0.702520 12.212157 5.022688

C 0.660742 12.064067 3.658073

C -0.035015 8.123879 0.492783

C -0.082015 6.623909 0.605339

C 0.642790 1.824313 2.016100

C 0.587123 0.896662 3.076609

C 0.724254 0.275841 7.746412

C 0.725926 0.463384 9.165751

C 0.362006 4.514334 12.344376

C 0.218016 5.919638 12.206404

C 0.875792 10.670980 10.817050

C 1.025667 11.644523 9.663961

C 0.152977 5.701301 1.610647

N 3.369822 7.642518 6.455573

C 4.301928 6.675956 6.252546

C 4.238166 5.230553 6.374810

C 5.629222 7.174584 5.958091

C 5.370318 4.487508 6.066347

H 3.380958 4.698329 6.752048

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H 5.806345 8.241953 6.125724

H 5.290450 3.397223 6.080202

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C 8.065024 6.827193 5.754869

C 8.470060 8.170378 5.674085

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Co 8.335789 4.039353 5.528042

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H 8.905601 5.376537 10.242947

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O 10.378070 5.473462 10.414322

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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 199

ATOMS\_TO 84

R\_0 [angstrom] 3.20

NN 10

ND 30

&END COORDINATION

&END COLVAR

&COLVAR

&COORDINATION

ATOMS\_FROM 84

ATOMS\_TO 69

R\_0 [angstrom] 2.10

NN 10

ND 30

&END COORDINATION

&END COLVAR

&END SUBSYS

&END FORCE\_EVAL

&GLOBAL

PROJECT co-grap-step3

RUN\_TYPE MD

PRINT\_LEVEL LOW

&END GLOBAL

&MOTION

&MD

ENSEMBLE NVT

STEPS 10000

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] 4.00

&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] 4.00

&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