Supporting Information

Screening of metal complexes and organic solvents using COSMOSAC-LANL model to enhance the energy density in non-aqueous redox flow cell: an insight into the solubility

Anwesa Karmakar*†, Rangachary Mukundan‡, Ping Yang*† and Enrique R. Batista*†

†Theoretical Division, Los Alamos National Laboratory, Los Alamos 87545
‡MPA-11 Division, Los Alamos National Laboratory, Los Alamos 87545
*E-mail: anwesa.karmakar@gmail.com; pyang@lanl.gov; erb@lanl.gov

Input files and co-ordinate for metal complexes and organic solvents

```
#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-I

ATOMS
1 V      9.728500000000     9.731800000000    12.193700000000    R=1.908
2 O     10.632300000000    10.717600000000    13.636500000000    R=1.72
3 O     11.225000000000     8.388600000000    12.254300000000    R=1.72
4 O     10.708700000000    10.925800000000    10.919000000000    R=1.72
5 O      9.016700000000     8.813400000000    10.582800000000    R=1.72
6 O      8.216900000000    11.024800000000    12.208900000000    R=1.72
7 O      8.713000000000     8.589800000000    13.425700000000    R=1.72
8 C     11.766000000000    10.477300000000    14.190100000000    R=2.00
9 C     12.541600000000     9.365700000000    13.949300000000    R=2.00
10 H    13.346100000000     9.273700000000    14.446000000000    R=1.30
11 C    12.231200000000     8.357000000000    13.022700000000    R=2.00
12 C    12.224400000000    11.527400000000    15.164100000000    R=2.00
13 H    12.251400000000    12.398800000000    14.716100000000    R=1.30
14 H    13.120200000000    11.300500000000    15.491900000000    R=1.30
15 H    11.600900000000    11.566700000000    15.919100000000    R=1.30
16 C    13.120500000000     7.155800000000    12.927100000000    R=2.00
17 H    12.862400000000     6.503100000000    13.611300000000    R=1.30
```

18 H 14.051200000000 7.426200000000 13.067900000000 R=1.30
19 H 13.029200000000 6.750600000000 12.040000000000 R=1.30
20 C 10.509300000000 11.122300000000 9.681400000000 R=2.00
21 C 9.657700000000 10.343900000000 8.898700000000 R=2.00
22 H 9.510000000000 10.606200000000 7.997200000000 R=1.30
23 C 9.013300000000 9.204000000000 9.367800000000 R=2.00
24 C 11.309300000000 12.232700000000 9.055000000000 R=2.00
25 H 11.273400000000 13.024900000000 9.630700000000 R=1.30
26 H 10.933800000000 12.449700000000 8.175600000000 R=1.30
27 H 12.240800000000 11.945300000000 8.951400000000 R=1.30
28 C 8.293800000000 8.303100000000 8.404300000000 R=2.00
29 H 8.762500000000 7.444900000000 8.347500000000 R=1.30
30 H 8.271200000000 8.722500000000 7.519300000000 R=1.30
31 H 7.378100000000 8.154000000000 8.717400000000 R=1.30
32 C 7.110300000000 10.957500000000 12.834800000000 R=2.00
33 C 6.740700000000 9.876900000000 13.653400000000 R=2.00
34 H 5.884600000000 9.907800000000 14.063000000000 R=1.30
35 C 7.532500000000 8.774700000000 13.903600000000 R=2.00
36 C 6.197000000000 12.134300000000 12.692600000000 R=2.00
37 H 6.398600000000 12.790800000000 13.392000000000 R=1.30
38 H 5.267500000000 11.838300000000 12.779800000000 R=1.30
39 H 6.327400000000 12.544600000000 11.812500000000 R=1.30
40 C 7.054400000000 7.674700000000 14.814500000000 R=2.00
41 H 7.203800000000 6.806800000000 14.385500000000 R=1.30
42 H 6.096900000000 7.790100000000 14.992700000000 R=1.30
43 H 7.549500000000 7.711100000000 15.658900000000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1
15 9 10 1
16 9 11 1.0
17 11 16 1

```
18 12 13 1
19 12 14 1
20 12 15 1
21 16 17 1
22 16 18 1
23 16 19 1
24 20 21 1.0
25 20 24 1
26 21 22 1
27 21 23 1.0
28 23 28 1
29 24 25 1
30 24 26 1
31 24 27 1
32 28 29 1
33 28 30 1
34 28 31 1
35 32 33 1.0
36 32 36 1
37 33 34 1
38 33 35 1.0
39 35 40 1
40 36 37 1
41 36 38 1
42 36 39 1
43 40 41 1
44 40 42 1
45 40 43 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
```

```
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21
```

```
# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-I

ATOMS
1 V      9.728500000000      9.731800000000     12.193700000000     R=1.908
2 O     10.632300000000     10.717600000000     13.636500000000     R=1.72
3 O     11.225000000000      8.388600000000     12.254300000000     R=1.72
4 O     10.708700000000     10.925800000000     10.919000000000     R=1.72
5 O      9.016700000000      8.813400000000     10.582800000000     R=1.72
6 O      8.216900000000     11.024800000000     12.208900000000     R=1.72
7 O      8.713000000000      8.589800000000     13.425700000000     R=1.72
8 C     11.766000000000     10.477300000000     14.190100000000     R=2.00
9 C     12.541600000000      9.365700000000     13.949300000000     R=2.00
10 H     13.346100000000      9.273700000000     14.446000000000     R=1.30
11 C     12.231200000000      8.357000000000     13.022700000000     R=2.00
12 C     12.224400000000     11.527400000000     15.164100000000     R=2.00
13 H     12.251400000000     12.398800000000     14.716100000000     R=1.30
14 H     13.120200000000     11.300500000000     15.491900000000     R=1.30
15 H     11.600900000000     11.566700000000     15.919100000000     R=1.30
16 C     13.120500000000      7.155800000000     12.927100000000     R=2.00
17 H     12.862400000000      6.503100000000     13.611300000000     R=1.30
18 H     14.051200000000      7.426200000000     13.067900000000     R=1.30
19 H     13.029200000000      6.750600000000     12.040000000000     R=1.30
20 C     10.509300000000     11.122300000000      9.681400000000     R=2.00
21 C      9.657700000000     10.343900000000      8.898700000000     R=2.00
22 H      9.510000000000     10.606200000000      7.997200000000     R=1.30
23 C      9.013300000000      9.204000000000      9.367800000000     R=2.00
24 C     11.309300000000     12.232700000000      9.055000000000     R=2.00
25 H     11.273400000000     13.024900000000      9.630700000000     R=1.30
26 H     10.933800000000     12.449700000000      8.175600000000     R=1.30
27 H     12.240800000000     11.945300000000      8.951400000000     R=1.30
28 C      8.293800000000      8.303100000000      8.404300000000     R=2.00
29 H      8.762500000000      7.444900000000      8.347500000000     R=1.30
30 H      8.271200000000      8.722500000000      7.519300000000     R=1.30
31 H      7.378100000000      8.154000000000      8.717400000000     R=1.30
32 C      7.110300000000     10.957500000000     12.834800000000     R=2.00
33 C      6.740700000000      9.876900000000     13.653400000000     R=2.00
34 H      5.884600000000      9.907800000000     14.063000000000     R=1.30
35 C      7.532500000000      8.774700000000     13.903600000000     R=2.00
36 C      6.197000000000     12.134300000000     12.692600000000     R=2.00
```

37 H 6.398600000000 12.790800000000 13.392000000000 R=1.30
38 H 5.267500000000 11.838300000000 12.779800000000 R=1.30
39 H 6.327400000000 12.544600000000 11.812500000000 R=1.30
40 C 7.054400000000 7.674700000000 14.814500000000 R=2.00
41 H 7.203800000000 6.806800000000 14.385500000000 R=1.30
42 H 6.096900000000 7.790100000000 14.992700000000 R=1.30
43 H 7.549500000000 7.711100000000 15.658900000000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1
15 9 10 1
16 9 11 1.0
17 11 16 1
18 12 13 1
19 12 14 1
20 12 15 1
21 16 17 1
22 16 18 1
23 16 19 1
24 20 21 1.0
25 20 24 1
26 21 22 1
27 21 23 1.0
28 23 28 1
29 24 25 1
30 24 26 1
31 24 27 1
32 28 29 1
33 28 30 1
34 28 31 1
35 32 33 1.0
36 32 36 1

```
37 33 34 1
38 33 35 1.0
39 35 40 1
40 36 37 1
41 36 38 1
42 36 39 1
43 40 41 1
44 40 42 1
45 40 43 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA

RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
```

```
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-III

ATOMS
1 Mn      0.029888372090      0.077986046510     -0.020172093020     R=1.867
2 O      -0.780711627900      1.045686047000      1.572027907000     R=1.72
3 O       1.001488372000     -1.096113953000      1.269527907000     R=1.72
4 O       1.486388372000      1.384986047000     -0.062372093020     R=1.72
5 O       0.918088372100     -0.934013953500     -1.525072093000     R=1.72
6 O      -0.948511627900      1.219386047000     -1.307372093000     R=1.72
7 O      -1.457111628000     -1.191013953000     -0.017472093020     R=1.72
8 C      -0.712211627900      0.698886046500      2.782127907000     R=2.00
9 C      -0.003011627907     -0.392613953500      3.255727907000     R=2.00
10 H     -0.081811627910     -0.586413953500      4.161127907000     R=1.30
11 C      0.801988372100     -1.209513953000      2.512627907000     R=2.00
12 C     -1.450811628000      1.593786047000      3.747727907000     R=2.00
```

13 H -0.823511627900 2.150986047000 4.213027907000 R=1.30
14 H -1.929811628000 1.054186047000 4.380327907000 R=1.30
15 H -2.070411628000 2.144286047000 3.262427907000 R=1.30
16 C 1.577688372000 -2.329313953000 3.165327907000 R=2.00
17 H 1.467988372000 -3.135413953000 2.654927907000 R=1.30
18 H 1.251688372000 -2.467913953000 4.057327907000 R=1.30
19 H 2.509488372000 -2.096413953000 3.197127907000 R=1.30
20 C 2.498588372000 1.399586047000 -0.817872093000 R=2.00
21 C 2.802988372000 0.420286046500 -1.731472093000 R=2.00
22 H 3.600288372000 0.515786046500 -2.200172093000 R=1.30
23 C 2.036588372000 -0.690013953500 -2.019472093000 R=2.00
24 C 3.393288372000 2.607186047000 -0.677272093000 R=2.00
25 H 3.079588372000 3.307086047000 -1.256272093000 R=1.30
26 H 4.290988372000 2.370386047000 -0.919872093000 R=1.30
27 H 3.377788372000 2.914086047000 0.231527907000 R=1.30
28 C 2.529488372000 -1.708813953000 -3.013572093000 R=2.00
29 H 2.339488372000 -2.591713953000 -2.687272093000 R=1.30
30 H 3.476688372000 -1.609213953000 -3.130772093000 R=1.30
31 H 2.086088372000 -1.576913953000 -3.853772093000 R=1.30
32 C -2.096711628000 1.005686047000 -1.785972093000 R=2.00
33 C -2.877511628000 -0.091213953490 -1.506172093000 R=2.00
34 H -3.706811628000 -0.135613953500 -1.925772093000 R=1.30
35 C -2.549411628000 -1.135513953000 -0.659672093000 R=2.00
36 C -2.574211628000 2.082386047000 -2.738472093000 R=2.00
37 H -2.424311628000 2.944986047000 -2.347472093000 R=1.30
38 H -3.512111628000 1.966586047000 -2.908172093000 R=1.30
39 H -2.090511628000 2.016386047000 -3.564172093000 R=1.30
40 C -3.468811628000 -2.298313953000 -0.476372093000 R=2.00
41 H -3.237011628000 -2.991413953000 -1.098972093000 R=1.30
42 H -4.374311628000 -2.019713953000 -0.632072093000 R=1.30
43 H -3.386911628000 -2.633413953000 0.420627907000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0

```
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0
```

```
UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA

GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
mv TAPE21 GASPHASE.t21

# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-III

ATOMS
1 Mn      0.029888372090      0.077986046510     -0.020172093020     R=1.867
2 O      -0.780711627900      1.045686047000      1.572027907000     R=1.72
3 O       1.001488372000     -1.096113953000      1.269527907000     R=1.72
4 O       1.486388372000      1.384986047000     -0.062372093020     R=1.72
5 O       0.918088372100     -0.934013953500     -1.525072093000     R=1.72
6 O      -0.948511627900      1.219386047000     -1.307372093000     R=1.72
7 O      -1.457111628000     -1.191013953000     -0.017472093020     R=1.72
8 C      -0.712211627900      0.698886046500      2.782127907000     R=2.00
9 C      -0.003011627907     -0.392613953500      3.255727907000     R=2.00
10 H     -0.081811627910     -0.586413953500      4.161127907000     R=1.30
11 C      0.801988372100     -1.209513953000      2.512627907000     R=2.00
12 C     -1.450811628000      1.593786047000      3.747727907000     R=2.00
13 H     -0.823511627900      2.150986047000      4.213027907000     R=1.30
14 H     -1.929811628000      1.054186047000      4.380327907000     R=1.30
15 H     -2.070411628000      2.144286047000      3.262427907000     R=1.30
16 C      1.577688372000     -2.329313953000      3.165327907000     R=2.00
17 H      1.467988372000     -3.135413953000      2.654927907000     R=1.30
18 H      1.251688372000     -2.467913953000      4.057327907000     R=1.30
19 H      2.509488372000     -2.096413953000      3.197127907000     R=1.30
20 C      2.498588372000      1.399586047000     -0.817872093000     R=2.00
21 C      2.802988372000      0.420286046500     -1.731472093000     R=2.00
22 H      3.600288372000      0.515786046500     -2.200172093000     R=1.30
23 C      2.036588372000     -0.690013953500     -2.019472093000     R=2.00
24 C      3.393288372000      2.607186047000     -0.677272093000     R=2.00
25 H      3.079588372000      3.307086047000     -1.256272093000     R=1.30
26 H      4.290988372000      2.370386047000     -0.919872093000     R=1.30
27 H      3.377788372000      2.914086047000      0.231527907000     R=1.30
28 C      2.529488372000     -1.708813953000     -3.013572093000     R=2.00
29 H      2.339488372000     -2.591713953000     -2.687272093000     R=1.30
30 H      3.476688372000     -1.609213953000     -3.130772093000     R=1.30
31 H      2.086088372000     -1.576913953000     -3.853772093000     R=1.30
32 C     -2.096711628000      1.005686047000     -1.785972093000     R=2.00
33 C     -2.877511628000     -0.091213953490     -1.506172093000     R=2.00
```

34 H -3.706811628000 -0.135613953500 -1.925772093000 R=1.30
35 C -2.549411628000 -1.135513953000 -0.659672093000 R=2.00
36 C -2.574211628000 2.082386047000 -2.738472093000 R=2.00
37 H -2.424311628000 2.944986047000 -2.347472093000 R=1.30
38 H -3.512111628000 1.966586047000 -2.908172093000 R=1.30
39 H -2.090511628000 2.016386047000 -3.564172093000 R=1.30
40 C -3.468811628000 -2.298313953000 -0.476372093000 R=2.00
41 H -3.237011628000 -2.991413953000 -1.098972093000 R=1.30
42 H -4.374311628000 -2.019713953000 -0.632072093000 R=1.30
43 H -3.386911628000 -2.633413953000 0.420627907000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0

```
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA

RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
```

```
END

BeckeGrid
   Quality Good
End

ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO

#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-II

ATOMS
1 Cr     -0.042834027000      0.581250438000     -0.336465180000     R=1.875
2 O      -1.447016477000     -0.172249582000      0.806430220000     R=1.72
3 O      -0.330203007000      2.351084198000      0.427810640000     R=1.72
4 O       1.307849023000      0.160012718000      1.021875770000     R=1.72
5 O       1.315384263000      1.394167848000     -1.473646640000     R=1.72
6 O       0.232332043000     -1.171523562000     -1.173021830000     R=1.72
7 O      -1.343183897000      1.064051278000     -1.705871330000     R=1.72
8 C      -1.223255767000      0.032185738000      2.142449670000     R=2.00
9 C      -0.599150467000      1.255399998000      2.650077980000     R=2.00
10 H     -0.482925017000      1.357288788000      3.722351360000     R=1.30
11 C     -0.229618007000      2.389461628000      1.795830270000     R=2.00
12 C     -1.871526587000     -0.896891282000      3.115767470000     R=2.00
13 H     -2.156270737000     -1.842890782000      2.608711880000     R=1.30
```

14 H -2.783127477000 -0.421947692000 3.534742240000 R=1.30
15 H -1.167247617000 -1.135421732000 3.940460060000 R=1.30
16 C 0.130139173000 3.697287108000 2.426504000000 R=2.00
17 H 1.146686133000 3.995808748000 2.096076380000 R=1.30
18 H 0.120789233000 3.635843098000 3.535333210000 R=1.30
19 H -0.596307877000 4.473315948000 2.107161040000 R=1.30
20 C 2.338556833000 -0.604352912000 0.541504850000 R=2.00
21 C 2.850177703000 -0.456824412000 -0.822405160000 R=2.00
22 H 3.684511023000 -1.080180442000 -1.120702220000 R=1.30
23 C 2.367826003000 0.562137018000 -1.761068350000 R=2.00
24 C 3.124495463000 -1.419629372000 1.515405570000 R=2.00
25 H 2.542481263000 -1.563788792000 2.450063840000 R=1.30
26 H -4.427960997000 -0.122727022000 -2.470649860000 R=1.30
27 H 3.350137193000 -2.416500692000 1.081418220000 R=1.30
28 C 3.132459313000 0.822619928000 -3.019999880000 R=2.00
29 H 2.461041043000 0.679824878000 -3.892062000000 R=1.30
30 H 3.999879573000 0.136875508000 -3.123941200000 R=1.30
31 H -3.505905127000 1.153045868000 -3.352392700000 R=1.30
32 C -0.921364977000 -1.894592542000 -1.330611660000 R=2.00
33 C -2.221152927000 -1.260538232000 -1.569736350000 R=2.00
34 H -3.093681257000 -1.896551832000 -1.654733420000 R=1.30
35 C -2.381957337000 0.175624138000 -1.817782650000 R=2.00
36 C -0.802891687000 -3.384074462000 -1.392116010000 R=2.00
37 H -0.104046687000 -3.665145712000 -2.207284310000 R=1.30
38 H -1.784727837000 -3.867071442000 -1.581820360000 R=1.30
39 H -0.402410227000 -3.759154452000 -0.427367460000 R=1.30
40 C -3.678464127000 0.689139948000 -2.358947360000 R=2.00
41 H -4.085769157000 1.455911868000 -1.667696940000 R=1.30
42 H 3.503754963000 1.868561198000 -3.016856050000 R=1.30
43 H 4.074499083000 -0.898840952000 1.757204270000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0

```
14 8 12 1
15 9 10 1
16 9 11 1.0
17 11 16 1
18 12 13 1
19 12 14 1
20 12 15 1
21 16 17 1
22 16 18 1
23 16 19 1
24 20 21 1.0
25 20 24 1
26 21 22 1
27 21 23 1.0
28 23 28 1
29 24 25 1
30 40 26 1
31 24 27 1
32 28 29 1
33 28 30 1
34 40 31 1
35 32 33 1.0
36 32 36 1
37 34 33 1.0
38 33 35 1.0
39 35 40 1
40 36 37 1
41 36 38 1
42 36 39 1
43 40 41 1
44 42 28 1.0
45 43 24 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0
```

```
UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
```

"\$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21

COSMO-RS Solvent calculation

==============================
The Molecule
==============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-II

