&FORCE\_EVAL

METHOD QS

&DFT

BASIS\_SET\_FILE\_NAME /ihome/gmpourmpakis/naa64/cp2k/BASIS\_MOLOPT

POTENTIAL\_FILE\_NAME /ihome/gmpourmpakis/naa64/cp2k/GTH\_POTENTIALS

&MGRID

CUTOFF 500

REL\_CUTOFF 60

NGRIDS 4

&END MGRID

&QS

EPS\_DEFAULT 1.0E-14

MAP\_CONSISTENT

&END QS

&SCF

SCF\_GUESS ATOMIC

EPS\_SCF 1.0E-8

MAX\_SCF 500

ADDED\_MOS 200

CHOLESKY INVERSE

&SMEAR ON

METHOD FERMI\_DIRAC

ELECTRONIC\_TEMPERATURE [K] 300

&END SMEAR

&DIAGONALIZATION

ALGORITHM STANDARD

&END DIAGONALIZATION

&MIXING

METHOD BROYDEN\_MIXING

ALPHA 0.1

BETA 1.5

NBROYDEN 8

&END MIXING

&END SCF

&XC

&XC\_FUNCTIONAL PBE

&END XC\_FUNCTIONAL

&END XC

&POISSON

POISSON\_SOLVER WAVELET

PERIODIC NONE

&END POISSON

UKS .TRUE.

CHARGE -1

&SCCS

DIELECTRIC\_CONSTANT 78.36

MAX\_ITER 500

METHOD ANDREUSSI

DERIVATIVE\_METHOD CD5

EPS\_SCCS 1.0E-8

&END SCCS

&PRINT

&SCCS on

&EACH

QS\_SCF 1

&END EACH

&END SCCS

&END PRINT

&END DFT

&SUBSYS

&CELL

ABC 30.00000 30.00000 30.00000

ALPHA\_BETA\_GAMMA 90.00 90.00 90.00

PERIODIC NONE

&END CELL

&TOPOLOGY

COORD\_FILE\_NAME ausrH\_COOH\_v3\_final.xyz

COORDINATE XYZ

&END TOPOLOGY

&KIND Au

ELEMENT Au

BASIS\_SET DZVP-MOLOPT-SR-GTH-q11

POTENTIAL GTH-PBE-q11

&END KIND

&KIND Se

ELEMENT Se

BASIS\_SET DZVP-MOLOPT-SR-GTH-q6

POTENTIAL GTH-PBE-q6

&END KIND

&KIND S

ELEMENT S

BASIS\_SET DZVP-MOLOPT-SR-GTH-q6

POTENTIAL GTH-PBE-q6

&END KIND

&KIND O

ELEMENT O

BASIS\_SET DZVP-MOLOPT-SR-GTH-q6

POTENTIAL GTH-PBE-q6

&END KIND

&KIND H

ELEMENT H

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

POTENTIAL GTH-PBE-q1

&END KIND

&KIND C

ELEMENT C

BASIS\_SET DZVP-MOLOPT-SR-GTH-q4

POTENTIAL GTH-PBE-q4

&END KIND

&END SUBSYS

&END FORCE\_EVAL

&GLOBAL

PROJECT au

RUN\_TYPE GEO\_OPT

PRINT\_LEVEL MEDIUM

&END GLOBAL

&MOTION

&GEO\_OPT

MAX\_FORCE 0.0004

MAX\_ITER 2000

OPTIMIZER BFGS

TYPE MINIMIZATION

&END GEO\_OPT

&END MOTION