

```

&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
C 1.269549 9.961778 5.812120
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
C	6.682652	6.319451	5.746542
H	5.806345	8.241953	6.125724
H	5.290450	3.397223	6.080202
N	6.559230	4.997980	5.711374
C	8.065024	6.827193	5.754869
C	8.470060	8.170378	5.674085
N	9.035454	5.836528	5.649177
O	7.775693	2.198609	5.485966
O	10.127316	3.304731	5.685525
O	8.093317	4.250621	3.602654

O	8.384720	4.222590	7.465636
C	9.784568	8.559252	5.547127
H	7.679350	8.943917	5.704760
C	10.341199	6.178979	5.586486
H	7.243882	2.099176	4.590757
H	8.169429	3.410111	3.089423
H	7.158968	4.550378	3.407479
H	9.310473	4.134003	7.872512
H	7.703601	3.677077	7.880852
C	10.742873	7.531041	5.460561
H	10.130636	9.589336	5.638805
H	11.058192	5.385203	5.434835
H	11.776680	7.851253	5.403687
Co	8.335789	4.039353	5.528042
O	11.161289	7.369277	8.342151
H	11.669061	7.313497	9.221044
H	10.670533	12.083358	5.611311
O	7.894422	5.188968	10.561764
H	8.905601	5.376537	10.242947
H	7.191252	5.539992	9.848385
O	10.378070	5.473462	10.414322
H	10.413999	5.072105	11.354994
H	10.768451	4.772043	9.834631
O	3.761115	6.743724	3.060337
H	3.286393	3.579649	5.081758
H	4.715637	6.371613	3.111997
O	7.684860	11.171682	10.139173
H	7.149967	10.288790	9.966561
H	7.155059	11.748556	10.833263
O	11.564878	8.269393	11.023520
H	11.721375	8.561968	13.438697
H	11.184030	9.154273	11.144059
O	6.521502	2.811288	8.684524
H	6.751661	2.859936	9.678427
H	7.027555	2.001064	8.365513
O	5.224060	1.810663	0.937106
H	4.469965	2.443136	1.230263
H	4.837224	1.461957	0.120429
O	3.751386	1.665950	8.779532
H	3.320547	2.475053	9.011849
H	4.670402	2.040598	8.795370
O	10.742345	12.102610	6.602701
H	10.808879	13.134020	6.537655
H	11.450383	10.757312	8.057715
O	8.368495	2.833875	11.074529
H	7.933954	4.193114	10.952260
H	8.579706	2.773898	12.052513
O	6.732400	8.140578	10.965064
H	7.572875	7.672992	10.668452
H	6.135876	7.464667	11.349486
O	4.093135	7.307976	9.385420
H	3.840367	7.898726	8.642202
H	3.723959	7.680046	10.267830
O	5.955430	-0.076976	8.900637
H	5.218619	-0.747660	8.974325
H	6.689804	-0.480989	9.383548
O	6.174873	2.448544	3.554916
H	5.322773	2.806142	3.991676
H	5.923746	1.472740	3.344644
O	10.429662	12.919344	4.186617
H	9.702019	13.115019	3.507808
H	11.184244	12.759292	3.575508
O	13.313102	10.988948	12.028027
H	11.649931	12.583100	9.995493
H	14.549990	11.023780	13.092929
O	10.556874	2.742790	3.032484

H	10.583564	2.568735	4.015808
H	10.861963	3.706641	2.992644
O	10.894357	1.845159	0.525733
H	10.880484	2.159407	1.534814
H	11.780889	1.936362	0.148708
O	10.408618	5.367393	2.450957
H	10.578235	6.334054	2.351926
H	9.563247	5.275772	2.909232
O	9.748643	9.909102	11.360018
H	9.323378	10.628818	10.871622
H	9.255316	9.063772	11.131798
O	3.280254	3.658085	11.920635
H	2.869318	4.176548	11.217119
H	2.783635	2.799755	12.112871
O	6.184647	12.493071	3.630585
H	6.180663	12.075353	2.697499
H	5.316276	12.099878	4.033753
O	2.790324	11.113959	0.577928
H	3.047367	10.310379	1.157214
H	3.615874	8.330354	5.731442
O	3.441408	0.803590	6.149216
H	4.491886	0.616064	6.199672
H	3.333710	1.144721	7.076736
O	11.021903	9.988647	8.451159
H	11.248911	9.975478	9.371673
H	11.269855	8.359140	8.026608
O	3.840945	12.573696	11.127508
H	4.174245	11.639533	11.304671
H	3.686270	12.634397	10.172522
O	3.127137	6.220455	0.696589
H	3.194800	12.049269	1.221633
H	3.119382	6.416097	1.708547
O	10.731977	12.808569	10.083249
H	10.287691	12.517065	10.969054
H	10.693477	14.309848	9.927810
O	6.721949	9.291226	3.449880
H	6.003792	9.325811	4.116423
H	7.323379	9.977745	3.854480