ATOMS
1 Cr -0.042834027000 0.581250438000 -0.336465180000 R=1.875
2 O -1.447016477000 -0.172249582000 0.806430220000 R=1.72
3 O -0.330203007000 2.351084198000 0.427810640000 R=1.72
4 O 1.307849023000 0.160012718000 1.021875770000 R=1.72
5 O 1.315384263000 1.394167848000 -1.473646640000 R=1.72
6 O 0.232332043000 -1.171523562000 -1.173021830000 R=1.72
7 O -1.343183897000 1.064051278000 -1.705871330000 R=1.72
8 C -1.223255767000 0.032185738000 2.142449670000 R=2.00
9 C -0.599150467000 1.255399998000 2.650077980000 R=2.00
10 H -0.482925017000 1.357288788000 3.722351360000 R=1.30
11 C -0.229618007000 2.389461628000 1.795830270000 R=2.00
12 C -1.871526587000 -0.896891282000 3.115767470000 R=2.00
13 H -2.156270737000 -1.842890782000 2.608711880000 R=1.30
14 H -2.783127477000 -0.421947692000 3.534742240000 R=1.30
15 H -1.167247617000 -1.135421732000 3.940460060000 R=1.30
16 C 0.130139173000 3.697287108000 2.426504000000 R=2.00
17 H 1.146686133000 3.995808748000 2.096076380000 R=1.30
18 H 0.120789233000 3.635843098000 3.535333210000 R=1.30
19 H -0.596307877000 4.473315948000 2.107161040000 R=1.30
20 C 2.338556833000 -0.604352912000 0.541504850000 R=2.00
21 C 2.850177703000 -0.456824412000 -0.822405160000 R=2.00
22 H 3.684511023000 -1.080180442000 -1.120702220000 R=1.30
23 C 2.367826003000 0.562137018000 -1.761068350000 R=2.00
24 C 3.124495463000 -1.419629372000 1.515405570000 R=2.00
25 H 2.542481263000 -1.563788792000 2.450063840000 R=1.30
26 H -4.427960997000 -0.122727022000 -2.470649860000 R=1.30
27 H 3.350137193000 -2.416500692000 1.081418220000 R=1.30
28 C 3.132459313000 0.822619928000 -3.019999880000 R=2.00
29 H 2.461041043000 0.679824878000 -3.892062000000 R=1.30
30 H 3.999879573000 0.136875508000 -3.123941200000 R=1.30
31 H -3.505905127000 1.153045868000 -3.352392700000 R=1.30
32 C -0.921364977000 -1.894592542000 -1.330611660000 R=2.00

33 C -2.221152927000 -1.260538232000 -1.569736350000 R=2.00
34 H -3.093681257000 -1.896551832000 -1.654733420000 R=1.30
35 C -2.381957337000 0.175624138000 -1.817782650000 R=2.00
36 C -0.802891687000 -3.384074462000 -1.392116010000 R=2.00
37 H -0.104046687000 -3.665145712000 -2.207284310000 R=1.30
38 H -1.784727837000 -3.867071442000 -1.581820360000 R=1.30
39 H -0.402410227000 -3.759154452000 -0.427367460000 R=1.30
40 C -3.678464127000 0.689139948000 -2.358947360000 R=2.00
41 H -4.085769157000 1.455911868000 -1.667696940000 R=1.30
42 H 3.503754963000 1.868561198000 -3.016856050000 R=1.30
43 H 4.074499083000 -0.898840952000 1.757204270000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1
15 9 10 1
16 9 11 1.0
17 11 16 1
18 12 13 1
19 12 14 1
20 12 15 1
21 16 17 1
22 16 18 1
23 16 19 1
24 20 21 1.0
25 20 24 1
26 21 22 1
27 21 23 1.0
28 23 28 1
29 24 25 1
30 40 26 1
31 24 27 1
32 28 29 1

```
33 28 30 1
34 40 31 1
35 32 33 1.0
36 32 36 1
37 34 33 1.0
38 33 35 1.0
39 35 40 1
40 36 37 1
41 36 38 1
42 36 39 1
43 40 41 1
44 42 28 1.0
45 43 24 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA

RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
```

```
diis
END

BeckeGrid
   Quality Good
End

ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-V

ATOMS
1 Fe      9.769071444000      9.800836796000     12.145676840000     R=1.858
2 O      10.688659690000     10.796634420000     13.595366370000     R=1.72
3 O      11.336517770000      8.524978993000     12.156565020000     R=1.72
4 O      10.720912190000     10.967024810000     10.802140970000     R=1.72
5 O       9.025227978000      8.795085679000     10.613006150000     R=1.72
6 O       8.272874534000     11.086480950000     12.212748590000     R=1.72
7 O       8.805908446000      8.610797375000     13.395914220000     R=1.72
8 C      11.657128390000     10.402192180000     14.370578730000     R=2.00
9 C      12.403771350000      9.238275033000     14.163872400000     R=2.00
10 H      13.210524190000      9.023057112000     14.862300990000     R=1.30
11 C      12.239002630000      8.370808062000     13.062270010000     R=2.00
```

12 C 11.964520200000 11.311835950000 15.529330990000 R=2.00
13 H 12.235355850000 12.309028740000 15.151433290000 R=1.30
14 H 12.781033770000 10.925585050000 16.148819160000 R=1.30
15 H 11.063127550000 11.434744260000 16.147991180000 R=1.30
16 C 13.166315580000 7.197547803000 12.880974740000 R=2.00
17 H 12.586493650000 6.263965758000 12.937706440000 R=1.30
18 H 13.956752060000 7.175475989000 13.638963790000 R=1.30
19 H 13.618709530000 7.237288670000 11.879468310000 R=1.30
20 C 10.492647480000 11.088623740000 9.540091836000 R=2.00
21 C 9.612465733000 10.253550530000 8.817964960000 R=2.00
22 H 9.500913123000 10.436471060000 7.750690047000 R=1.30
23 C 8.949205752000 9.149581834000 9.361944843000 R=2.00
24 C 11.259403420000 12.172754890000 8.828253483000 R=2.00
25 H 11.041313150000 13.144883600000 9.294210079000 R=1.30
26 H 11.014149000000 12.217883560000 7.761661287000 R=1.30
27 H 12.338502930000 11.992477250000 8.944144759000 R=1.30
28 C 8.106733144000 8.256309428000 8.492023433000 R=2.00
29 H 8.515154469000 7.234783460000 8.511980855000 R=1.30
30 H 8.068478118000 8.610185722000 7.456145627000 R=1.30
31 H 7.085990799000 8.203943402000 8.898788842000 R=1.30
32 C 7.155495349000 10.987950670000 12.869550160000 R=2.00
33 C 6.811752205000 9.895704661000 13.682108700000 R=2.00
34 H 5.842723158000 9.923880773000 14.177877030000 R=1.30
35 C 7.624342459000 8.772460924000 13.910281570000 R=2.00
36 C 6.209236716000 12.148373780000 12.713630950000 R=2.00
37 H 6.702692391000 13.072291200000 13.050334190000 R=1.30
38 H 5.285056553000 12.004337510000 13.283690580000 R=1.30
39 H 5.963096912000 12.282772720000 11.649863380000 R=1.30
40 C 7.146871852000 7.656161473000 14.800247010000 R=2.00
41 H 7.131254747000 6.714899762000 14.230796610000 R=1.30
42 H 6.147419211000 7.850800779000 15.203876190000 R=1.30
43 H 7.853974653000 7.519248648000 15.631903820000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0

```
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END
```

```
CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====
```

```
rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21

# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-V

ATOMS
1 Fe      9.769071444000      9.800836796000     12.145676840000    R=1.858
2 O      10.688659690000     10.796634420000     13.595366370000    R=1.72
3 O      11.336517770000      8.524978993000     12.156565020000    R=1.72
4 O      10.720912190000     10.967024810000     10.802140970000    R=1.72
5 O       9.025227978000      8.795085679000     10.613006150000    R=1.72
6 O       8.272874534000     11.086480950000     12.212748590000    R=1.72
7 O       8.805908446000      8.610797375000     13.395914220000    R=1.72
8 C      11.657128390000     10.402192180000     14.370578730000    R=2.00
9 C      12.403771350000      9.238275033000     14.163872400000    R=2.00
10 H     13.210524190000      9.023057112000     14.862300990000    R=1.30
11 C     12.239002630000      8.370808062000     13.062270010000    R=2.00
12 C     11.964520200000     11.311835950000     15.529330990000    R=2.00
13 H     12.235355850000     12.309028740000     15.151433290000    R=1.30
14 H     12.781033770000     10.925585050000     16.148819160000    R=1.30
15 H     11.063127550000     11.434744260000     16.147991180000    R=1.30
16 C     13.166315580000      7.197547803000     12.880974740000    R=2.00
17 H     12.586493650000      6.263965758000     12.937706440000    R=1.30
18 H     13.956752060000      7.175475989000     13.638963790000    R=1.30
19 H     13.618709530000      7.237288670000     11.879468310000    R=1.30
20 C     10.492647480000     11.088623740000      9.540091836000    R=2.00
21 C      9.612465733000     10.253550530000      8.817964960000    R=2.00
22 H      9.500913123000     10.436471060000      7.750690047000    R=1.30
23 C      8.949205752000      9.149581834000      9.361944843000    R=2.00
24 C     11.259403420000     12.172754890000      8.828253483000    R=2.00
25 H     11.041313150000     13.144883600000      9.294210079000    R=1.30
26 H     11.014149000000     12.217883560000      7.761661287000    R=1.30
27 H     12.338502930000     11.992477250000      8.944144759000    R=1.30
28 C      8.106733144000      8.256309428000      8.492023433000    R=2.00
29 H      8.515154469000      7.234783460000      8.511980855000    R=1.30
30 H      8.068478118000      8.610185722000      7.456145627000    R=1.30
```

31 H 7.085990799000 8.203943402000 8.898788842000 R=1.30
32 C 7.155495349000 10.987950670000 12.869550160000 R=2.00
33 C 6.811752205000 9.895704661000 13.682108700000 R=2.00
34 H 5.842723158000 9.923880773000 14.177877030000 R=1.30
35 C 7.624342459000 8.772460924000 13.910281570000 R=2.00
36 C 6.209236716000 12.148373780000 12.713630950000 R=2.00
37 H 6.702692391000 13.072291200000 13.050334190000 R=1.30
38 H 5.285056553000 12.004337510000 13.283690580000 R=1.30
39 H 5.963096912000 12.282772720000 11.649863380000 R=1.30
40 C 7.146871852000 7.656161473000 14.800247010000 R=2.00
41 H 7.131254747000 6.714899762000 14.230796610000 R=1.30
42 H 6.147419211000 7.850800779000 15.203876190000 R=1.30
43 H 7.853974653000 7.519248648000 15.631903820000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0

```
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21
```

```
SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-IV

ATOMS
1 Ru      0.109518418000      0.008697842000     -0.053327540000     R=1.950
2 O       1.029106664000      1.004495466000      1.396361990000     R=1.72
3 O       1.676964744000     -1.267159961000     -0.042439360000     R=1.72
4 O       1.061359164000      1.174885856000     -1.396863410000     R=1.72
5 O      -0.634325048000     -0.997053275000     -1.585998230000     R=1.72
6 O      -1.386678492000      1.294341996000      0.013744210000     R=1.72
```

7 O -0.853644580000 -1.181341579000 1.196909840000 R=1.72
8 C 1.997575364000 0.610053226000 2.171574350000 R=2.00
9 C 2.744218324000 -0.553863921000 1.964868020000 R=2.00
10 H 3.550971164000 -0.769081842000 2.663296610000 R=1.30
11 C 2.579449604000 -1.421330892000 0.863265630000 R=2.00
12 C 2.304967174000 1.519696996000 3.330326610000 R=2.00
13 H 2.575802824000 2.516889786000 2.952428910000 R=1.30
14 H 3.121480744000 1.133446096000 3.949814780000 R=1.30
15 H 1.403574524000 1.642605306000 3.948986800000 R=1.30
16 C 3.506762554000 -2.594591151000 0.681970360000 R=2.00
17 H 2.926940624000 -3.528173196000 0.738702060000 R=1.30
18 H 4.297199034000 -2.616662965000 1.439959410000 R=1.30
19 H 3.959156504000 -2.554850284000 -0.319536070000 R=1.30
20 C 0.833094454000 1.296484786000 -2.658912544000 R=2.00
21 C -0.047087293000 0.461411576000 -3.381039420000 R=2.00
22 H -0.158639903000 0.644332106000 -4.448314333000 R=1.30
23 C -0.710347274000 -0.642557120000 -2.837059537000 R=2.00
24 C 1.599850394000 2.380615936000 -3.370750897000 R=2.00
25 H 1.381760124000 3.352744646000 -2.904794301000 R=1.30
26 H 1.354595974000 2.425744606000 -4.437343093000 R=1.30
27 H 2.678949904000 2.200338296000 -3.254859621000 R=1.30
28 C -1.552819882000 -1.535829526000 -3.706980947000 R=2.00
29 H -1.144398557000 -2.557355494000 -3.687023525000 R=1.30
30 H -1.591074908000 -1.181953232000 -4.742858753000 R=1.30
31 H -2.573562227000 -1.588195552000 -3.300215538000 R=1.30
32 C -2.504057677000 1.195811716000 0.670545780000 R=2.00
33 C -2.847800821000 0.103565707000 1.483104320000 R=2.00
34 H -3.816829868000 0.131741819000 1.978872650000 R=1.30
35 C -2.035210567000 -1.019678030000 1.711277190000 R=2.00
36 C -3.450316310000 2.356234826000 0.514626570000 R=2.00
37 H -2.956860635000 3.280152246000 0.851329810000 R=1.30
38 H -4.374496473000 2.212198556000 1.084686200000 R=1.30
39 H -3.696456114000 2.490633766000 -0.549141000000 R=1.30
40 C -2.512681174000 -2.135977481000 2.601242630000 R=2.00
41 H -2.528298279000 -3.077239192000 2.031792230000 R=1.30
42 H -3.512133815000 -1.941338175000 3.004871810000 R=1.30
43 H -1.805578373000 -2.272890306000 3.432899440000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0

7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
  Surf Delley
  Div ndiv=4
  Solvent name=CRS cav0=0.0 cav1=0.0
  Charged method=CONJ conv=1.0E-06 iter=300 corr

```
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE
```

```
eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21

# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-IV

ATOMS
1 Ru      0.109518418000      0.008697842000     -0.053327540000    R=1.950
2 O       1.029106664000      1.004495466000      1.396361990000    R=1.72
3 O       1.676964744000     -1.267159961000     -0.042439360000    R=1.72
4 O       1.061359164000      1.174885856000     -1.396863410000    R=1.72
5 O      -0.634325048000     -0.997053275000     -1.585998230000    R=1.72
6 O      -1.386678492000      1.294341996000      0.013744210000    R=1.72
7 O      -0.853644580000     -1.181341579000      1.196909840000    R=1.72
8 C       1.997575364000      0.610053226000      2.171574350000    R=2.00
9 C       2.744218324000     -0.553863921000      1.964868020000    R=2.00
10 H      3.550971164000     -0.769081842000      2.663296610000    R=1.30
11 C      2.579449604000     -1.421330892000      0.863265630000    R=2.00
12 C      2.304967174000      1.519696996000      3.330326610000    R=2.00
13 H      2.575802824000      2.516889786000      2.952428910000    R=1.30
14 H      3.121480744000      1.133446096000      3.949814780000    R=1.30
15 H      1.403574524000      1.642605306000      3.948986800000    R=1.30
16 C      3.506762554000     -2.594591151000      0.681970360000    R=2.00
17 H      2.926940624000     -3.528173196000      0.738702060000    R=1.30
18 H      4.297199034000     -2.616662965000      1.439959410000    R=1.30
19 H      3.959156504000     -2.554850284000     -0.319536070000    R=1.30
20 C      0.833094454000      1.296484786000     -2.658912544000    R=2.00
21 C     -0.047087293000      0.461411576000     -3.381039420000    R=2.00
22 H     -0.158639903000      0.644332106000     -4.448314333000    R=1.30
23 C     -0.710347274000     -0.642557120000     -2.837059537000    R=2.00
24 C      1.599850394000      2.380615936000     -3.370750897000    R=2.00
25 H      1.381760124000      3.352744646000     -2.904794301000    R=1.30
```

```
26 H      1.354595974000      2.425744606000     -4.437343093000    R=1.30
27 H      2.678949904000      2.200338296000     -3.254859621000    R=1.30
28 C     -1.552819882000     -1.535829526000     -3.706980947000    R=2.00
29 H     -1.144398557000     -2.557355494000     -3.687023525000    R=1.30
30 H     -1.591074908000     -1.181953232000     -4.742858753000    R=1.30
31 H     -2.573562227000     -1.588195552000     -3.300215538000    R=1.30
32 C     -2.504057677000      1.195811716000      0.670545780000    R=2.00
33 C     -2.847800821000      0.103565707000      1.483104320000    R=2.00
34 H     -3.816829868000      0.131741819000      1.978872650000    R=1.30
35 C     -2.035210567000     -1.019678030000      1.711277190000    R=2.00
36 C     -3.450316310000      2.356234826000      0.514626570000    R=2.00
37 H     -2.956860635000      3.280152246000      0.851329810000    R=1.30
38 H     -4.374496473000      2.212198556000      1.084686200000    R=1.30
39 H     -3.696456114000      2.490633766000     -0.549141000000    R=1.30
40 C     -2.512681174000     -2.135977481000      2.601242630000    R=2.00
41 H     -2.528298279000     -3.077239192000      2.031792230000    R=1.30
42 H     -3.512133815000     -1.941338175000      3.004871810000    R=1.30
43 H     -1.805578373000     -2.272890306000      3.432899440000    R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 9 10 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
```

```
26 21 22 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 24 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 28 31 1.0
35 32 33 1.0
36 32 36 1.0
37 33 34 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 40 42 1.0
45 40 43 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-VI
```

ATOMS

1 Cr	0.193747440000	0.413827560000	0.403846490000	R=1.875
2 O	-0.650481560000	0.036987790000	2.136073870000	R=1.72
3 O	0.458931650000	2.315845320000	0.833650210000	R=1.72
4 O	1.954364390000	-0.107764820000	1.097352670000	R=1.72
5 O	0.926799510000	0.702080560000	-1.383165760000	R=1.72
6 O	-0.077314470000	-1.483217430000	0.000229650000	R=1.72
7 O	-1.575249380000	0.962631850000	-0.238046970000	R=1.72
8 C	0.008230770000	0.565961630000	3.247498760000	R=2.00
9 C	-0.039083210000	2.102433620000	3.210557240000	R=2.00
10 H	-1.041677560000	4.519625140000	4.090839070000	R=1.30
11 C	0.943346610000	2.579903980000	2.127514170000	R=2.00
12 C	-0.631198360000	0.000028600000	4.520019390000	R=2.00
13 H	-0.547765570000	-1.107616690000	4.517181630000	R=1.30
14 H	-1.706025010000	0.263796200000	4.592221230000	R=1.30
15 H	-0.102258940000	0.382155850000	5.418044930000	R=1.30
16 C	1.231191070000	4.079497200000	2.241084150000	R=2.00
17 H	2.015719670000	4.364853110000	1.508040120000	R=1.30
18 H	1.598519350000	4.330810140000	3.258913350000	R=1.30
19 H	0.320749360000	4.675659890000	2.022210310000	R=1.30
20 C	3.057053780000	0.053947960000	0.234761340000	R=2.00
21 C	3.085315600000	1.440064420000	-0.456570770000	R=2.00
22 H	-4.528562800000	-1.471360050000	-2.107622870000	R=1.30
23 C	1.952405970000	1.647416230000	-1.513346110000	R=2.00
24 C	3.225481610000	-1.144446270000	-0.706088740000	R=2.00
25 H	2.451403510000	-1.180398340000	-1.489565040000	R=1.30
26 H	-3.825106850000	-1.523500860000	0.097488220000	R=1.30
27 H	4.216770160000	-1.098243380000	-1.204217920000	R=1.30
28 C	2.415355510000	1.564353340000	-2.976646070000	R=2.00
29 H	1.535022660000	1.646410020000	-3.649801500000	R=1.30
30 H	2.909277940000	0.590656960000	-3.178250950000	R=1.30
31 H	-3.398186980000	-0.191882040000	1.202426980000	R=1.30
32 C	-0.526896030000	-1.817745010000	-1.291208850000	R=2.00
33 C	-1.638308510000	-0.861429470000	-1.815035290000	R=2.00
34 C	-2.533638880000	-1.407792480000	-2.969328120000	R=2.00
35 C	-2.386563420000	-0.076118510000	-0.718289580000	R=2.00
36 C	-0.927353660000	-3.296971700000	-1.245651310000	R=2.00
37 H	-0.061929470000	-3.899566840000	-0.895729190000	R=1.30
38 H	-1.206026440000	-3.682853490000	-2.246852990000	R=1.30
39 H	-1.757207960000	-3.458322860000	-0.527902380000	R=1.30
40 C	-2.986963930000	-0.889822700000	0.442367630000	R=2.00
41 H	-2.255029340000	-1.544566920000	0.946858730000	R=1.30
42 H	3.102164000000	2.391094420000	-3.243446160000	R=1.30
43 H	3.176022850000	-2.087913330000	-0.122273120000	R=1.30
44 C	-1.484808290000	2.665071000000	3.004980250000	R=2.00
45 H	-2.252375440000	1.864068440000	3.061982450000	R=1.30

