&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