O	6.095748	8.119677	1.214005
H	6.395291	8.775311	1.892658
H	6.366926	8.517323	0.349967
O	5.077157	5.895409	11.616285
H	4.659957	5.509759	10.816972
H	4.362558	5.917354	12.315609
O	9.237813	-0.134841	12.208658
H	8.903924	-0.767533	12.898209
H	9.740148	0.586521	12.686029
O	3.235726	8.198011	-1.060793
H	3.074297	7.597529	-0.305626
H	3.864982	8.900648	-0.901178
O	10.211029	7.869440	2.141887
H	10.524391	8.713343	2.591400
H	9.247269	7.756755	2.414023
O	2.142318	1.413326	12.171213
H	2.735382	0.573562	12.001248
H	1.621313	1.251949	12.989363
O	3.634637	2.822632	4.588274
H	3.483164	1.982302	5.259884
H	3.724484	-0.426440	2.885488
O	3.731587	4.635036	9.237189
H	3.712079	5.641976	9.084254
H	4.679575	4.394982	9.217311
O	10.971042	4.405252	7.953473
H	10.957675	3.907347	7.076775
H	11.283768	5.345366	7.708680
O	3.615082	0.116476	1.966683

H	3.517008	3.111356	3.108283
H	4.463705	0.606671	1.704445
O	8.371704	11.623663	7.429731
H	9.443100	11.681859	7.113349
H	8.074524	11.260955	8.294374
O	8.798215	7.799725	9.717669
H	9.653134	7.493239	9.343527
H	8.391815	8.331178	8.960356
O	5.639317	10.534877	6.365472
H	5.165495	10.173014	5.571299
H	5.734204	11.517629	6.333741
O	5.949643	0.408812	6.419185
H	5.998469	0.311155	7.486996
H	6.675579	1.160125	6.158554
O	3.665304	9.255603	1.914923
H	3.069948	8.513471	2.130329
H	4.444826	8.763209	1.430660
O	7.809031	3.068496	1.313170
H	6.888449	2.714241	1.153523
H	7.842650	3.988028	0.901956
O	8.596757	1.191412	8.169863
H	9.165064	0.887886	8.948586
H	8.365285	-0.025072	7.874452
O	7.887741	7.084375	2.867808
H	7.362474	7.019186	2.026444
H	7.543034	7.895257	3.288964
O	5.271115	10.044797	11.875587
H	5.683497	10.403768	12.688605
H	5.975611	9.464728	11.466338
O	6.483486	9.388496	8.431189
H	6.111034	9.722091	7.573265
H	6.097300	8.587094	8.787846
O	6.717625	0.391884	11.606775
H	7.649560	0.700764	11.681878
H	6.269139	1.155274	11.200661
O	4.037930	9.348274	4.706447
H	2.630055	5.425757	0.507224
H	4.004117	8.930520	3.821067
O	3.685286	3.440523	2.160960
H	3.314625	6.236824	3.781901
H	2.769840	3.701824	1.850530
O	10.166351	4.379304	0.122245
H	10.580473	3.492194	0.167307
H	10.451011	4.771549	0.962494
O	10.056305	10.324907	2.928171
H	9.621812	10.843185	3.619882
H	10.745944	10.909534	2.529200
O	5.735915	3.072640	11.221177
H	4.682654	3.204139	11.332601
H	6.105076	3.405770	12.035594
O	3.767831	11.681595	4.161662
H	3.389434	12.135257	4.972850
H	3.812638	10.494491	4.321245
O	10.516094	2.573750	9.733800
H	9.318019	2.757807	10.556746
H	10.813835	2.905133	8.872311
O	8.787498	0.771741	2.262458
H	8.698268	1.740707	2.177508
H	7.883518	0.398611	2.247959
O	10.142776	1.919135	6.211250
H	9.340177	1.431819	7.830748
H	8.692541	1.708003	5.393766
O	9.170424	7.344587	12.568619
H	9.725947	7.710679	13.321298
H	9.851894	6.955381	11.945004
O	8.128335	11.186378	4.726532

H	7.483216	11.836322	4.333199
H	7.884314	11.264714	5.681141
O	11.588967	11.706635	1.094512
H	12.222776	11.411664	0.369115
H	11.179075	12.531888	0.826938
O	4.047053	10.888709	8.694850
H	4.357296	10.318754	7.952998
H	3.134556	11.082611	8.463662
O	5.732122	5.148958	2.856640
H	6.168452	5.450101	2.057000
H	5.098990	4.444916	2.584033
O	7.276050	5.535267	0.649090
H	8.081965	6.095843	0.363452
H	6.679528	5.557267	-0.106995
O	6.098690	11.701038	1.142033
H	6.997861	11.253293	1.120342
H	6.109159	12.338997	0.410396
O	6.388152	6.078883	8.816294
H	5.588985	6.689877	9.041855
H	7.114520	6.706663	8.562225
O	8.412402	10.522364	0.943596
H	8.609341	9.777198	0.350614
H	9.034610	10.341575	1.721806

&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
```