46 H	-1.597329710000	3.086853730000	1.983509490000	R=1.30
47 C	-2.164517200000	3.206808870000	5.366660010000	R=2.00
48 H	-2.754311780000	4.303112080000	3.625396930000	R=1.30
49 H	-0.673900040000	1.544392840000	9.253151040000	R=1.30
50 C	-1.856277020000	3.769510500000	4.007774420000	R=2.00
51 O	-1.105526740000	2.923392250000	6.229404780000	R=1.72
52 H	0.347257500000	1.322241380000	7.778869320000	R=1.30
53 H	0.204889280000	2.955939170000	8.544226980000	R=1.30
54 H	-2.076048040000	1.367349840000	7.220543620000	R=1.30
55 C	-1.545165270000	2.324054520000	7.430695570000	R=2.00
56 C	-0.339662850000	2.017726080000	8.305855750000	R=2.00
57 H	-2.216070370000	3.014733610000	7.990578050000	R=1.30
58 O	-3.336866780000	3.032035810000	5.682880080000	R=1.72
59 C	4.520570080000	1.811606270000	-0.934290960000	R=2.00
60 H	4.770221720000	1.297626070000	-1.885707320000	R=1.30
61 H	5.268075600000	1.453057970000	-0.192794560000	R=1.30
62 C	4.717847350000	3.332937570000	-1.055708530000	R=2.00
63 H	4.658075620000	3.789300290000	-0.042500220000	R=1.30
64 H	3.921015200000	3.795527300000	-1.672192860000	R=1.30
65 C	6.047422400000	3.645808770000	-1.676146930000	R=2.00
66 H	7.548201540000	3.584045140000	-4.570637390000	R=1.30
67 C	7.571396770000	3.559075800000	-3.460706650000	R=2.00
68 O	6.257597000000	3.285227170000	-3.009027500000	R=1.72
69 H	8.634638030000	2.418148700000	-1.935225790000	R=1.30
70 O	-3.726460940000	-3.917732970000	-4.326222590000	R=1.72
71 O	6.898404160000	4.215252750000	-1.001638940000	R=1.72
72 C	-3.794024320000	-2.180323090000	-2.546925050000	R=2.00
73 C	-4.416547970000	-2.860745180000	-3.731295950000	R=2.00
74 H	7.940970480000	4.559988430000	-3.140825870000	R=1.30
75 H	-4.174347970000	-6.050784890000	-6.871864930000	R=1.30
76 H	1.057955420000	0.210407380000	3.269239150000	R=1.30
77 H	0.366531960000	2.452884660000	4.185472430000	R=1.30
78 H	1.915865090000	2.072751050000	2.286647720000	R=1.30
79 H	3.940120280000	0.014388310000	0.909189090000	R=1.30
80 H	2.891738350000	2.165763170000	0.349712500000	R=1.30
81 H	-3.565234470000	-2.955075220000	-1.792730600000	R=1.30
82 H	1.517461230000	2.661682410000	-1.382768590000	R=1.30
83 H	0.331180900000	-1.760152960000	-1.992205770000	R=1.30
84 H	-1.076991860000	-0.072504920000	-2.359528700000	R=1.30
85 H	-1.908074300000	-2.025845810000	-3.649615100000	R=1.30
86 H	-2.876220280000	-0.544882670000	-3.584900400000	R=1.30
87 H	-3.247618260000	0.427468100000	-1.209384410000	R=1.30
88 H	8.166488830000	1.469808980000	-3.402075810000	R=1.30
89 H	9.537807280000	2.643809630000	-3.479678310000	R=1.30
90 C	8.536277650000	2.452518590000	-3.040112160000	R=2.00
91 H	-2.640865140000	-5.240482930000	-6.362121420000	R=1.30

92 C -4.433582230000 -4.465462680000 -5.419614710000 R=2.00
93 H -4.584341930000 -3.697979570000 -6.212800020000 R=1.30
94 H -5.418603310000 -4.867053090000 -5.088657380000 R=1.30
95 C -3.627286530000 -5.611324310000 -6.011155170000 R=2.00
96 H -3.468604740000 -6.399528510000 -5.244730460000 R=1.30
97 O -5.512983380000 -2.480430760000 -4.129137050000 R=1.72
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0

38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0

```
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 90 89 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21

# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-VI

ATOMS
1 Cr       0.193747440000       0.413827560000       0.403846490000     R=1.875
2 O      -0.650481560000       0.036987790000       2.136073870000     R=1.72
```

3 O	0.458931650000	2.315845320000	0.833650210000	R=1.72
4 O	1.954364390000	-0.107764820000	1.097352670000	R=1.72
5 O	0.926799510000	0.702080560000	-1.383165760000	R=1.72
6 O	-0.077314470000	-1.483217430000	0.000229650000	R=1.72
7 O	-1.575249380000	0.962631850000	-0.238046970000	R=1.72
8 C	0.008230770000	0.565961630000	3.247498760000	R=2.00
9 C	-0.039083210000	2.102433620000	3.210557240000	R=2.00
10 H	-1.041677560000	4.519625140000	4.090839070000	R=1.30
11 C	0.943346610000	2.579903980000	2.127514170000	R=2.00
12 C	-0.631198360000	0.000028600000	4.520019390000	R=2.00
13 H	-0.547765570000	-1.107616690000	4.517181630000	R=1.30
14 H	-1.706025010000	0.263796200000	4.592221230000	R=1.30
15 H	-0.102258940000	0.382155850000	5.418044930000	R=1.30
16 C	1.231191070000	4.079497200000	2.241084150000	R=2.00
17 H	2.015719670000	4.364853110000	1.508040120000	R=1.30
18 H	1.598519350000	4.330810140000	3.258913350000	R=1.30
19 H	0.320749360000	4.675659890000	2.022210310000	R=1.30
20 C	3.057053780000	0.053947960000	0.234761340000	R=2.00
21 C	3.085315600000	1.440064420000	-0.456570770000	R=2.00
22 H	-4.528562800000	-1.471360050000	-2.107622870000	R=1.30
23 C	1.952405970000	1.647416230000	-1.513346110000	R=2.00
24 C	3.225481610000	-1.144446270000	-0.706088740000	R=2.00
25 H	2.451403510000	-1.180398340000	-1.489565040000	R=1.30
26 H	-3.825106850000	-1.523500860000	0.097488220000	R=1.30
27 H	4.216770160000	-1.098243380000	-1.204217920000	R=1.30
28 C	2.415355510000	1.564353340000	-2.976646070000	R=2.00
29 H	1.535022660000	1.646410020000	-3.649801500000	R=1.30
30 H	2.909277940000	0.590656960000	-3.178250950000	R=1.30
31 H	-3.398186980000	-0.191882040000	1.202426980000	R=1.30
32 C	-0.526896030000	-1.817745010000	-1.291208850000	R=2.00
33 C	-1.638308510000	-0.861429470000	-1.815035290000	R=2.00
34 C	-2.533638880000	-1.407792480000	-2.969328120000	R=2.00
35 C	-2.386563420000	-0.076118510000	-0.718289580000	R=2.00
36 C	-0.927353660000	-3.296971700000	-1.245651310000	R=2.00
37 H	-0.061929470000	-3.899566840000	-0.895729190000	R=1.30
38 H	-1.206026440000	-3.682853490000	-2.246852990000	R=1.30
39 H	-1.757207960000	-3.458322860000	-0.527902380000	R=1.30
40 C	-2.986963930000	-0.889822700000	0.442367630000	R=2.00
41 H	-2.255029340000	-1.544566920000	0.946858730000	R=1.30
42 H	3.102164000000	2.391094420000	-3.243446160000	R=1.30
43 H	3.176022850000	-2.087913330000	-0.122273120000	R=1.30
44 C	-1.484808290000	2.665071000000	3.004980250000	R=2.00
45 H	-2.252375440000	1.864068440000	3.061982450000	R=1.30
46 H	-1.597329710000	3.086853730000	1.983509490000	R=1.30
47 C	-2.164517200000	3.206808870000	5.366660010000	R=2.00
48 H	-2.754311780000	4.303112080000	3.625396930000	R=1.30

49 H	-0.673900040000	1.544392840000	9.253151040000	R=1.30
50 C	-1.856277020000	3.769510500000	4.007774420000	R=2.00
51 O	-1.105526740000	2.923392250000	6.229404780000	R=1.72
52 H	0.347257500000	1.322241380000	7.778869320000	R=1.30
53 H	0.204889280000	2.955939170000	8.544226980000	R=1.30
54 H	-2.076048040000	1.367349840000	7.220543620000	R=1.30
55 C	-1.545165270000	2.324054520000	7.430695570000	R=2.00
56 C	-0.339662850000	2.017726080000	8.305855750000	R=2.00
57 H	-2.216070370000	3.014733610000	7.990578050000	R=1.30
58 O	-3.336866780000	3.032035810000	5.682880080000	R=1.72
59 C	4.520570080000	1.811606270000	-0.934290960000	R=2.00
60 H	4.770221720000	1.297626070000	-1.885707320000	R=1.30
61 H	5.268075600000	1.453057970000	-0.192794560000	R=1.30
62 C	4.717847350000	3.332937570000	-1.055708530000	R=2.00
63 H	4.658075620000	3.789300290000	-0.042500220000	R=1.30
64 H	3.921015200000	3.795527300000	-1.672192860000	R=1.30
65 C	6.047422400000	3.645808770000	-1.676146930000	R=2.00
66 H	7.548201540000	3.584045140000	-4.570637390000	R=1.30
67 C	7.571396770000	3.559075800000	-3.460706650000	R=2.00
68 O	6.257597000000	3.285227170000	-3.009027500000	R=1.72
69 H	8.634638030000	2.418148700000	-1.935225790000	R=1.30
70 O	-3.726460940000	-3.917732970000	-4.326222590000	R=1.72
71 O	6.898404160000	4.215252750000	-1.001638940000	R=1.72
72 C	-3.794024320000	-2.180323090000	-2.546925050000	R=2.00
73 C	-4.416547970000	-2.860745180000	-3.731295950000	R=2.00
74 H	7.940970480000	4.559988430000	-3.140825870000	R=1.30
75 H	-4.174347970000	-6.050784890000	-6.871864930000	R=1.30
76 H	1.057955420000	0.210407380000	3.269239150000	R=1.30
77 H	0.366531960000	2.452884660000	4.185472430000	R=1.30
78 H	1.915865090000	2.072751050000	2.286647720000	R=1.30
79 H	3.940120280000	0.014388310000	0.909189090000	R=1.30
80 H	2.891738350000	2.165763170000	0.349712500000	R=1.30
81 H	-3.565234470000	-2.955075220000	-1.792730600000	R=1.30
82 H	1.517461230000	2.661682410000	-1.382768590000	R=1.30
83 H	0.331180900000	-1.760152960000	-1.992205770000	R=1.30
84 H	-1.076991860000	-0.072504920000	-2.359528700000	R=1.30
85 H	-1.908074300000	-2.025845810000	-3.649615100000	R=1.30
86 H	-2.876220280000	-0.544882670000	-3.584900400000	R=1.30
87 H	-3.247618260000	0.427468100000	-1.209384410000	R=1.30
88 H	8.166488830000	1.469808980000	-3.402075810000	R=1.30
89 H	9.537807280000	2.643809630000	-3.479678310000	R=1.30
90 C	8.536277650000	2.452518590000	-3.040112160000	R=2.00
91 H	-2.640865140000	-5.240482930000	-6.362121420000	R=1.30
92 C	-4.433582230000	-4.465462680000	-5.419614710000	R=2.00
93 H	-4.584341930000	-3.697979570000	-6.212800020000	R=1.30
94 H	-5.418603310000	-4.867053090000	-5.088657380000	R=1.30

95 C -3.627286530000 -5.611324310000 -6.011155170000 R=2.00
96 H -3.468604740000 -6.399528510000 -5.244730460000 R=1.30
97 O -5.512983380000 -2.480430760000 -4.129137050000 R=1.72
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0

41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0

```
87 86 34 1.0
88 87 35 1.0
89 90 89 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
```

```
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-VII

ATOMS
1 Cr     -0.278775080000      0.100558910000      0.263361200000     R=1.875
2 O      -1.205685760000     -0.366235990000      1.927830880000     R=1.72
3 O       0.064054630000      1.941555830000      0.859981340000     R=1.72
4 O       1.418575590000     -0.573775630000      0.974685060000     R=1.72
5 O       0.541790710000      0.497823640000     -1.463239490000     R=1.72
6 O      -0.636253630000     -1.736530860000     -0.308321000000     R=1.72
7 O      -1.986450490000      0.794475830000     -0.397807860000     R=1.72
```

8 C	-0.569235010000	0.038689390000	3.105280680000	R=2.00
9 C	-0.527183950000	1.579996940000	3.196950080000	R=2.00
10 H	-1.647535500000	4.982394960000	3.576285510000	R=1.30
11 C	0.527453470000	2.064323530000	2.179989980000	R=2.00
12 C	-1.293778700000	-0.598934410000	4.291596170000	R=2.00
13 H	-1.256603300000	-1.705245140000	4.198402570000	R=1.30
14 H	-2.359894070000	-0.295431180000	4.322398610000	R=1.30
15 H	-0.794006030000	-0.320509510000	5.242294770000	R=1.30
16 C	0.942760740000	3.518203190000	2.411856800000	R=2.00
17 H	1.765040930000	3.785468350000	1.715737190000	R=1.30
18 H	1.310776560000	3.659857450000	3.449796280000	R=1.30
19 H	0.100069430000	4.208898490000	2.212114510000	R=1.30
20 C	2.555870630000	-0.438223290000	0.155023230000	R=2.00
21 C	2.721558460000	0.990554780000	-0.421238460000	R=2.00
22 H	-5.518468720000	-0.704890430000	-2.270013350000	R=1.30
23 C	1.621923100000	1.390254110000	-1.462705840000	R=2.00
24 C	2.663080810000	-1.570211900000	-0.874275850000	R=2.00
25 H	2.017733270000	-1.409554310000	-1.752840070000	R=1.30
26 H	-4.465260510000	-1.448604980000	-0.271909510000	R=1.30
27 H	3.709149560000	-1.647795940000	-1.239188050000	R=1.30
28 C	2.102195580000	1.468038060000	-2.919482580000	R=2.00
29 H	1.239334410000	1.692746640000	-3.582714030000	R=1.30
30 H	2.536789100000	0.499812740000	-3.245432000000	R=1.30
31 H	-3.776532490000	-0.385584200000	0.971015400000	R=1.30
32 C	-1.011289300000	-1.917184940000	-1.651937830000	R=2.00
33 C	-2.096380250000	-0.897878430000	-2.116260620000	R=2.00
34 C	-2.982033780000	-1.318282940000	-3.330625880000	R=2.00
35 C	-2.835077320000	-0.160532210000	-0.978631160000	R=2.00
36 C	-1.392386200000	-3.392501560000	-1.811543810000	R=2.00
37 H	-0.533445300000	-4.026409210000	-1.503370080000	R=1.30
38 H	-1.615658200000	-3.644749920000	-2.867155430000	R=1.30
39 H	-2.247215210000	-3.656547390000	-1.157169130000	R=1.30
40 C	-3.514207160000	-1.023252900000	0.100212580000	R=2.00
41 H	-2.883976980000	-1.855806490000	0.461384990000	R=1.30
42 H	2.838678850000	2.280528000000	-3.066335080000	R=1.30
43 H	2.390146350000	-2.537739660000	-0.402247200000	R=1.30
44 C	-1.934471100000	2.243380470000	2.982958800000	R=2.00
45 H	-2.692865450000	1.471805820000	2.729491150000	R=1.30
46 H	-1.919665250000	2.909543700000	2.093816440000	R=1.30
47 C	-2.697979070000	2.240077300000	5.418943960000	R=2.00
48 H	-3.505976660000	3.418679770000	3.846145080000	R=1.30
49 H	-1.027075460000	0.573781090000	9.232193860000	R=1.30
50 C	-2.500292160000	3.065776750000	4.170784540000	R=2.00
51 O	-1.611887340000	2.024569380000	6.269407610000	R=1.72
52 H	0.013297770000	0.535762260000	7.754239460000	R=1.30
53 H	-0.318107400000	2.107329190000	8.589116420000	R=1.30

54 H	-2.396016390000	0.322465060000	7.185545080000	R=1.30
55 C	-1.981457150000	1.324662620000	7.439485480000	R=2.00
56 C	-0.749661700000	1.123239270000	8.307949850000	R=2.00
57 H	-2.730681060000	1.906847500000	8.022892340000	R=1.30
58 O	-3.817079360000	1.798853350000	5.660962310000	R=1.72
59 C	4.196844910000	1.244594260000	-0.865906040000	R=2.00
60 H	4.376965920000	0.769261840000	-1.852810590000	R=1.30
61 H	4.899608180000	0.722844020000	-0.179623920000	R=1.30
62 C	4.590743310000	2.745205560000	-0.886987210000	R=2.00
63 H	5.807806160000	2.679058520000	0.941945080000	R=1.30
64 H	3.733102950000	3.356887590000	-1.239019860000	R=1.30
65 C	5.725825280000	2.958748320000	-1.866178510000	R=2.00
66 H	6.260979340000	3.145431430000	-5.081948730000	R=1.30
67 C	6.584592850000	2.886356100000	-4.051780040000	R=2.00
68 O	5.432245400000	2.875909050000	-3.229233980000	R=1.72
69 H	7.625582330000	1.220403870000	-3.103116920000	R=1.30
70 O	-4.077724900000	-4.686578910000	-3.637221970000	R=1.72
71 O	6.857040830000	3.195991550000	-1.453191910000	R=1.72
72 C	-4.183683710000	-2.263984210000	-3.044441150000	R=2.00
73 C	-4.244435480000	-3.370670790000	-4.070413920000	R=2.00
74 H	7.320884300000	3.668284010000	-3.757433690000	R=1.30
75 H	-3.648233080000	-7.709036920000	-5.019555220000	R=1.30
76 H	0.457355230000	-0.378768760000	3.140368670000	R=1.30
77 H	-0.138739720000	1.833872800000	4.205950160000	R=1.30
78 H	1.453267580000	1.471710200000	2.317719510000	R=1.30
79 H	3.408447220000	-0.602643280000	0.849844370000	R=1.30
80 H	2.577022190000	1.659823830000	0.441560550000	R=1.30
81 H	-4.067779150000	-2.741598040000	-2.055677140000	R=1.30
82 H	1.243742910000	2.405409780000	-1.216566440000	R=1.30
83 H	-0.117949410000	-1.779343260000	-2.293683540000	R=1.30
84 H	-1.500898240000	-0.084324080000	-2.586737280000	R=1.30
85 H	-2.304458480000	-1.769216680000	-4.090107230000	R=1.30
86 H	-3.359562010000	-0.393865770000	-3.823975950000	R=1.30
87 H	-3.648727860000	0.429933070000	-1.450534450000	R=1.30
88 H	6.488213670000	0.747860400000	-4.427186820000	R=1.30
89 H	8.076112880000	1.513529040000	-4.824626270000	R=1.30
90 C	7.233382520000	1.504473540000	-4.101756480000	R=2.00
91 H	-2.765690060000	-6.998372690000	-3.611153040000	R=1.30
92 C	-3.989991300000	-5.592473090000	-4.717663950000	R=2.00
93 H	-3.150844520000	-5.316539270000	-5.397145450000	R=1.30
94 H	-4.946917040000	-5.613957610000	-5.286987740000	R=1.30
95 C	-3.721113630000	-6.988379470000	-4.177726960000	R=2.00
96 H	-4.547510300000	-7.301710530000	-3.505061690000	R=1.30
97 O	-4.431951240000	-3.085561640000	-5.249846000000	R=1.72
98 C	4.954064930000	3.252945660000	0.521573000000	R=2.00
99 H	5.233188680000	4.327494940000	0.477126260000	R=1.30

100 H 4.093674710000 3.158174760000 1.213332650000 R=1.30
101 C -1.691890240000 4.331858670000 4.474418700000 R=2.00
102 H -2.186636500000 4.909879850000 5.284291210000 R=1.30
103 H -0.662523250000 4.085044290000 4.804480970000 R=1.30
104 C -5.521968220000 -1.508142160000 -3.032785280000 R=2.00
105 H -5.724244450000 -1.046605060000 -4.023356580000 R=1.30
106 H -6.351035760000 -2.207240440000 -2.790431930000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0

37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 10 101 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 63 98 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 104 1.0

```
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 90 89 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 99 98 1.0
101 100 98 1.0
102 98 62 1.0
103 102 101 1.0
104 103 101 1.0
105 101 50 1.0
106 105 104 1.0
107 106 104 1.0
108 104 72 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
```

```
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

mv TAPE21 GASPHASE.t21

COSMO-RS Solvent calculation

==============================
The Molecule
==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-VII

ATOMS
1 Cr -0.278775080000 0.100558910000 0.263361200000 R=1.875
2 O -1.205685760000 -0.366235990000 1.927830880000 R=1.72
3 O 0.064054630000 1.941555830000 0.859981340000 R=1.72
4 O 1.418575590000 -0.573775630000 0.974685060000 R=1.72
5 O 0.541790710000 0.497823640000 -1.463239490000 R=1.72
6 O -0.636253630000 -1.736530860000 -0.308321000000 R=1.72
7 O -1.986450490000 0.794475830000 -0.397807860000 R=1.72
8 C -0.569235010000 0.038689390000 3.105280680000 R=2.00
9 C -0.527183950000 1.579996940000 3.196950080000 R=2.00
10 H -1.647535500000 4.982394960000 3.576285510000 R=1.30
11 C 0.527453470000 2.064323530000 2.179989980000 R=2.00
12 C -1.293778700000 -0.598934410000 4.291596170000 R=2.00
13 H -1.256603300000 -1.705245140000 4.198402570000 R=1.30
14 H -2.359894070000 -0.295431180000 4.322398610000 R=1.30
15 H -0.794006030000 -0.320509510000 5.242294770000 R=1.30
16 C 0.942760740000 3.518203190000 2.411856800000 R=2.00
17 H 1.765040930000 3.785468350000 1.715737190000 R=1.30
18 H 1.310776560000 3.659857450000 3.449796280000 R=1.30
19 H 0.100069430000 4.208898490000 2.212114510000 R=1.30
20 C 2.555870630000 -0.438223290000 0.155023230000 R=2.00
21 C 2.721558460000 0.990554780000 -0.421238460000 R=2.00
22 H -5.518468720000 -0.704890430000 -2.270013350000 R=1.30
23 C 1.621923100000 1.390254110000 -1.462705840000 R=2.00
24 C 2.663080810000 -1.570211900000 -0.874275850000 R=2.00
25 H 2.017733270000 -1.409554310000 -1.752840070000 R=1.30
26 H -4.465260510000 -1.448604980000 -0.271909510000 R=1.30
27 H 3.709149560000 -1.647795940000 -1.239188050000 R=1.30
28 C 2.102195580000 1.468038060000 -2.919482580000 R=2.00
29 H 1.239334410000 1.692746640000 -3.582714030000 R=1.30
30 H 2.536789100000 0.499812740000 -3.245432000000 R=1.30

31 H	-3.776532490000	-0.385584200000	0.971015400000	R=1.30
32 C	-1.011289300000	-1.917184940000	-1.651937830000	R=2.00
33 C	-2.096380250000	-0.897878430000	-2.116260620000	R=2.00
34 C	-2.982033780000	-1.318282940000	-3.330625880000	R=2.00
35 C	-2.835077320000	-0.160532210000	-0.978631160000	R=2.00
36 C	-1.392386200000	-3.392501560000	-1.811543810000	R=2.00
37 H	-0.533445300000	-4.026409210000	-1.503370080000	R=1.30
38 H	-1.615658200000	-3.644749920000	-2.867155430000	R=1.30
39 H	-2.247215210000	-3.656547390000	-1.157169130000	R=1.30
40 C	-3.514207160000	-1.023252900000	0.100212580000	R=2.00
41 H	-2.883976980000	-1.855806490000	0.461384990000	R=1.30
42 H	2.838678850000	2.280528000000	-3.066335080000	R=1.30
43 H	2.390146350000	-2.537739660000	-0.402247200000	R=1.30
44 C	-1.934471100000	2.243380470000	2.982958800000	R=2.00
45 H	-2.692865450000	1.471805820000	2.729491150000	R=1.30
46 H	-1.919665250000	2.909543700000	2.093816440000	R=1.30
47 C	-2.697979070000	2.240077300000	5.418943960000	R=2.00
48 H	-3.505976660000	3.418679770000	3.846145080000	R=1.30
49 H	-1.027075460000	0.573781090000	9.232193860000	R=1.30
50 C	-2.500292160000	3.065776750000	4.170784540000	R=2.00
51 O	-1.611887340000	2.024569380000	6.269407610000	R=1.72
52 H	0.013297770000	0.535762260000	7.754239460000	R=1.30
53 H	-0.318107400000	2.107329190000	8.589116420000	R=1.30
54 H	-2.396016390000	0.322465060000	7.185545080000	R=1.30
55 C	-1.981457150000	1.324662620000	7.439485480000	R=2.00
56 C	-0.749661700000	1.123239270000	8.307949850000	R=2.00
57 H	-2.730681060000	1.906847500000	8.022892340000	R=1.30
58 O	-3.817079360000	1.798853350000	5.660962310000	R=1.72
59 C	4.196844910000	1.244594260000	-0.865906040000	R=2.00
60 H	4.376965920000	0.769261840000	-1.852810590000	R=1.30
61 H	4.899608180000	0.722844020000	-0.179623920000	R=1.30
62 C	4.590743310000	2.745205560000	-0.886987210000	R=2.00
63 H	5.807806160000	2.679058520000	0.941945080000	R=1.30
64 H	3.733102950000	3.356887590000	-1.239019860000	R=1.30
65 C	5.725825280000	2.958748320000	-1.866178510000	R=2.00
66 H	6.260979340000	3.145431430000	-5.081948730000	R=1.30
67 C	6.584592850000	2.886356100000	-4.051780040000	R=2.00
68 O	5.432245400000	2.875909050000	-3.229233980000	R=1.72
69 H	7.625582330000	1.220403870000	-3.103116920000	R=1.30
70 O	-4.077724900000	-4.686578910000	-3.637221970000	R=1.72
71 O	6.857040830000	3.195991550000	-1.453191910000	R=1.72
72 C	-4.183683710000	-2.263984210000	-3.044441150000	R=2.00
73 C	-4.244435480000	-3.370670790000	-4.070413920000	R=2.00
74 H	7.320884300000	3.668284010000	-3.757433690000	R=1.30
75 H	-3.648233080000	-7.709036920000	-5.019555220000	R=1.30
76 H	0.457355230000	-0.378768760000	3.140368670000	R=1.30

77 H -0.138739720000 1.833872800000 4.205950160000 R=1.30
78 H 1.453267580000 1.471710200000 2.317719510000 R=1.30
79 H 3.408447220000 -0.602643280000 0.849844370000 R=1.30
80 H 2.577022190000 1.659823830000 0.441560550000 R=1.30
81 H -4.067779150000 -2.741598040000 -2.055677140000 R=1.30
82 H 1.243742910000 2.405409780000 -1.216566440000 R=1.30
83 H -0.117949410000 -1.779343260000 -2.293683540000 R=1.30
84 H -1.500898240000 -0.084324080000 -2.586737280000 R=1.30
85 H -2.304458480000 -1.769216680000 -4.090107230000 R=1.30
86 H -3.359562010000 -0.393865770000 -3.823975950000 R=1.30
87 H -3.648727860000 0.429933070000 -1.450534450000 R=1.30
88 H 6.488213670000 0.747860400000 -4.427186820000 R=1.30
89 H 8.076112880000 1.513529040000 -4.824626270000 R=1.30
90 C 7.233382520000 1.504473540000 -4.101756480000 R=2.00
91 H -2.765690060000 -6.998372690000 -3.611153040000 R=1.30
92 C -3.989991300000 -5.592473090000 -4.717663950000 R=2.00
93 H -3.150844520000 -5.316539270000 -5.397145450000 R=1.30
94 H -4.946917040000 -5.613957610000 -5.286987740000 R=1.30
95 C -3.721113630000 -6.988379470000 -4.177726960000 R=2.00
96 H -4.547510300000 -7.301710530000 -3.505061690000 R=1.30
97 O -4.431951240000 -3.085561640000 -5.249846000000 R=1.72
98 C 4.954064930000 3.252945660000 0.521573000000 R=2.00
99 H 5.233188680000 4.327494940000 0.477126260000 R=1.30
100 H 4.093674710000 3.158174760000 1.213332650000 R=1.30
101 C -1.691890240000 4.331858670000 4.474418700000 R=2.00
102 H -2.186636500000 4.909879850000 5.284291210000 R=1.30
103 H -0.662523250000 4.085044290000 4.804480970000 R=1.30
104 C -5.521968220000 -1.508142160000 -3.032785280000 R=2.00
105 H -5.724244450000 -1.046605060000 -4.023356580000 R=1.30
106 H -6.351035760000 -2.207240440000 -2.790431930000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0

14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 10 101 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0

60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 63 98 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 104 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 90 89 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 99 98 1.0
101 100 98 1.0
102 98 62 1.0
103 102 101 1.0
104 103 101 1.0
105 101 50 1.0

```
106 105 104 1.0
107 106 104 1.0
108 104 72 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End
```

```
ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-VIII

ATOMS
1 Cr     -0.384795260000     -0.045905740000      0.244362340000    R=1.875
2 O      -1.313780350000     -0.603588010000      1.882238260000    R=1.72
3 O      -0.157532260000      1.802686400000      0.879424840000    R=1.72
4 O       1.341088240000     -0.630231980000      0.972654570000    R=1.72
5 O       0.438246900000      0.428649610000     -1.461534210000    R=1.72
6 O      -0.618402790000     -1.891598430000     -0.368074770000    R=1.72
7 O      -2.123558260000      0.560353410000     -0.428343110000    R=1.72
8 C      -0.721442810000     -0.185345150000      3.075489880000    R=2.00
9 C      -0.781133380000      1.346780810000      3.189156650000    R=2.00
10 H     -1.876430900000      3.664930770000      4.238816310000    R=1.30
11 C      0.255645300000      1.933841540000      2.216844910000    R=2.00
12 C     -1.424423820000     -0.876480540000      4.248819750000    R=2.00
13 H     -1.324558110000     -1.977940380000      4.145842510000    R=1.30
14 H     -2.505375310000     -0.630535590000      4.281521780000    R=1.30
15 H     -0.954507340000     -0.576841600000      5.208864990000    R=1.30
16 C      0.525418530000      3.414443910000      2.498914860000    R=2.00
17 H      1.345574270000      3.775391070000      1.842157190000    R=1.30
```

18 H	0.836164230000	3.560406360000	3.555427970000	R=1.30
19 H	-0.376615920000	4.028105170000	2.294160170000	R=1.30
20 C	2.485137190000	-0.382092160000	0.188308500000	R=2.00
21 C	2.543323010000	1.067608350000	-0.355144390000	R=2.00
22 H	-4.951220480000	-1.682001000000	-2.714056270000	R=1.30
23 C	1.460449530000	1.385938360000	-1.437479370000	R=2.00
24 C	2.707354920000	-1.478138470000	-0.860355960000	R=2.00
25 H	1.988753030000	-1.420162090000	-1.693719720000	R=1.30
26 H	-4.360602570000	-1.959785960000	-0.484094860000	R=1.30
27 H	3.730248680000	-1.394128350000	-1.284265950000	R=1.30
28 C	1.992147210000	1.466767740000	-2.877530890000	R=2.00
29 H	1.144003670000	1.624785270000	-3.577913320000	R=1.30
30 H	2.498451550000	0.520952890000	-3.163650790000	R=1.30
31 H	-4.014634550000	-0.748492250000	0.777163880000	R=1.30
32 C	-0.992532140000	-2.087950920000	-1.711118040000	R=2.00
33 C	-2.083686250000	-1.085661330000	-2.190140890000	R=2.00
34 C	-2.909014230000	-1.507390540000	-3.443433240000	R=2.00
35 C	-2.897766850000	-0.424680350000	-1.059450070000	R=2.00
36 C	-1.377794990000	-3.565627970000	-1.848061370000	R=2.00
37 H	-0.525055800000	-4.197773530000	-1.519824400000	R=1.30
38 H	-1.598780740000	-3.841677490000	-2.898983680000	R=1.30
39 H	-2.242082380000	-3.808925810000	-1.197131840000	R=1.30
40 C	-3.551947530000	-1.359888940000	-0.026583360000	R=2.00
41 H	-2.841205270000	-2.058599400000	0.448408830000	R=1.30
42 H	2.687410830000	2.317386290000	-3.017461760000	R=1.30
43 H	2.612176640000	-2.476853580000	-0.384004330000	R=1.30
44 C	-2.218760040000	1.921838080000	2.958318360000	R=2.00
45 H	-2.978157430000	1.114973790000	2.878067510000	R=1.30
46 H	-2.275721130000	2.458430600000	1.987437610000	R=1.30
47 C	-2.978845850000	2.185255160000	5.337907990000	R=2.00
48 H	-3.570760410000	3.439791130000	3.710787450000	R=1.30
49 H	-1.611775220000	-7.482183890000	-6.403106020000	R=1.30
50 C	-2.661643300000	2.900845950000	4.056757010000	R=2.00
51 O	-1.969009660000	2.043423780000	6.289336050000	R=1.72
52 H	-2.348816080000	-0.522001740000	9.307591670000	R=1.30
53 H	-4.051092950000	-5.474380190000	-8.064287120000	R=1.30
54 H	-2.686634570000	0.226763880000	7.014691070000	R=1.30
55 C	-2.371702380000	1.233857660000	7.375196950000	R=2.00
56 H	1.501744130000	-0.399564130000	8.654679770000	R=1.30
57 H	-3.212514890000	1.717360090000	7.923802660000	R=1.30
58 O	-4.110908330000	1.743525100000	5.505808970000	R=1.72
59 C	3.998657220000	1.475975330000	-0.729214640000	R=2.00
60 H	4.287831270000	1.055869450000	-1.715089940000	R=1.30
61 H	4.713425490000	1.039579350000	0.002773820000	R=1.30
62 C	4.205998360000	3.000355840000	-0.688741080000	R=2.00
63 H	4.159410260000	3.345550170000	0.368095420000	R=1.30

64 H	3.407897250000	3.533140630000	-1.244306380000	R=1.30
65 C	5.532035380000	3.362880940000	-1.287520440000	R=2.00
66 H	7.089848740000	3.371080480000	-4.155274380000	R=1.30
67 C	7.070412840000	3.233664480000	-3.052682420000	R=2.00
68 O	5.711582620000	3.172744080000	-2.658438330000	R=1.72
69 O	-5.813755920000	-2.529394740000	-4.865219370000	R=1.72
70 O	-3.940597920000	-3.835004370000	-5.142402040000	R=1.72
71 O	6.403733790000	3.834814240000	-0.566222240000	R=1.72
72 C	-4.179266770000	-2.332740270000	-3.178700100000	R=2.00
73 C	-4.713770840000	-2.894345320000	-4.463439880000	R=2.00
74 H	7.597544050000	4.118252520000	-2.627439840000	R=1.30
75 H	0.229390790000	-1.542023770000	8.077981480000	R=1.30
76 H	0.328907930000	-0.537427920000	3.119419790000	R=1.30
77 H	-0.434864190000	1.599064690000	4.216423340000	R=1.30
78 H	1.222351140000	1.415123730000	2.374281860000	R=1.30
79 H	3.332683990000	-0.491189390000	0.899712950000	R=1.30
80 H	2.312802860000	1.708963910000	0.511923320000	R=1.30
81 H	-3.981476820000	-3.179439230000	-2.496766260000	R=1.30
82 H	1.011294340000	2.378410740000	-1.218385230000	R=1.30
83 H	-0.098177480000	-1.950929820000	-2.353095570000	R=1.30
84 H	-1.502045330000	-0.240826910000	-2.616284850000	R=1.30
85 H	-2.237593320000	-2.040477900000	-4.151645350000	R=1.30
86 H	-3.230307680000	-0.584720210000	-3.978538840000	R=1.30
87 H	-3.736169850000	0.124492510000	-1.540841090000	R=1.30
88 O	-0.112790790000	0.445564840000	7.676224320000	R=1.72
89 H	0.314372290000	0.153651920000	10.583205570000	R=1.30
90 H	9.915816020000	1.456716020000	-2.509593220000	R=1.30
91 H	10.075857630000	0.469322520000	-4.629022380000	R=1.30
92 C	-4.496088910000	-4.179915820000	-6.395669620000	R=2.00
93 H	-4.651213580000	-3.274182730000	-7.027078820000	R=1.30
94 H	-5.470646170000	-4.699595770000	-6.251872000000	R=1.30
95 O	7.097694340000	0.834090410000	-3.272243190000	R=1.72
96 H	7.836546990000	1.800052020000	-1.610358900000	R=1.30
97 C	7.964924860000	0.161200190000	-4.154693960000	R=2.00
98 C	9.144233320000	1.054079250000	-4.467494600000	R=2.00
99 C	9.232723910000	1.924236870000	-3.253522320000	R=2.00
100 C	7.804851960000	1.922930290000	-2.714811700000	R=2.00
101 H	9.612559070000	2.939120420000	-3.505318720000	R=1.30
102 H	7.421021860000	-0.102860560000	-5.086449560000	R=1.30
103 H	8.316047570000	-0.775978660000	-3.670023170000	R=1.30
104 H	8.923548050000	1.674285210000	-5.364486530000	R=1.30
105 C	-3.547652570000	-5.130635640000	-7.133187400000	R=2.00
106 C	-2.230826100000	-4.459100940000	-7.512155030000	R=2.00
107 C	-1.228717550000	-5.550753550000	-7.308227130000	R=2.00
108 C	-1.884426320000	-6.415789560000	-6.254233220000	R=2.00
109 O	-3.283009640000	-6.265524120000	-6.335511810000	R=1.72

110 H -2.238306590000 -4.103661450000 -8.565733750000 R=1.30
111 H -1.991014480000 -3.607372550000 -6.836624490000 R=1.30
112 H -0.246733030000 -5.155809650000 -6.967837770000 R=1.30
113 H -1.100286340000 -6.130504970000 -8.249224640000 R=1.30
114 H -1.547619440000 -6.100213640000 -5.242355660000 R=1.30
115 H -0.463589110000 -1.471468010000 10.317070550000 R=1.30
116 C -1.194070390000 1.065237990000 8.337804360000 R=2.00
117 C 0.406780280000 -0.544405030000 8.535314800000 R=2.00
118 C -0.287546130000 -0.464311930000 9.880220800000 R=2.00
119 C -1.569646260000 0.233915250000 9.555242570000 R=2.00
120 H -1.917665220000 0.869648520000 10.398549800000 R=1.30
121 H -0.863856880000 2.072719980000 8.678242800000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0

32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 105 92 1.0
54 75 117 1.0
55 55 54 1.0
56 51 47 1.0
57 120 119 1.0
58 53 105 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 81 72 1.0
68 68 65 1.0
69 95 97 1.0
70 90 99 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0

78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 69 73 2.0
90 67 68 1.0
91 70 73 1.0
92 116 119 1.0
93 88 116 1.0
94 92 93 1.0
95 92 94 1.0
96 117 88 1.0
97 101 99 1.0
98 97 98 1.0
99 98 99 1.0
100 96 100 1.0
101 100 67 1.0
102 100 95 1.0
103 100 99 1.0
104 102 97 1.0
105 103 97 1.0
106 104 98 1.0
107 91 98 1.0
108 106 107 1.0
109 107 108 1.0
110 108 109 1.0
111 109 105 1.0
112 105 106 1.0
113 110 106 1.0
114 111 106 1.0
115 112 107 1.0
116 113 107 1.0
117 114 108 1.0
118 49 108 1.0
119 56 117 1.0
120 117 118 1.0
121 118 119 1.0
122 89 118 1.0
123 115 118 1.0

```
124 52 119 1.0
125 116 55 1.0
126 121 116 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
```

```
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-VIII

ATOMS
1 Cr     -0.384795260000     -0.045905740000      0.244362340000     R=1.875
2 O      -1.313780350000     -0.603588010000      1.882238260000     R=1.72
3 O      -0.157532260000      1.802686400000      0.879424840000     R=1.72
4 O       1.341088240000     -0.630231980000      0.972654570000     R=1.72
5 O       0.438246900000      0.428649610000     -1.461534210000     R=1.72
6 O      -0.618402790000     -1.891598430000     -0.368074770000     R=1.72
7 O      -2.123558260000      0.560353410000     -0.428343110000     R=1.72
```

8 C	-0.721442810000	-0.185345150000	3.075489880000	R=2.00
9 C	-0.781133380000	1.346780810000	3.189156650000	R=2.00
10 H	-1.876430900000	3.664930770000	4.238816310000	R=1.30
11 C	0.255645300000	1.933841540000	2.216844910000	R=2.00
12 C	-1.424423820000	-0.876480540000	4.248819750000	R=2.00
13 H	-1.324558110000	-1.977940380000	4.145842510000	R=1.30
14 H	-2.505375310000	-0.630535590000	4.281521780000	R=1.30
15 H	-0.954507340000	-0.576841600000	5.208864990000	R=1.30
16 C	0.525418530000	3.414443910000	2.498914860000	R=2.00
17 H	1.345574270000	3.775391070000	1.842157190000	R=1.30
18 H	0.836164230000	3.560406360000	3.555427970000	R=1.30
19 H	-0.376615920000	4.028105170000	2.294160170000	R=1.30
20 C	2.485137190000	-0.382092160000	0.188308500000	R=2.00
21 C	2.543323010000	1.067608350000	-0.355144390000	R=2.00
22 H	-4.951220480000	-1.682001000000	-2.714056270000	R=1.30
23 C	1.460449530000	1.385938360000	-1.437479370000	R=2.00
24 C	2.707354920000	-1.478138470000	-0.860355960000	R=2.00
25 H	1.988753030000	-1.420162090000	-1.693719720000	R=1.30
26 H	-4.360602570000	-1.959785960000	-0.484094860000	R=1.30
27 H	3.730248680000	-1.394128350000	-1.284265950000	R=1.30
28 C	1.992147210000	1.466767740000	-2.877530890000	R=2.00
29 H	1.144003670000	1.624785270000	-3.577913320000	R=1.30
30 H	2.498451550000	0.520952890000	-3.163650790000	R=1.30
31 H	-4.014634550000	-0.748492250000	0.777163880000	R=1.30
32 C	-0.992532140000	-2.087950920000	-1.711118040000	R=2.00
33 C	-2.083686250000	-1.085661330000	-2.190140890000	R=2.00
34 C	-2.909014230000	-1.507390540000	-3.443433240000	R=2.00
35 C	-2.897766850000	-0.424680350000	-1.059450070000	R=2.00
36 C	-1.377794990000	-3.565627970000	-1.848061370000	R=2.00
37 H	-0.525055800000	-4.197773530000	-1.519824400000	R=1.30
38 H	-1.598780740000	-3.841677490000	-2.898983680000	R=1.30
39 H	-2.242082380000	-3.808925810000	-1.197131840000	R=1.30
40 C	-3.551947530000	-1.359888940000	-0.026583360000	R=2.00
41 H	-2.841205270000	-2.058599400000	0.448408830000	R=1.30
42 H	2.687410830000	2.317386290000	-3.017461760000	R=1.30
43 H	2.612176640000	-2.476853580000	-0.384004330000	R=1.30
44 C	-2.218760040000	1.921838080000	2.958318360000	R=2.00
45 H	-2.978157430000	1.114973790000	2.878067510000	R=1.30
46 H	-2.275721130000	2.458430600000	1.987437610000	R=1.30
47 C	-2.978845850000	2.185255160000	5.337907990000	R=2.00
48 H	-3.570760410000	3.439791130000	3.710787450000	R=1.30
49 H	-1.611775220000	-7.482183890000	-6.403106020000	R=1.30
50 C	-2.661643300000	2.900845950000	4.056757010000	R=2.00
51 O	-1.969009660000	2.043423780000	6.289336050000	R=1.72
52 H	-2.348816080000	-0.522001740000	9.307591670000	R=1.30
53 H	-4.051092950000	-5.474380190000	-8.064287120000	R=1.30

54 H	-2.686634570000	0.226763880000	7.014691070000	R=1.30
55 C	-2.371702380000	1.233857660000	7.375196950000	R=2.00
56 H	1.501744130000	-0.399564130000	8.654679770000	R=1.30
57 H	-3.212514890000	1.717360090000	7.923802660000	R=1.30
58 O	-4.110908330000	1.743525100000	5.505808970000	R=1.72
59 C	3.998657220000	1.475975330000	-0.729214640000	R=2.00
60 H	4.287831270000	1.055869450000	-1.715089940000	R=1.30
61 H	4.713425490000	1.039579350000	0.002773820000	R=1.30
62 C	4.205998360000	3.000355840000	-0.688741080000	R=2.00
63 H	4.159410260000	3.345550170000	0.368095420000	R=1.30
64 H	3.407897250000	3.533140630000	-1.244306380000	R=1.30
65 C	5.532035380000	3.362880940000	-1.287520440000	R=2.00
66 H	7.089848740000	3.371080480000	-4.155274380000	R=1.30
67 C	7.070412840000	3.233664480000	-3.052682420000	R=2.00
68 O	5.711582620000	3.172744080000	-2.658438330000	R=1.72
69 O	-5.813755920000	-2.529394740000	-4.865219370000	R=1.72
70 O	-3.940597920000	-3.835004370000	-5.142402040000	R=1.72
71 O	6.403733790000	3.834814240000	-0.566222240000	R=1.72
72 C	-4.179266770000	-2.332740270000	-3.178700100000	R=2.00
73 C	-4.713770840000	-2.894345320000	-4.463439880000	R=2.00
74 H	7.597544050000	4.118252520000	-2.627439840000	R=1.30
75 H	0.229390790000	-1.542023770000	8.077981480000	R=1.30
76 H	0.328907930000	-0.537427920000	3.119419790000	R=1.30
77 H	-0.434864190000	1.599064690000	4.216423340000	R=1.30
78 H	1.222351140000	1.415123730000	2.374281860000	R=1.30
79 H	3.332683990000	-0.491189390000	0.899712950000	R=1.30
80 H	2.312802860000	1.708963910000	0.511923320000	R=1.30
81 H	-3.981476820000	-3.179439230000	-2.496766260000	R=1.30
82 H	1.011294340000	2.378410740000	-1.218385230000	R=1.30
83 H	-0.098177480000	-1.950929820000	-2.353095570000	R=1.30
84 H	-1.502045330000	-0.240826910000	-2.616284850000	R=1.30
85 H	-2.237593320000	-2.040477900000	-4.151645350000	R=1.30
86 H	-3.230307680000	-0.584720210000	-3.978538840000	R=1.30
87 H	-3.736169850000	0.124492510000	-1.540841090000	R=1.30
88 O	-0.112790790000	0.445564840000	7.676224320000	R=1.72
89 H	0.314372290000	0.153651920000	10.583205570000	R=1.30
90 H	9.915816020000	1.456716020000	-2.509593220000	R=1.30
91 H	10.075857630000	0.469322520000	-4.629022380000	R=1.30
92 C	-4.496088910000	-4.179915820000	-6.395669620000	R=2.00
93 H	-4.651213580000	-3.274182730000	-7.027078820000	R=1.30
94 H	-5.470646170000	-4.699595770000	-6.251872000000	R=1.30
95 O	7.097694340000	0.834090410000	-3.272243190000	R=1.72
96 H	7.836546990000	1.800052020000	-1.610358900000	R=1.30
97 C	7.964924860000	0.161200190000	-4.154693960000	R=2.00
98 C	9.144233320000	1.054079250000	-4.467494600000	R=2.00
99 C	9.232723910000	1.924236870000	-3.253522320000	R=2.00

100 C 7.804851960000 1.922930290000 -2.714811700000 R=2.00
101 H 9.612559070000 2.939120420000 -3.505318720000 R=1.30
102 H 7.421021860000 -0.102860560000 -5.086449560000 R=1.30
103 H 8.316047570000 -0.775978660000 -3.670023170000 R=1.30
104 H 8.923548050000 1.674285210000 -5.364486530000 R=1.30
105 C -3.547652570000 -5.130635640000 -7.133187400000 R=2.00
106 C -2.230826100000 -4.459100940000 -7.512155030000 R=2.00
107 C -1.228717550000 -5.550753550000 -7.308227130000 R=2.00
108 C -1.884426320000 -6.415789560000 -6.254233220000 R=2.00
109 O -3.283009640000 -6.265524120000 -6.335511810000 R=1.72
110 H -2.238306590000 -4.103661450000 -8.565733750000 R=1.30
111 H -1.991014480000 -3.607372550000 -6.836624490000 R=1.30
112 H -0.246733030000 -5.155809650000 -6.967837770000 R=1.30
113 H -1.100286340000 -6.130504970000 -8.249224640000 R=1.30
114 H -1.547619440000 -6.100213640000 -5.242355660000 R=1.30
115 H -0.463589110000 -1.471468010000 10.317070550000 R=1.30
116 C -1.194070390000 1.065237990000 8.337804360000 R=2.00
117 C 0.406780280000 -0.544405030000 8.535314800000 R=2.00
118 C -0.287546130000 -0.464311930000 9.880220800000 R=2.00
119 C -1.569646260000 0.233915250000 9.555242570000 R=2.00
120 H -1.917665220000 0.869648520000 10.398549800000 R=1.30
121 H -0.863856880000 2.072719980000 8.678242800000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0

22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 105 92 1.0
54 75 117 1.0
55 55 54 1.0
56 51 47 1.0
57 120 119 1.0
58 53 105 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 81 72 1.0

68 68 65 1.0
69 95 97 1.0
70 90 99 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 69 73 2.0
90 67 68 1.0
91 70 73 1.0
92 116 119 1.0
93 88 116 1.0
94 92 93 1.0
95 92 94 1.0
96 117 88 1.0
97 101 99 1.0
98 97 98 1.0
99 98 99 1.0
100 96 100 1.0
101 100 67 1.0
102 100 95 1.0
103 100 99 1.0
104 102 97 1.0
105 103 97 1.0
106 104 98 1.0
107 91 98 1.0
108 106 107 1.0
109 107 108 1.0
110 108 109 1.0
111 109 105 1.0
112 105 106 1.0
113 110 106 1.0

```
114 111 106 1.0
115 112 107 1.0
116 113 107 1.0
117 114 108 1.0
118 49 108 1.0
119 56 117 1.0
120 117 118 1.0
121 118 119 1.0
122 89 118 1.0
123 115 118 1.0
124 52 119 1.0
125 116 55 1.0
126 121 116 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
```

```
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-IX

ATOMS
1 Cr     -0.416229660000     -0.261169180000      0.462879750000     R=1.875
2 O      -1.332286570000     -0.485379880000      2.185521120000     R=1.72
3 O      -0.096273160000      1.656022570000      0.768487810000     R=1.72
4 O       1.298667190000     -0.791386750000      1.255267110000     R=1.72
5 O       0.389880270000     -0.123643060000     -1.310160880000     R=1.72
6 O      -0.742473940000     -2.171410450000      0.182148460000     R=1.72
7 O      -2.142222190000      0.299553570000     -0.280387530000     R=1.72
```

8 C	-0.691236260000	0.097639170000	3.280858130000	R=2.00
9 C	-0.675109340000	1.628019030000	3.134167390000	R=2.00
10 H	-1.637840740000	4.134459590000	3.819743640000	R=1.30
11 C	0.359208040000	1.991128220000	2.055686640000	R=2.00
12 C	-1.396673200000	-0.348655010000	4.566239460000	R=2.00
13 H	-1.341537860000	-1.454452560000	4.655809300000	R=1.30
14 H	-2.466689310000	-0.056875710000	4.568406590000	R=1.30
15 H	-0.897315910000	0.094593490000	5.453858950000	R=1.30
16 C	0.702910150000	3.483185620000	2.076865580000	R=2.00
17 H	1.517435350000	3.688233190000	1.349708070000	R=1.30
18 H	1.052594250000	3.788832170000	3.086018640000	R=1.30
19 H	-0.176903460000	4.097518110000	1.792841100000	R=1.30
20 C	2.433962350000	-0.738835940000	0.422183960000	R=2.00
21 C	2.547238720000	0.591613070000	-0.363963280000	R=2.00
22 H	-5.103589280000	-2.170180620000	-2.149273450000	R=1.30
23 C	1.451996870000	0.776090350000	-1.464977030000	R=2.00
24 C	2.580870290000	-2.008079870000	-0.425229410000	R=2.00
25 H	1.857921180000	-2.050471730000	-1.255699520000	R=1.30
26 H	-4.483625270000	-2.093691240000	0.106506610000	R=1.30
27 H	3.601690160000	-2.056035350000	-0.859610840000	R=1.30
28 C	1.948800880000	0.591961050000	-2.907913470000	R=2.00
29 H	1.090389480000	0.673442060000	-3.608918050000	R=1.30
30 H	2.403768730000	-0.411881320000	-3.042242790000	R=1.30
31 H	-4.077549870000	-0.697396220000	1.138320440000	R=1.30
32 C	-1.149505950000	-2.578612460000	-1.102310450000	R=2.00
33 C	-2.201396560000	-1.622578620000	-1.737143630000	R=2.00
34 C	-3.060755080000	-2.213216860000	-2.895202950000	R=2.00
35 C	-2.968316740000	-0.741751750000	-0.730158060000	R=2.00
36 C	-1.605665050000	-4.036772050000	-0.976157350000	R=2.00
37 H	-0.777964590000	-4.643403980000	-0.550232340000	R=1.30
38 H	-1.857140690000	-4.479391700000	-1.961088190000	R=1.30
39 H	-2.469429840000	-4.120825030000	-0.285692620000	R=1.30
40 C	-3.647552890000	-1.456842290000	0.451126710000	R=2.00
41 H	-2.958623790000	-2.089662510000	1.037720040000	R=1.30
42 H	2.677695620000	1.372620570000	-3.200439220000	R=1.30
43 H	2.435280830000	-2.904577300000	0.213897920000	R=1.30
44 C	-2.090243730000	2.229283540000	2.841215750000	R=2.00
45 H	-2.887522030000	1.458039250000	2.901921960000	R=1.30
46 H	-2.146949040000	2.610317420000	1.799361960000	R=1.30
47 C	-2.765950250000	2.898799410000	5.166915020000	R=2.00
48 H	-3.355661070000	3.906160910000	3.375295560000	R=1.30
49 H	-2.067986860000	4.217855730000	9.623813030000	R=1.30
50 C	-2.459251440000	3.387783570000	3.780680120000	R=2.00
51 O	-1.734697340000	2.867577500000	6.105679440000	R=1.72
52 H	-0.181045300000	1.642426220000	7.861634150000	R=1.30
53 H	-1.275390000000	1.791611600000	9.258996460000	R=1.30

54 H	-2.519578500000	1.278425640000	7.201069680000	R=1.30
55 C	-2.154849040000	2.322042210000	7.339701010000	R=2.00
56 C	-0.971716830000	2.284984390000	8.304714870000	R=2.00
57 H	-2.965928340000	2.940226350000	7.786158100000	R=1.30
58 O	-3.907121270000	2.531289980000	5.426850470000	R=1.72
59 C	4.010603170000	0.852720880000	-0.828450620000	R=2.00
60 H	4.251666710000	0.259925600000	-1.735295930000	R=1.30
61 H	4.722053630000	0.506206370000	-0.046842960000	R=1.30
62 C	4.295887550000	2.348768290000	-1.047557190000	R=2.00
63 H	4.281572930000	2.868975330000	-0.063956370000	R=1.30
64 H	3.518015560000	2.821619940000	-1.680509060000	R=1.30
65 C	5.630741940000	2.536455620000	-1.705124940000	R=2.00
66 H	7.115181810000	2.110708920000	-4.578740540000	R=1.30
67 C	7.127928320000	2.142493010000	-3.468532820000	R=2.00
68 O	5.783817310000	2.106744020000	-3.025013830000	R=1.72
69 H	7.910657870000	0.878585590000	-1.855785330000	R=1.30
70 O	-4.221503410000	-4.796362190000	-4.117433150000	R=1.72
71 O	6.535073780000	3.072564430000	-1.074189020000	R=1.72
72 C	-4.361715330000	-2.925032240000	-2.489002710000	R=2.00
73 C	-4.921873560000	-3.682259070000	-3.657036190000	R=2.00
74 H	7.643182860000	3.092066500000	-3.199730660000	R=1.30
75 H	-4.153048490000	-6.715214670000	-6.880377450000	R=1.30
76 H	0.342145780000	-0.294242710000	3.366979100000	R=1.30
77 H	-0.286291950000	2.031002780000	4.096006880000	R=1.30
78 H	1.305357120000	1.459985740000	2.280705750000	R=1.30
79 H	3.291814070000	-0.766529110000	1.129048860000	R=1.30
80 H	2.370046250000	1.382856050000	0.383836350000	R=1.30
81 H	-4.196828410000	-3.644416710000	-1.666595910000	R=1.30
82 H	1.051660710000	1.811010030000	-1.407083750000	R=1.30
83 H	-0.261856230000	-2.598661670000	-1.767276270000	R=1.30
84 H	-1.590288230000	-0.890339520000	-2.305667250000	R=1.30
85 H	-2.421714490000	-2.887828690000	-3.506246310000	R=1.30
86 H	-3.348871300000	-1.381343740000	-3.577871500000	R=1.30
87 H	-3.788719020000	-0.244727130000	-1.292489660000	R=1.30
88 H	7.356220350000	0.005579010000	-3.303859520000	R=1.30
89 H	-0.605140260000	3.643916690000	10.555781120000	R=1.30
90 C	7.900550220000	0.914894610000	-2.970991690000	R=2.00
91 H	-0.585983060000	5.223728730000	9.706629500000	R=1.30
92 C	-4.685565770000	-5.227595120000	-5.380146730000	R=2.00
93 H	-4.648849800000	-4.396172560000	-6.120472380000	R=1.30
94 H	-5.730386640000	-5.604872350000	-5.301232870000	R=1.30
95 C	-3.800824150000	-6.368937910000	-5.879449570000	R=2.00
96 H	-3.926264740000	-7.231600340000	-5.190912180000	R=1.30
97 O	-5.984290840000	-3.321203290000	-4.152302070000	R=1.72
98 O	9.192267610000	0.881672940000	-3.548072300000	R=1.72
99 C	10.136675150000	1.455798650000	-2.671282060000	R=2.00

100 H 10.263593180000 0.827046680000 -1.762528860000 R=1.30
101 H 11.117055450000 1.502459170000 -3.188117390000 R=1.30
102 H 9.854769120000 2.494022730000 -2.387865090000 R=1.30
103 O -2.436316690000 -5.990575210000 -5.857268320000 R=1.72
104 C -2.038082280000 -5.504300410000 -7.119967460000 R=2.00
105 H -0.991486230000 -5.144083730000 -7.045605690000 R=1.30
106 H -2.062445320000 -6.314757550000 -7.881346310000 R=1.30
107 H -2.666393320000 -4.646201070000 -7.444970670000 R=1.30
108 O -0.433012500000 3.582668110000 8.480606440000 R=1.72
109 C -0.956454270000 4.179817910000 9.646594970000 R=2.00
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0

34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 108 56 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 91 109 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0

```
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 89 109 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 100 99 1.0
101 101 99 1.0
102 102 99 1.0
103 99 98 1.0
104 103 95 1.0
105 105 104 1.0
106 106 104 1.0
107 107 104 1.0
108 104 103 1.0
109 109 108 1.0
110 49 109 1.0
111 98 90 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0
```

```
UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
```

"$ADFBIN/cpkf" TAPE21 COSKF COSMO

mv TAPE21 GASPHASE.t21

COSMO-RS Solvent calculation

==============================
The Molecule
==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-IX

ATOMS
1 Cr -0.416229660000 -0.261169180000 0.462879750000 R=1.875
2 O -1.332286570000 -0.485379880000 2.185521120000 R=1.72
3 O -0.096273160000 1.656022570000 0.768487810000 R=1.72
4 O 1.298667190000 -0.791386750000 1.255267110000 R=1.72
5 O 0.389880270000 -0.123643060000 -1.310160880000 R=1.72
6 O -0.742473940000 -2.171410450000 0.182148460000 R=1.72
7 O -2.142222190000 0.299553570000 -0.280387530000 R=1.72
8 C -0.691236260000 0.097639170000 3.280858130000 R=2.00
9 C -0.675109340000 1.628019030000 3.134167390000 R=2.00
10 H -1.637840740000 4.134459590000 3.819743640000 R=1.30
11 C 0.359208040000 1.991128220000 2.055686640000 R=2.00
12 C -1.396673200000 -0.348655010000 4.566239460000 R=2.00
13 H -1.341537860000 -1.454452560000 4.655809300000 R=1.30
14 H -2.466689310000 -0.056875710000 4.568406590000 R=1.30
15 H -0.897315910000 0.094593490000 5.453858950000 R=1.30
16 C 0.702910150000 3.483185620000 2.076865580000 R=2.00
17 H 1.517435350000 3.688233190000 1.349708070000 R=1.30
18 H 1.052594250000 3.788832170000 3.086018640000 R=1.30
19 H -0.176903460000 4.097518110000 1.792841100000 R=1.30
20 C 2.433962350000 -0.738835940000 0.422183960000 R=2.00
21 C 2.547238720000 0.591613070000 -0.363963280000 R=2.00
22 H -5.103589280000 -2.170180620000 -2.149273450000 R=1.30
23 C 1.451996870000 0.776090350000 -1.464977030000 R=2.00
24 C 2.580870290000 -2.008079870000 -0.425229410000 R=2.00

25 H	1.857921180000	-2.050471730000	-1.255699520000	R=1.30
26 H	-4.483625270000	-2.093691240000	0.106506610000	R=1.30
27 H	3.601690160000	-2.056035350000	-0.859610840000	R=1.30
28 C	1.948800880000	0.591961050000	-2.907913470000	R=2.00
29 H	1.090389480000	0.673442060000	-3.608918050000	R=1.30
30 H	2.403768730000	-0.411881320000	-3.042242790000	R=1.30
31 H	-4.077549870000	-0.697396220000	1.138320440000	R=1.30
32 C	-1.149505950000	-2.578612460000	-1.102310450000	R=2.00
33 C	-2.201396560000	-1.622578620000	-1.737143630000	R=2.00
34 C	-3.060755080000	-2.213216860000	-2.895202950000	R=2.00
35 C	-2.968316740000	-0.741751750000	-0.730158060000	R=2.00
36 C	-1.605665050000	-4.036772050000	-0.976157350000	R=2.00
37 H	-0.777964590000	-4.643403980000	-0.550232340000	R=1.30
38 H	-1.857140690000	-4.479391700000	-1.961088190000	R=1.30
39 H	-2.469429840000	-4.120825030000	-0.285692620000	R=1.30
40 C	-3.647552890000	-1.456842290000	0.451126710000	R=2.00
41 H	-2.958623790000	-2.089662510000	1.037720040000	R=1.30
42 H	2.677695620000	1.372620570000	-3.200439220000	R=1.30
43 H	2.435280830000	-2.904577300000	0.213897920000	R=1.30
44 C	-2.090243730000	2.229283540000	2.841215750000	R=2.00
45 H	-2.887522030000	1.458039250000	2.901921960000	R=1.30
46 H	-2.146949040000	2.610317420000	1.799361960000	R=1.30
47 C	-2.765950250000	2.898799410000	5.166915020000	R=2.00
48 H	-3.355661070000	3.906160910000	3.375295560000	R=1.30
49 H	-2.067986860000	4.217855730000	9.623813030000	R=1.30
50 C	-2.459251440000	3.387783570000	3.780680120000	R=2.00
51 O	-1.734697340000	2.867577500000	6.105679440000	R=1.72
52 H	-0.181045300000	1.642426220000	7.861634150000	R=1.30
53 H	-1.275390000000	1.791611600000	9.258996460000	R=1.30
54 H	-2.519578500000	1.278425640000	7.201069680000	R=1.30
55 C	-2.154849040000	2.322042210000	7.339701010000	R=2.00
56 C	-0.971716830000	2.284984390000	8.304714870000	R=2.00
57 H	-2.965928340000	2.940226350000	7.786158100000	R=1.30
58 O	-3.907121270000	2.531289980000	5.426850470000	R=1.72
59 C	4.010603170000	0.852720880000	-0.828450620000	R=2.00
60 H	4.251666710000	0.259925600000	-1.735295930000	R=1.30
61 H	4.722053630000	0.506206370000	-0.046842960000	R=1.30
62 C	4.295887550000	2.348768290000	-1.047557190000	R=2.00
63 H	4.281572930000	2.868975330000	-0.063956370000	R=1.30
64 H	3.518015560000	2.821619940000	-1.680509060000	R=1.30
65 C	5.630741940000	2.536455620000	-1.705124940000	R=2.00
66 H	7.115181810000	2.110708920000	-4.578740540000	R=1.30
67 C	7.127928320000	2.142493010000	-3.468532820000	R=2.00
68 O	5.783817310000	2.106744020000	-3.025013830000	R=1.72
69 H	7.910657870000	0.878585590000	-1.855785330000	R=1.30
70 O	-4.221503410000	-4.796362190000	-4.117433150000	R=1.72

71 O 6.535073780000 3.072564430000 -1.074189020000 R=1.72
72 C -4.361715330000 -2.925032240000 -2.489002710000 R=2.00
73 C -4.921873560000 -3.682259070000 -3.657036190000 R=2.00
74 H 7.643182860000 3.092066500000 -3.199730660000 R=1.30
75 H -4.153048490000 -6.715214670000 -6.880377450000 R=1.30
76 H 0.342145780000 -0.294242710000 3.366979100000 R=1.30
77 H -0.286291950000 2.031002780000 4.096006880000 R=1.30
78 H 1.305357120000 1.459985740000 2.280705750000 R=1.30
79 H 3.291814070000 -0.766529110000 1.129048860000 R=1.30
80 H 2.370046250000 1.382856050000 0.383836350000 R=1.30
81 H -4.196828410000 -3.644416710000 -1.666595910000 R=1.30
82 H 1.051660710000 1.811010030000 -1.407083750000 R=1.30
83 H -0.261856230000 -2.598661670000 -1.767276270000 R=1.30
84 H -1.590288230000 -0.890339520000 -2.305667250000 R=1.30
85 H -2.421714490000 -2.887828690000 -3.506246310000 R=1.30
86 H -3.348871300000 -1.381343740000 -3.577871500000 R=1.30
87 H -3.788719020000 -0.244727130000 -1.292489660000 R=1.30
88 H 7.356220350000 0.005579010000 -3.303859520000 R=1.30
89 H -0.605140260000 3.643916690000 10.555781120000 R=1.30
90 C 7.900550220000 0.914894610000 -2.970991690000 R=2.00
91 H -0.585983060000 5.223728730000 9.706629500000 R=1.30
92 C -4.685565770000 -5.227595120000 -5.380146730000 R=2.00
93 H -4.648849800000 -4.396172560000 -6.120472380000 R=1.30
94 H -5.730386640000 -5.604872350000 -5.301232870000 R=1.30
95 C -3.800824150000 -6.368937910000 -5.879449570000 R=2.00
96 H -3.926264740000 -7.231600340000 -5.190912180000 R=1.30
97 O -5.984290840000 -3.321203290000 -4.152302070000 R=1.72
98 O 9.192267610000 0.881672940000 -3.548072300000 R=1.72
99 C 10.136675150000 1.455798650000 -2.671282060000 R=2.00
100 H 10.263593180000 0.827046680000 -1.762528860000 R=1.30
101 H 11.117055450000 1.502459170000 -3.188117390000 R=1.30
102 H 9.854769120000 2.494022730000 -2.387865090000 R=1.30
103 O -2.436316690000 -5.990575210000 -5.857268320000 R=1.72
104 C -2.038082280000 -5.504300410000 -7.119967460000 R=2.00
105 H -0.991486230000 -5.144083730000 -7.045605690000 R=1.30
106 H -2.062445320000 -6.314757550000 -7.881346310000 R=1.30
107 H -2.666393320000 -4.646201070000 -7.444970670000 R=1.30
108 O -0.433012500000 3.582668110000 8.480606440000 R=1.72
109 C -0.956454270000 4.179817910000 9.646594970000 R=2.00
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0

5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 50 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0

51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 108 56 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 56 53 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 62 63 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 91 109 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 22 72 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 89 109 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 95 96 1.0

```
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 100 99 1.0
101 101 99 1.0
102 102 99 1.0
103 99 98 1.0
104 103 95 1.0
105 105 104 1.0
106 106 104 1.0
107 107 104 1.0
108 104 103 1.0
109 109 108 1.0
110 49 109 1.0
111 98 90 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.0E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21
```

```
SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-X

ATOMS
1 Cr     -0.481724850000     -0.054489550000      0.496061880000     R=1.875
2 O      -1.425382660000     -0.313682690000      2.197771230000     R=1.72
3 O      -0.318681110000      1.885508040000      0.773969320000     R=1.72
4 O       1.247155560000     -0.439579310000      1.341938280000     R=1.72
5 O       0.360836170000      0.110834720000     -1.257606930000     R=1.72
```

6 O	-0.656341180000	-1.989802170000	0.245633060000	R=1.72
7 O	-2.221165650000	0.364643470000	-0.303513900000	R=1.72
8 C	-0.850421090000	0.325028140000	3.298194070000	R=2.00
9 C	-0.941558450000	1.851010120000	3.131339270000	R=2.00
10 H	-2.588154680000	-9.020788830000	-1.622233690000	R=1.30
11 C	0.079642490000	2.277878020000	2.063665300000	R=2.00
12 C	-1.545616650000	-0.164416070000	4.574219450000	R=2.00
13 H	-1.415449430000	-1.263490240000	4.668684060000	R=1.30
14 H	-2.633043570000	0.051343580000	4.562094250000	R=1.30
15 H	-1.094248750000	0.310932780000	5.468570240000	R=1.30
16 C	0.303965460000	3.792435700000	2.060051680000	R=2.00
17 H	1.148337810000	4.042301380000	1.382705890000	R=1.30
18 H	0.555890830000	4.155223920000	3.078873720000	R=1.30
19 H	-0.599982570000	4.324011980000	1.695987290000	R=1.30
20 C	2.397860810000	-0.310179310000	0.538727770000	R=2.00
21 C	2.427783210000	1.012203110000	-0.267968720000	R=2.00
22 O	-4.129645850000	-11.172004930000	-1.667324310000	R=1.72
23 C	1.349616100000	1.092970600000	-1.398692990000	R=2.00
24 C	2.665717300000	-1.576927560000	-0.282502450000	R=2.00
25 H	1.958013360000	-1.698965220000	-1.118719240000	R=1.30
26 H	-4.400032380000	-2.172735980000	0.099555820000	R=1.30
27 H	3.692077670000	-1.543733810000	-0.704939320000	R=1.30
28 C	1.897967190000	0.936145340000	-2.825841530000	R=2.00
29 H	1.055206930000	0.943260840000	-3.550072480000	R=1.30
30 H	2.434316830000	-0.029787960000	-2.936640420000	R=1.30
31 H	-4.100655640000	-0.733159800000	1.106601500000	R=1.30
32 C	-1.010764270000	-2.455066010000	-1.035087650000	R=2.00
33 C	-2.110094780000	-1.587945660000	-1.714813750000	R=2.00
34 C	-2.902004600000	-2.264471880000	-2.875597740000	R=2.00
35 C	-2.960160340000	-0.742685420000	-0.743855790000	R=2.00
36 C	-1.376243250000	-3.936501330000	-0.879039960000	R=2.00
37 H	-0.524819350000	-4.476409770000	-0.412067630000	R=1.30
38 H	-1.569520130000	-4.422294610000	-1.856690060000	R=1.30
39 H	-2.254224070000	-4.058178290000	-0.212728530000	R=1.30
40 C	-3.611698950000	-1.476779090000	0.441873770000	R=2.00
41 H	-2.893569080000	-2.052431350000	1.051780800000	R=1.30
42 H	2.570788350000	1.770770390000	-3.105713040000	R=1.30
43 H	2.591274320000	-2.470400730000	0.372901060000	R=1.30
44 C	-2.393380930000	2.348357910000	2.825791490000	R=2.00
45 H	-3.143278360000	1.540387070000	2.956587540000	R=1.30
46 H	-2.483085400000	2.643219730000	1.758534440000	R=1.30
47 C	-3.098565510000	3.167186090000	5.112366700000	R=2.00
48 H	-3.750793100000	3.980837210000	3.238683990000	R=1.30
49 H	-1.438381170000	2.262721300000	9.174972650000	R=1.30
50 C	-2.825890380000	3.551263140000	3.682960770000	R=2.00
51 O	-2.014375580000	2.902525780000	5.946399920000	R=1.72

52 H	-0.758846100000	1.372957700000	7.769542510000	R=1.30
53 H	1.315316720000	2.076849140000	8.455863470000	R=1.30
54 H	-3.089439540000	1.799311900000	7.352520920000	R=1.30
55 C	-2.399330320000	2.671379330000	7.284888060000	R=2.00
56 C	-1.152553130000	2.361178690000	8.105915640000	R=2.00
57 H	-2.891662430000	3.575883350000	7.709363560000	R=1.30
58 O	-4.258774510000	3.122159580000	5.507215520000	R=1.72
59 C	3.877239560000	1.381784210000	-0.701473310000	R=2.00
60 H	4.186987760000	0.798297550000	-1.593741260000	R=1.30
61 H	4.594924000000	1.104270770000	0.101595560000	R=1.30
62 C	4.045047120000	2.893151970000	-0.940073750000	R=2.00
63 H	-6.036519830000	-11.747532340000	-2.277700910000	R=1.30
64 H	3.188331850000	3.302479010000	-1.514606110000	R=1.30
65 C	5.314636660000	3.175734050000	-1.686103420000	R=2.00
66 H	6.358085880000	4.311168130000	-4.557396240000	R=1.30
67 C	6.473747010000	3.648367230000	-3.673446790000	R=2.00
68 O	5.221540680000	3.595812560000	-3.014363170000	R=1.72
69 H	7.053110940000	1.596849750000	-3.298875340000	R=1.30
70 O	-4.011498000000	-4.993707900000	-3.983462100000	R=1.72
71 O	6.387579520000	3.012166150000	-1.115593400000	R=1.72
72 C	-4.176657130000	-3.025123600000	-2.477310440000	R=2.00
73 C	-4.690007160000	-3.825542250000	-3.637393300000	R=2.00
74 H	7.274401190000	4.109377540000	-3.050915350000	R=1.30
75 H	-4.213563300000	-7.351338750000	-6.341594600000	R=1.30
76 H	0.207037140000	0.012487060000	3.409827450000	R=1.30
77 H	-0.587066890000	2.290419310000	4.084232760000	R=1.30
78 H	1.058468660000	1.826907130000	2.319802080000	R=1.30
79 H	3.235849120000	-0.258408150000	1.267883000000	R=1.30
80 H	2.172211170000	1.799662160000	0.460539180000	R=1.30
81 H	-3.992542120000	-3.721000800000	-1.638029780000	R=1.30
82 H	0.864521130000	2.091981450000	-1.365498690000	R=1.30
83 H	-0.109294130000	-2.432950600000	-1.681834350000	R=1.30
84 H	-1.536463340000	-0.827700660000	-2.286020010000	R=1.30
85 H	-2.215647980000	-2.927878410000	-3.445812900000	R=1.30
86 H	-3.212380860000	-1.472481100000	-3.594959590000	R=1.30
87 H	-3.801136000000	-0.317347820000	-1.333638060000	R=1.30
88 H	6.050905500000	1.856024600000	-4.792560320000	R=1.30
89 H	9.510105910000	1.944775140000	-7.110218300000	R=1.30
90 C	6.884304840000	2.263240890000	-4.174657580000	R=2.00
91 H	-2.750843590000	-6.742005130000	-5.522497770000	R=1.30
92 C	-4.569691740000	-5.619259490000	-5.120300570000	R=2.00
93 H	-4.449511760000	-4.965214540000	-6.013643440000	R=1.30
94 H	-5.650240300000	-5.844484620000	-4.964610860000	R=1.30
95 C	-3.842007800000	-6.934618820000	-5.381452720000	R=2.00
96 H	-2.201193610000	-8.545742850000	-4.063182670000	R=1.30
97 O	-5.692003860000	-3.441454410000	-4.231753030000	R=1.72

98 H 4.066863800000 3.424315530000 0.036651360000 R=1.30
99 H -5.947837650000 -10.191335660000 -1.325108410000 R=1.30
100 C -5.523006470000 -11.212053470000 -1.448893820000 R=2.00
101 H -4.294280280000 -8.479624330000 -1.797247340000 R=1.30
102 C -3.828140250000 -10.362711980000 -2.788829080000 R=2.00
103 H -2.052788490000 4.347260350000 3.660428230000 R=1.30
104 H -4.956731040000 -2.298039630000 -2.164325390000 R=1.30
105 H -5.718971980000 -11.773841220000 -0.512690060000 R=1.30
106 H -2.956601870000 -10.816895400000 -3.306883650000 R=1.30
107 O 8.064583630000 2.380810540000 -4.940211480000 R=1.72
108 H 12.325489900000 1.198114780000 -4.301082690000 R=1.30
109 H 8.603744290000 0.389553730000 -4.619380130000 R=1.30
110 H 7.627139370000 0.714088880000 -6.112829370000 R=1.30
111 C 8.426225750000 1.113127800000 -5.446928800000 R=2.00
112 H 9.955593260000 0.260946480000 -6.739956370000 R=1.30
113 H 12.119566280000 0.245037260000 -5.806430760000 R=1.30
114 C 9.705341520000 1.242994800000 -6.271464300000 R=2.00
115 O 10.751271960000 1.782454820000 -5.484094860000 R=1.72
116 C 11.571740920000 0.751075740000 -4.981116630000 R=2.00
117 H 10.984635560000 0.010897870000 -4.393837790000 R=1.30
118 O -0.230255500000 3.430258970000 7.975069230000 R=1.72
119 C 1.094158690000 2.959396030000 7.810519380000 R=2.00
120 H 3.504499250000 3.146343430000 6.395129720000 R=1.30
121 H 1.780222900000 3.769039490000 8.138850130000 R=1.30
122 C 1.375895740000 2.650174240000 6.333465530000 R=2.00
123 H 1.103343200000 3.533652110000 5.717000850000 R=1.30
124 H 0.751530890000 1.792697790000 6.010543870000 R=1.30
125 C 2.846049160000 2.295105260000 6.096799250000 R=2.00
126 H 3.114888300000 1.442785850000 6.756783100000 R=1.30
127 H 4.547506550000 3.210188150000 4.255718220000 R=1.30
128 O 3.032388930000 1.874777250000 4.757369700000 R=1.72
129 C 3.508288860000 2.941037290000 3.965692930000 R=2.00
130 H 3.525482390000 2.615718390000 2.904859610000 R=1.30
131 H 2.846460320000 3.832067350000 4.034919780000 R=1.30
132 O -4.147137480000 -7.864715740000 -4.358081530000 R=1.72
133 C -3.036001060000 -8.060874190000 -3.507653750000 R=2.00
134 H -2.678741790000 -7.090771400000 -3.092802190000 R=1.30
135 H -4.652342290000 -10.320550330000 -3.541044790000 R=1.30
136 C -3.441403600000 -8.950831130000 -2.331585960000 R=2.00
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0

5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0
15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 136 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0

51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 119 118 1.0
59 55 57 1.0
60 58 47 2.0
61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 22 102 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 99 100 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 111 107 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 133 132 1.0

97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 105 100 1.0
101 63 100 1.0
102 98 62 1.0
103 102 106 1.0
104 136 102 1.0
105 136 101 1.0
106 136 133 1.0
107 100 22 1.0
108 104 72 1.0
109 116 115 1.0
110 111 109 1.0
111 111 110 1.0
112 107 90 1.0
113 111 114 1.0
114 114 89 1.0
115 115 114 1.0
116 114 112 1.0
117 117 116 1.0
118 113 116 1.0
119 108 116 1.0
120 125 120 1.0
121 121 119 1.0
122 53 119 1.0
123 118 56 1.0
124 122 125 1.0
125 122 123 1.0
126 122 124 1.0
127 125 126 1.0
128 129 128 1.0
129 122 119 1.0
130 130 129 1.0
131 131 129 1.0
132 127 129 1.0
133 128 125 1.0
134 134 133 1.0
135 102 135 1.0
136 96 133 1.0
137 132 95 1.0
138 103 50 1.0
END

SOLVATION
Surf Delley

```
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
```

```
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-X

ATOMS
1 Cr     -0.481724850000     -0.054489550000      0.496061880000    R=1.875
2 O      -1.425382660000     -0.313682690000      2.197771230000    R=1.72
3 O      -0.318681110000      1.885508040000      0.773969320000    R=1.72
4 O       1.247155560000     -0.439579310000      1.341938280000    R=1.72
5 O       0.360836170000      0.110834720000     -1.257606930000    R=1.72
6 O      -0.656341180000     -1.989802170000      0.245633060000    R=1.72
7 O      -2.221165650000      0.364643470000     -0.303513900000    R=1.72
8 C      -0.850421090000      0.325028140000      3.298194070000    R=2.00
9 C      -0.941558450000      1.851010120000      3.131339270000    R=2.00
10 H     -2.588154680000     -9.020788830000     -1.622233690000    R=1.30
11 C      0.079642490000      2.277878020000      2.063665300000    R=2.00
12 C     -1.545616650000     -0.164416070000      4.574219450000    R=2.00
13 H     -1.415449430000     -1.263490240000      4.668684060000    R=1.30
14 H     -2.633043570000      0.051343580000      4.562094250000    R=1.30
15 H     -1.094248750000      0.310932780000      5.468570240000    R=1.30
```

16 C	0.303965460000	3.792435700000	2.060051680000	R=2.00
17 H	1.148337810000	4.042301380000	1.382705890000	R=1.30
18 H	0.555890830000	4.155223920000	3.078873720000	R=1.30
19 H	-0.599982570000	4.324011980000	1.695987290000	R=1.30
20 C	2.397860810000	-0.310179310000	0.538727770000	R=2.00
21 C	2.427783210000	1.012203110000	-0.267968720000	R=2.00
22 O	-4.129645850000	-11.172004930000	-1.667324310000	R=1.72
23 C	1.349616100000	1.092970600000	-1.398692990000	R=2.00
24 C	2.665717300000	-1.576927560000	-0.282502450000	R=2.00
25 H	1.958013360000	-1.698965220000	-1.118719240000	R=1.30
26 H	-4.400032380000	-2.172735980000	0.099555820000	R=1.30
27 H	3.692077670000	-1.543733810000	-0.704939320000	R=1.30
28 C	1.897967190000	0.936145340000	-2.825841530000	R=2.00
29 H	1.055206930000	0.943260840000	-3.550072480000	R=1.30
30 H	2.434316830000	-0.029787960000	-2.936640420000	R=1.30
31 H	-4.100655640000	-0.733159800000	1.106601500000	R=1.30
32 C	-1.010764270000	-2.455066010000	-1.035087650000	R=2.00
33 C	-2.110094780000	-1.587945660000	-1.714813750000	R=2.00
34 C	-2.902004600000	-2.264471880000	-2.875597740000	R=2.00
35 C	-2.960160340000	-0.742685420000	-0.743855790000	R=2.00
36 C	-1.376243250000	-3.936501330000	-0.879039960000	R=2.00
37 H	-0.524819350000	-4.476409770000	-0.412067630000	R=1.30
38 H	-1.569520130000	-4.422294610000	-1.856690060000	R=1.30
39 H	-2.254224070000	-4.058178290000	-0.212728530000	R=1.30
40 C	-3.611698950000	-1.476779090000	0.441873770000	R=2.00
41 H	-2.893569080000	-2.052431350000	1.051780800000	R=1.30
42 H	2.570788350000	1.770770390000	-3.105713040000	R=1.30
43 H	2.591274320000	-2.470400730000	0.372901060000	R=1.30
44 C	-2.393380930000	2.348357910000	2.825791490000	R=2.00
45 H	-3.143278360000	1.540387070000	2.956587540000	R=1.30
46 H	-2.483085400000	2.643219730000	1.758534440000	R=1.30
47 C	-3.098565510000	3.167186090000	5.112366700000	R=2.00
48 H	-3.750793100000	3.980837210000	3.238683990000	R=1.30
49 H	-1.438381170000	2.262721300000	9.174972650000	R=1.30
50 C	-2.825890380000	3.551263140000	3.682960770000	R=2.00
51 O	-2.014375580000	2.902525780000	5.946399920000	R=1.72
52 H	-0.758846100000	1.372957700000	7.769542510000	R=1.30
53 H	1.315316720000	2.076849140000	8.455863470000	R=1.30
54 H	-3.089439540000	1.799311900000	7.352520920000	R=1.30
55 C	-2.399330320000	2.671379330000	7.284888060000	R=2.00
56 C	-1.152553130000	2.361178690000	8.105915640000	R=2.00
57 H	-2.891662430000	3.575883350000	7.709363560000	R=1.30
58 O	-4.258774510000	3.122159580000	5.507215520000	R=1.72
59 C	3.877239560000	1.381784210000	-0.701473310000	R=2.00
60 H	4.186987760000	0.798297550000	-1.593741260000	R=1.30
61 H	4.594924000000	1.104270770000	0.101595560000	R=1.30

62 C	4.045047120000	2.893151970000	-0.940073750000	R=2.00
63 H	-6.036519830000	-11.747532340000	-2.277700910000	R=1.30
64 H	3.188331850000	3.302479010000	-1.514606110000	R=1.30
65 C	5.314636660000	3.175734050000	-1.686103420000	R=2.00
66 H	6.358085880000	4.311168130000	-4.557396240000	R=1.30
67 C	6.473747010000	3.648367230000	-3.673446790000	R=2.00
68 O	5.221540680000	3.595812560000	-3.014363170000	R=1.72
69 H	7.053110940000	1.596849750000	-3.298875340000	R=1.30
70 O	-4.011498000000	-4.993707900000	-3.983462100000	R=1.72
71 O	6.387579520000	3.012166150000	-1.115593400000	R=1.72
72 C	-4.176657130000	-3.025123600000	-2.477310440000	R=2.00
73 C	-4.690007160000	-3.825542250000	-3.637393300000	R=2.00
74 H	7.274401190000	4.109377540000	-3.050915350000	R=1.30
75 H	-4.213563300000	-7.351338750000	-6.341594600000	R=1.30
76 H	0.207037140000	0.012487060000	3.409827450000	R=1.30
77 H	-0.587066890000	2.290419310000	4.084232760000	R=1.30
78 H	1.058468660000	1.826907130000	2.319802080000	R=1.30
79 H	3.235849120000	-0.258408150000	1.267883000000	R=1.30
80 H	2.172211170000	1.799662160000	0.460539180000	R=1.30
81 H	-3.992542120000	-3.721000800000	-1.638029780000	R=1.30
82 H	0.864521130000	2.091981450000	-1.365498690000	R=1.30
83 H	-0.109294130000	-2.432950600000	-1.681834350000	R=1.30
84 H	-1.536463340000	-0.827700660000	-2.286020010000	R=1.30
85 H	-2.215647980000	-2.927878410000	-3.445812900000	R=1.30
86 H	-3.212380860000	-1.472481100000	-3.594959590000	R=1.30
87 H	-3.801136000000	-0.317347820000	-1.333638060000	R=1.30
88 H	6.050905500000	1.856024600000	-4.792560320000	R=1.30
89 H	9.510105910000	1.944775140000	-7.110218300000	R=1.30
90 C	6.884304840000	2.263240890000	-4.174657580000	R=2.00
91 H	-2.750843590000	-6.742005130000	-5.522497770000	R=1.30
92 C	-4.569691740000	-5.619259490000	-5.120300570000	R=2.00
93 H	-4.449511760000	-4.965214540000	-6.013643440000	R=1.30
94 H	-5.650240300000	-5.844484620000	-4.964610860000	R=1.30
95 C	-3.842007800000	-6.934618820000	-5.381452720000	R=2.00
96 H	-2.201193610000	-8.545742850000	-4.063182670000	R=1.30
97 O	-5.692003860000	-3.441454410000	-4.231753030000	R=1.72
98 H	4.066863800000	3.424315530000	0.036651360000	R=1.30
99 H	-5.947837650000	-10.191335660000	-1.325108410000	R=1.30
100 C	-5.523006470000	-11.212053470000	-1.448893820000	R=2.00
101 H	-4.294280280000	-8.479624330000	-1.797247340000	R=1.30
102 C	-3.828140250000	-10.362711980000	-2.788829080000	R=2.00
103 H	-2.052788490000	4.347260350000	3.660428230000	R=1.30
104 H	-4.956731040000	-2.298039630000	-2.164325390000	R=1.30
105 H	-5.718971980000	-11.773841220000	-0.512690060000	R=1.30
106 H	-2.956601870000	-10.816895400000	-3.306883650000	R=1.30
107 O	8.064583630000	2.380810540000	-4.940211480000	R=1.72

108 H 12.325489900000 1.198114780000 -4.301082690000 R=1.30
109 H 8.603744290000 0.389553730000 -4.619380130000 R=1.30
110 H 7.627139370000 0.714088880000 -6.112829370000 R=1.30
111 C 8.426225750000 1.113127800000 -5.446928800000 R=2.00
112 H 9.955593260000 0.260946480000 -6.739956370000 R=1.30
113 H 12.119566280000 0.245037260000 -5.806430760000 R=1.30
114 C 9.705341520000 1.242994800000 -6.271464300000 R=2.00
115 O 10.751271960000 1.782454820000 -5.484094860000 R=1.72
116 C 11.571740920000 0.751075740000 -4.981116630000 R=2.00
117 H 10.984635560000 0.010897870000 -4.393837790000 R=1.30
118 O -0.230255500000 3.430258970000 7.975069230000 R=1.72
119 C 1.094158690000 2.959396030000 7.810519380000 R=2.00
120 H 3.504499250000 3.146343430000 6.395129720000 R=1.30
121 H 1.780222900000 3.769039490000 8.138850130000 R=1.30
122 C 1.375895740000 2.650174240000 6.333465530000 R=2.00
123 H 1.103343200000 3.533652110000 5.717000850000 R=1.30
124 H 0.751530890000 1.792697790000 6.010543870000 R=1.30
125 C 2.846049160000 2.295105260000 6.096799250000 R=2.00
126 H 3.114888300000 1.442785850000 6.756783100000 R=1.30
127 H 4.547506550000 3.210188150000 4.255718220000 R=1.30
128 O 3.032388930000 1.874777250000 4.757369700000 R=1.72
129 C 3.508288860000 2.941037290000 3.965692930000 R=2.00
130 H 3.525482390000 2.615718390000 2.904859610000 R=1.30
131 H 2.846460320000 3.832067350000 4.034919780000 R=1.30
132 O -4.147137480000 -7.864715740000 -4.358081530000 R=1.72
133 C -3.036001060000 -8.060874190000 -3.507653750000 R=2.00
134 H -2.678741790000 -7.090771400000 -3.092802190000 R=1.30
135 H -4.652342290000 -10.320550330000 -3.541044790000 R=1.30
136 C -3.441403600000 -8.950831130000 -2.331585960000 R=2.00
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 20 1.0
10 5 23 1.0
11 6 32 1.0
12 7 35 1.0
13 8 9 1.0
14 8 12 1.0

15 55 51 1.0
16 9 11 1.0
17 11 16 1.0
18 12 13 1.0
19 12 14 1.0
20 12 15 1.0
21 16 17 1.0
22 16 18 1.0
23 16 19 1.0
24 20 21 1.0
25 20 24 1.0
26 59 61 1.0
27 21 23 1.0
28 23 28 1.0
29 24 25 1.0
30 40 26 1.0
31 24 27 1.0
32 28 29 1.0
33 28 30 1.0
34 40 31 1.0
35 32 33 1.0
36 32 36 1.0
37 34 33 1.0
38 33 35 1.0
39 35 40 1.0
40 36 37 1.0
41 36 38 1.0
42 36 39 1.0
43 40 41 1.0
44 42 28 1.0
45 43 24 1.0
46 136 10 1.0
47 44 45 1.0
48 44 46 1.0
49 50 44 1.0
50 50 48 1.0
51 44 9 1.0
52 50 47 1.0
53 56 52 1.0
54 56 49 1.0
55 55 54 1.0
56 51 47 1.0
57 55 56 1.0
58 119 118 1.0
59 55 57 1.0
60 58 47 2.0

61 59 21 1.0
62 59 60 1.0
63 62 65 1.0
64 22 102 1.0
65 62 64 1.0
66 62 59 1.0
67 90 69 1.0
68 68 65 1.0
69 95 91 1.0
70 67 90 1.0
71 67 66 1.0
72 71 65 2.0
73 72 73 1.0
74 72 34 1.0
75 67 74 1.0
76 92 70 1.0
77 76 8 1.0
78 77 9 1.0
79 78 11 1.0
80 79 20 1.0
81 80 21 1.0
82 99 100 1.0
83 82 23 1.0
84 83 32 1.0
85 84 33 1.0
86 85 34 1.0
87 86 34 1.0
88 87 35 1.0
89 111 107 1.0
90 67 68 1.0
91 70 73 1.0
92 90 88 1.0
93 92 95 1.0
94 92 93 1.0
95 92 94 1.0
96 133 132 1.0
97 95 75 1.0
98 97 73 2.0
99 81 72 1.0
100 105 100 1.0
101 63 100 1.0
102 98 62 1.0
103 102 106 1.0
104 136 102 1.0
105 136 101 1.0
106 136 133 1.0

```
107 100 22 1.0
108 104 72 1.0
109 116 115 1.0
110 111 109 1.0
111 111 110 1.0
112 107 90 1.0
113 111 114 1.0
114 114 89 1.0
115 115 114 1.0
116 114 112 1.0
117 117 116 1.0
118 113 116 1.0
119 108 116 1.0
120 125 120 1.0
121 121 119 1.0
122 53 119 1.0
123 118 56 1.0
124 122 125 1.0
125 122 123 1.0
126 122 124 1.0
127 125 126 1.0
128 129 128 1.0
129 122 119 1.0
130 130 129 1.0
131 131 129 1.0
132 127 129 1.0
133 128 125 1.0
134 134 133 1.0
135 102 135 1.0
136 96 133 1.0
137 132 95 1.0
138 103 50 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 2.0
```

```
UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-XI

ATOMS
1 Cr      4.052500000000     10.421400000000      4.466000000000    R=1.875
2 O       3.869200000000     12.367700000000      4.522000000000    R=1.72
3 O       2.465000000000     10.345300000000      3.347800000000    R=1.72
4 O       2.943400000000     10.305600000000      6.065100000000    R=1.72
5 O       4.063700000000      8.457200000000      4.436700000000    R=1.72
6 O       5.674800000000     10.545300000000      5.551600000000    R=1.72
7 O       5.162400000000     10.494300000000      2.856900000000    R=1.72
8 H       7.354900000000      9.442800000000      1.164600000000    R=1.30
9 C       7.908800000000     10.619900000000      6.278400000000    R=2.00
10 H      7.608300000000     11.021500000000      1.208000000000    R=1.30
11 C      2.847800000000     13.065900000000      4.198900000000    R=2.00
12 C      1.709700000000     12.584800000000      3.519800000000    R=2.00
13 C      1.614000000000     11.251900000000      3.081200000000    R=2.00
14 C      2.035900000000      9.415300000000      6.249100000000    R=2.00
15 C      1.973600000000      8.199400000000      5.536500000000    R=2.00
16 C      3.026400000000      7.755800000000      4.723200000000    R=2.00
17 C      6.893400000000     10.467300000000      5.172900000000    R=2.00
18 C      7.312600000000     10.279800000000      3.848300000000    R=2.00
19 C      6.425500000000     10.359100000000      2.754200000000    R=2.00
20 C      2.930900000000     14.512200000000      4.598100000000    R=2.00
21 H      3.760000000000     14.666200000000      5.097700000000    R=1.30
22 H      2.162700000000     14.739800000000      5.161400000000    R=1.30
23 H      2.925400000000     15.073900000000      3.794800000000    R=1.30
24 Br     0.768519625100      7.374586859000      5.704917848000    R=2.16
25 C      6.941900000000     10.314900000000      1.335400000000    R=2.00
26 H      6.197500000000     10.451300000000      0.713100000000    R=1.30
27 Br     8.744355785000     10.080526050000      3.581344454000    R=2.16
28 C      0.445300000000     10.784700000000      2.252700000000    R=2.00
29 H      0.611900000000      9.870500000000      1.938700000000    R=1.30
30 H      0.332400000000     11.378600000000      1.481800000000    R=1.30
31 H     -0.369300000000     10.799300000000      2.798300000000    R=1.30
32 C      1.024800000000      9.749400000000      7.301700000000    R=2.00
33 H      1.316900000000     10.544800000000      7.794300000000    R=1.30
34 H      0.936400000000      8.995300000000      7.921700000000    R=1.30
```

35 H 0.159400000000 9.927200000000 6.877800000000 R=1.30
36 H 8.555700000000 11.314200000000 6.034500000000 R=1.30
37 H 7.454000000000 10.875900000000 7.106900000000 R=1.30
38 Br 0.639354397300 13.529755920000 3.170059245000 R=2.16
39 H 8.377500000000 9.769300000000 6.411400000000 R=1.30
40 C 3.010000000000 6.369200000000 4.128700000000 R=2.00
41 H 3.846700000000 6.212000000000 3.642900000000 R=1.30
42 H 2.253500000000 6.287100000000 3.511400000000 R=1.30
43 H 2.919500000000 5.707700000000 4.845500000000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 11 1.0
8 3 13 1.0
9 4 14 1.0
10 5 16 1.0
11 6 17 1.0
12 7 19 1.0
13 25 10 1.0
14 24 15 1.0
15 40 41 1.0
16 11 12 1.0
17 11 20 1.0
18 12 13 1.0
19 9 37 1.0
20 13 28 1.0
21 14 15 1.0
22 14 32 1.0
23 15 16 1.0
24 40 43 1.0
25 16 40 1.0
26 17 18 1.0
27 17 9 1.0
28 18 19 1.0
29 40 42 1.0
30 19 25 1.0
31 20 21 1.0
32 20 22 1.0
33 20 23 1.0
34 27 18 1.0

```
35 25 26 1.0
36 25 8 1.0
37 28 29 1.0
38 28 30 1.0
39 28 31 1.0
40 32 33 1.0
41 32 34 1.0
42 32 35 1.0
43 9 36 1.0
44 9 39 1.0
45 38 12 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END
```

```
SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-XI
```

ATOMS

1 Cr	4.052500000000	10.421400000000	4.466000000000	R=1.875
2 O	3.869200000000	12.367700000000	4.522000000000	R=1.72
3 O	2.465000000000	10.345300000000	3.347800000000	R=1.72
4 O	2.943400000000	10.305600000000	6.065100000000	R=1.72
5 O	4.063700000000	8.457200000000	4.436700000000	R=1.72
6 O	5.674800000000	10.545300000000	5.551600000000	R=1.72
7 O	5.162400000000	10.494300000000	2.856900000000	R=1.72
8 H	7.354900000000	9.442800000000	1.164600000000	R=1.30
9 C	7.908800000000	10.619900000000	6.278400000000	R=2.00
10 H	7.608300000000	11.021500000000	1.208000000000	R=1.30
11 C	2.847800000000	13.065900000000	4.198900000000	R=2.00
12 C	1.709700000000	12.584800000000	3.519800000000	R=2.00
13 C	1.614000000000	11.251900000000	3.081200000000	R=2.00
14 C	2.035900000000	9.415300000000	6.249100000000	R=2.00
15 C	1.973600000000	8.199400000000	5.536500000000	R=2.00
16 C	3.026400000000	7.755800000000	4.723200000000	R=2.00
17 C	6.893400000000	10.467300000000	5.172900000000	R=2.00
18 C	7.312600000000	10.279800000000	3.848300000000	R=2.00
19 C	6.425500000000	10.359100000000	2.754200000000	R=2.00
20 C	2.930900000000	14.512200000000	4.598100000000	R=2.00
21 H	3.760000000000	14.666200000000	5.097700000000	R=1.30
22 H	2.162700000000	14.739800000000	5.161400000000	R=1.30
23 H	2.925400000000	15.073900000000	3.794800000000	R=1.30
24 Br	0.768519625100	7.374586859000	5.704917848000	R=2.16
25 C	6.941900000000	10.314900000000	1.335400000000	R=2.00
26 H	6.197500000000	10.451300000000	0.713100000000	R=1.30
27 Br	8.744355785000	10.080526050000	3.581344454000	R=2.16
28 C	0.445300000000	10.784700000000	2.252700000000	R=2.00
29 H	0.611900000000	9.870500000000	1.938700000000	R=1.30
30 H	0.332400000000	11.378600000000	1.481800000000	R=1.30
31 H	-0.369300000000	10.799300000000	2.798300000000	R=1.30
32 C	1.024800000000	9.749400000000	7.301700000000	R=2.00
33 H	1.316900000000	10.544800000000	7.794300000000	R=1.30
34 H	0.936400000000	8.995300000000	7.921700000000	R=1.30
35 H	0.159400000000	9.927200000000	6.877800000000	R=1.30
36 H	8.555700000000	11.314200000000	6.034500000000	R=1.30
37 H	7.454000000000	10.875900000000	7.106900000000	R=1.30
38 Br	0.639354397300	13.529755920000	3.170059245000	R=2.16
39 H	8.377500000000	9.769300000000	6.411400000000	R=1.30
40 C	3.010000000000	6.369200000000	4.128700000000	R=2.00
41 H	3.846700000000	6.212000000000	3.642900000000	R=1.30
42 H	2.253500000000	6.287100000000	3.511400000000	R=1.30
43 H	2.919500000000	5.707700000000	4.845500000000	R=1.30

END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 11 1.0
8 3 13 1.0
9 4 14 1.0
10 5 16 1.0
11 6 17 1.0
12 7 19 1.0
13 25 10 1.0
14 24 15 1.0
15 40 41 1.0
16 11 12 1.0
17 11 20 1.0
18 12 13 1.0
19 9 37 1.0
20 13 28 1.0
21 14 15 1.0
22 14 32 1.0
23 15 16 1.0
24 40 43 1.0
25 16 40 1.0
26 17 18 1.0
27 17 9 1.0
28 18 19 1.0
29 40 42 1.0
30 19 25 1.0
31 20 21 1.0
32 20 22 1.0
33 20 23 1.0
34 27 18 1.0
35 25 26 1.0
36 25 8 1.0
37 28 29 1.0
38 28 30 1.0
39 28 31 1.0
40 32 33 1.0
41 32 34 1.0
42 32 35 1.0
43 9 36 1.0
44 9 39 1.0
45 38 12 1.0

```
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End
```

```
ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-XII

ATOMS
1 Cr      0.101825870000     -0.003777540000      1.046791430000     R=1.875
2 O       1.377543370000      0.807682430000     -0.149331940000     R=1.72
3 O      -1.341346240000      0.792147930000      0.047114350000     R=1.72
4 O       0.026185460000     -1.560045590000     -0.087808450000     R=1.72
5 O       2.551022640000      1.999468320000     -2.073157230000     R=1.72
6 O      -2.889226810000      1.708887320000     -1.822055330000     R=1.72
7 O      -0.236595830000     -3.168778010000     -2.103426370000     R=1.72
8 C       3.696395310000      1.322982920000     -0.103322540000     R=2.00
9 C      -2.849565830000      2.590393600000      0.380197900000     R=2.00
10 C     -0.793010720000     -3.775242480000      0.121976630000     R=2.00
11 C      2.591156990000      0.769413420000      0.498062830000     R=2.00
12 C     -1.792403630000      1.847276220000      0.805811400000     R=2.00
13 C     -0.599169670000     -2.537046830000      0.651710030000     R=2.00
14 C      3.603735610000      1.969097760000     -1.452831660000     R=2.00
15 C     -3.503998180000      2.305135700000     -0.949608150000     R=2.00
16 C     -0.380983570000     -4.077512390000     -1.298465510000     R=2.00
17 C      2.604933430000      0.101767810000      1.855328590000     R=2.00
18 C     -1.089105980000      2.114811040000      2.114670310000     R=2.00
19 C     -1.024985460000     -2.181249480000      2.055888320000     R=2.00
20 C      4.818257720000      2.596919170000     -2.074186250000     R=2.00
```

21 C -4.910114150000 2.743874430000 -1.251025630000 R=2.00
22 C -0.146073650000 -5.484625950000 -1.773512810000 R=2.00
23 O 5.353272330000 0.192023950000 0.720284940000 R=1.72
24 O -3.314847430000 4.687711950000 0.568580240000 R=1.72
25 O -2.386433010000 -5.210462800000 0.350646910000 R=1.72
26 H 3.587237250000 0.074562250000 2.358660820000 R=1.30
27 H 2.261168410000 -0.947595950000 1.744266220000 R=1.30
28 H 1.902049720000 0.634801580000 2.528621260000 R=1.30
29 H -1.151439940000 1.210668900000 2.755351880000 R=1.30
30 H -1.513860660000 2.966038020000 2.683791630000 R=1.30
31 H -0.020990920000 2.339276350000 1.914313500000 R=1.30
32 H -0.135802400000 -1.860219620000 2.637368640000 R=1.30
33 H -1.506058510000 -3.017470800000 2.601975300000 R=1.30
34 H -1.748598250000 -1.340822120000 2.015223300000 R=1.30
35 H 5.197233240000 3.408750100000 -1.418538250000 R=1.30
36 H 4.573759990000 3.029222860000 -3.068194360000 R=1.30
37 H 5.610523340000 1.830566170000 -2.206548740000 R=1.30
38 H -5.611906580000 2.283705180000 -0.524815760000 R=1.30
39 H -5.208983650000 2.421869490000 -2.271725890000 R=1.30
40 H -4.991041610000 3.848840500000 -1.202088870000 R=1.30
41 H 0.164401040000 -5.489425520000 -2.840487220000 R=1.30
42 H -1.074189660000 -6.084988490000 -1.683665080000 R=1.30
43 H 0.663590300000 -5.953564920000 -1.176752010000 R=1.30
44 N 5.010223760000 1.330343420000 0.506710540000 R=1.83
45 O 4.950286380000 1.904029070000 1.568040590000 R=1.72
46 N -1.420596130000 -4.788833350000 0.940214280000 R=1.83
47 O -0.649660230000 -5.708321630000 1.073224770000 R=1.72
48 N -3.321126870000 3.669979040000 1.218506070000 R=1.83
49 O -4.466743210000 3.446169490000 1.526634270000 R=1.72
END

GUIBONDS
1 2 11 1
2 3 12 1
3 4 13 1
4 5 14 2
5 6 15 2
6 7 16 2
7 8 11 2
8 8 14 1
9 9 12 2
10 9 15 1
11 10 13 2
12 10 16 1
13 11 17 1
14 12 18 1

```
15 13 19 1
16 14 20 1
17 15 21 1
18 16 22 1
19 2 1 1.0
20 3 1 1.0
21 4 1 1.0
22 23 44 2.0
23 24 48 2.0
24 25 46 2.0
25 26 17 1.0
26 27 17 1.0
27 28 17 1.0
28 29 18 1.0
29 30 18 1.0
30 31 18 1.0
31 32 19 1.0
32 33 19 1.0
33 34 19 1.0
34 35 20 1.0
35 36 20 1.0
36 37 20 1.0
37 38 21 1.0
38 39 21 1.0
39 40 21 1.0
40 41 22 1.0
41 42 22 1.0
42 43 22 1.0
43 45 44 2.0
44 44 8 1.0
45 47 46 2.0
46 46 10 1.0
47 49 48 2.0
48 48 9 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END
```

```
CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====
```

```
rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-XII

ATOMS
1 Cr      0.101825870000     -0.003777540000      1.046791430000     R=1.875
2 O       1.377543370000      0.807682430000     -0.149331940000     R=1.72
3 O      -1.341346240000      0.792147930000      0.047114350000     R=1.72
4 O       0.026185460000     -1.560045590000     -0.087808450000     R=1.72
5 O       2.551022640000      1.999468320000     -2.073157230000     R=1.72
6 O      -2.889226810000      1.708887320000     -1.822055330000     R=1.72
7 O      -0.236595830000     -3.168778010000     -2.103426370000     R=1.72
8 C       3.696395310000      1.322982920000     -0.103322540000     R=2.00
9 C      -2.849565830000      2.590393600000      0.380197900000     R=2.00
10 C     -0.793010720000     -3.775242480000      0.121976630000     R=2.00
11 C      2.591156990000      0.769413420000      0.498062830000     R=2.00
12 C     -1.792403630000      1.847276220000      0.805811400000     R=2.00
13 C     -0.599169670000     -2.537046830000      0.651710030000     R=2.00
14 C      3.603735610000      1.969097760000     -1.452831660000     R=2.00
15 C     -3.503998180000      2.305135700000     -0.949608150000     R=2.00
16 C     -0.380983570000     -4.077512390000     -1.298465510000     R=2.00
17 C      2.604933430000      0.101767810000      1.855328590000     R=2.00
18 C     -1.089105980000      2.114811040000      2.114670310000     R=2.00
19 C     -1.024985460000     -2.181249480000      2.055888320000     R=2.00
20 C      4.818257720000      2.596919170000     -2.074186250000     R=2.00
21 C     -4.910114150000      2.743874430000     -1.251025630000     R=2.00
22 C     -0.146073650000     -5.484625950000     -1.773512810000     R=2.00
```

23 O 5.353272330000 0.192023950000 0.720284940000 R=1.72
24 O -3.314847430000 4.687711950000 0.568580240000 R=1.72
25 O -2.386433010000 -5.210462800000 0.350646910000 R=1.72
26 H 3.587237250000 0.074562250000 2.358660820000 R=1.30
27 H 2.261168410000 -0.947595950000 1.744266220000 R=1.30
28 H 1.902049720000 0.634801580000 2.528621260000 R=1.30
29 H -1.151439940000 1.210668900000 2.755351880000 R=1.30
30 H -1.513860660000 2.966038020000 2.683791630000 R=1.30
31 H -0.020990920000 2.339276350000 1.914313500000 R=1.30
32 H -0.135802400000 -1.860219620000 2.637368640000 R=1.30
33 H -1.506058510000 -3.017470800000 2.601975300000 R=1.30
34 H -1.748598250000 -1.340822120000 2.015223300000 R=1.30
35 H 5.197233240000 3.408750100000 -1.418538250000 R=1.30
36 H 4.573759990000 3.029222860000 -3.068194360000 R=1.30
37 H 5.610523340000 1.830566170000 -2.206548740000 R=1.30
38 H -5.611906580000 2.283705180000 -0.524815760000 R=1.30
39 H -5.208983650000 2.421869490000 -2.271725890000 R=1.30
40 H -4.991041610000 3.848840500000 -1.202088870000 R=1.30
41 H 0.164401040000 -5.489425520000 -2.840487220000 R=1.30
42 H -1.074189660000 -6.084988490000 -1.683665080000 R=1.30
43 H 0.663590300000 -5.953564920000 -1.176752010000 R=1.30
44 N 5.010223760000 1.330343420000 0.506710540000 R=1.83
45 O 4.950286380000 1.904029070000 1.568040590000 R=1.72
46 N -1.420596130000 -4.788833350000 0.940214280000 R=1.83
47 O -0.649660230000 -5.708321630000 1.073224770000 R=1.72
48 N -3.321126870000 3.669979040000 1.218506070000 R=1.83
49 O -4.466743210000 3.446169490000 1.526634270000 R=1.72
END

GUIBONDS
1 2 11 1
2 3 12 1
3 4 13 1
4 5 14 2
5 6 15 2
6 7 16 2
7 8 11 2
8 8 14 1
9 9 12 2
10 9 15 1
11 10 13 2
12 10 16 1
13 11 17 1
14 12 18 1
15 13 19 1
16 14 20 1

```
17 15 21 1
18 16 22 1
19 2 1 1.0
20 3 1 1.0
21 4 1 1.0
22 23 44 2.0
23 24 48 2.0
24 25 46 2.0
25 26 17 1.0
26 27 17 1.0
27 28 17 1.0
28 29 18 1.0
29 30 18 1.0
30 31 18 1.0
31 32 19 1.0
32 33 19 1.0
33 34 19 1.0
34 35 20 1.0
35 36 20 1.0
36 37 20 1.0
37 38 21 1.0
38 39 21 1.0
39 40 21 1.0
40 41 22 1.0
41 42 22 1.0
42 43 22 1.0
43 45 44 2.0
44 44 8 1.0
45 47 46 2.0
46 46 10 1.0
47 49 48 2.0
48 48 9 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0
```

```
UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-XIII

ATOMS
1 Cr      4.052500000000     10.421400000000      4.466000000000    R=1.875
2 O       3.869200000000     12.367700000000      4.522000000000    R=1.72
3 O       2.465000000000     10.345300000000      3.347800000000    R=1.72
4 O       2.943400000000     10.305600000000      6.065100000000    R=1.72
5 O       4.063700000000      8.457200000000      4.436700000000    R=1.72
6 O       5.674800000000     10.545300000000      5.551600000000    R=1.72
7 O       5.162400000000     10.494300000000      2.856900000000    R=1.72
8 N       1.276600000000     14.995600000000      1.085000000000    R=1.83
9 N      -1.236500000000      8.415000000000      4.346700000000    R=1.83
10 N     10.023300000000     12.339300000000      3.115400000000    R=1.83
11 C      2.847800000000     13.065900000000      4.198900000000    R=2.00
12 C      1.709700000000     12.584800000000      3.519800000000    R=2.00
13 C      1.614000000000     11.251900000000      3.081200000000    R=2.00
14 C      2.035900000000      9.415300000000      6.249100000000    R=2.00
15 C      1.973600000000      8.199400000000      5.536500000000    R=2.00
16 C      3.026400000000      7.755800000000      4.723200000000    R=2.00
17 C      6.893400000000     10.467300000000      5.172900000000    R=2.00
18 C      7.312600000000     10.279800000000      3.848300000000    R=2.00
19 C      6.425500000000     10.359100000000      2.754200000000    R=2.00
20 C      2.930900000000     14.512200000000      4.598100000000    R=2.00
21 H      3.760000000000     14.666200000000      5.097700000000    R=1.30
22 H      2.162700000000     14.739800000000      5.161400000000    R=1.30
23 H      2.925400000000     15.073900000000      3.794800000000    R=1.30
24 C      0.600000000000     13.564500000000      3.157200000000    R=2.00
25 H     -0.232700000000     13.061500000000      2.975900000000    R=1.30
26 H      0.432800000000     14.166600000000      3.924900000000    R=1.30
27 C      0.946100000000     14.364600000000      1.982000000000    R=2.00
28 C      0.445300000000     10.784700000000      2.252700000000    R=2.00
29 H      0.611900000000      9.870500000000      1.938700000000    R=1.30
30 H      0.332400000000     11.378600000000      1.481800000000    R=1.30
31 H     -0.369300000000     10.799300000000      2.798300000000    R=1.30
32 C      1.024800000000      9.749400000000      7.301700000000    R=2.00
33 H      1.316900000000     10.544800000000      7.794300000000    R=1.30
34 H      0.936400000000      8.995300000000      7.921700000000    R=1.30
35 H      0.159400000000      9.927200000000      6.877800000000    R=1.30
```

36 C 0.725000000000 7.344800000000 5.711000000000 R=2.00
37 H 0.906100000000 6.423500000000 5.397300000000 R=1.30
38 H 0.484300000000 7.301700000000 6.670300000000 R=1.30
39 C -0.396700000000 7.915400000000 4.945100000000 R=2.00
40 C 3.010000000000 6.369200000000 4.128700000000 R=2.00
41 H 3.846700000000 6.212000000000 3.642900000000 R=1.30
42 H 2.253500000000 6.287100000000 3.511400000000 R=1.30
43 H 2.919500000000 5.707700000000 4.845500000000 R=1.30
44 C 7.908800000000 10.619900000000 6.278400000000 R=2.00
45 H 7.454000000000 10.875900000000 7.106900000000 R=1.30
46 H 8.555700000000 11.314200000000 6.034500000000 R=1.30
47 H 8.377500000000 9.769300000000 6.411400000000 R=1.30
48 C 8.793400000000 10.073700000000 3.572200000000 R=2.00
49 H 9.207400000000 9.622200000000 4.349300000000 R=1.30
50 H 8.896500000000 9.481200000000 2.786100000000 R=1.30
51 C 9.500400000000 11.338600000000 3.317900000000 R=2.00
52 C 6.941900000000 10.314900000000 1.335400000000 R=2.00
53 H 6.197500000000 10.451300000000 0.713100000000 R=1.30
54 H 7.354900000000 9.442800000000 1.164600000000 R=1.30
55 H 7.608300000000 11.021500000000 1.208000000000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 11 1.0
8 3 13 1.0
9 4 14 1.0
10 5 16 1.0
11 6 17 1.0
12 7 19 1.0
13 8 27 3
14 9 39 3
15 10 51 3
16 11 12 1.0
17 11 20 1
18 12 13 1.0
19 12 24 1
20 13 28 1
21 14 15 1.0
22 14 32 1
23 15 16 1.0

```
24 15 36 1
25 16 40 1
26 17 18 1.0
27 17 44 1
28 18 19 1.0
29 18 48 1
30 19 52 1
31 20 21 1
32 20 22 1
33 20 23 1
34 24 25 1
35 24 26 1
36 24 27 1
37 28 29 1
38 28 30 1
39 28 31 1
40 32 33 1
41 32 34 1
42 32 35 1
43 36 37 1
44 36 38 1
45 36 39 1
46 40 41 1
47 40 42 1
48 40 43 1
49 44 45 1
50 44 46 1
51 44 47 1
52 48 49 1
53 48 50 1
54 48 51 1
55 52 53 1
56 52 54 1
57 52 55 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END
```

```
CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====
```

```
rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-XIII

ATOMS
1 Cr      4.052500000000     10.421400000000      4.466000000000     R=1.875
2 O       3.869200000000     12.367700000000      4.522000000000     R=1.72
3 O       2.465000000000     10.345300000000      3.347800000000     R=1.72
4 O       2.943400000000     10.305600000000      6.065100000000     R=1.72
5 O       4.063700000000      8.457200000000      4.436700000000     R=1.72
6 O       5.674800000000     10.545300000000      5.551600000000     R=1.72
7 O       5.162400000000     10.494300000000      2.856900000000     R=1.72
8 N       1.276600000000     14.995600000000      1.085000000000     R=1.83
9 N      -1.236500000000      8.415000000000      4.346700000000     R=1.83
10 N     10.023300000000     12.339300000000      3.115400000000     R=1.83
11 C      2.847800000000     13.065900000000      4.198900000000     R=2.00
12 C      1.709700000000     12.584800000000      3.519800000000     R=2.00
13 C      1.614000000000     11.251900000000      3.081200000000     R=2.00
14 C      2.035900000000      9.415300000000      6.249100000000     R=2.00
15 C      1.973600000000      8.199400000000      5.536500000000     R=2.00
16 C      3.026400000000      7.755800000000      4.723200000000     R=2.00
17 C      6.893400000000     10.467300000000      5.172900000000     R=2.00
18 C      7.312600000000     10.279800000000      3.848300000000     R=2.00
19 C      6.425500000000     10.359100000000      2.754200000000     R=2.00
20 C      2.930900000000     14.512200000000      4.598100000000     R=2.00
21 H      3.760000000000     14.666200000000      5.097700000000     R=1.30
22 H      2.162700000000     14.739800000000      5.161400000000     R=1.30
```

```
23 H       2.925400000000     15.073900000000      3.794800000000    R=1.30
24 C       0.600000000000     13.564500000000      3.157200000000    R=2.00
25 H      -0.232700000000     13.061500000000      2.975900000000    R=1.30
26 H       0.432800000000     14.166600000000      3.924900000000    R=1.30
27 C       0.946100000000     14.364600000000      1.982000000000    R=2.00
28 C       0.445300000000     10.784700000000      2.252700000000    R=2.00
29 H       0.611900000000      9.870500000000      1.938700000000    R=1.30
30 H       0.332400000000     11.378600000000      1.481800000000    R=1.30
31 H      -0.369300000000     10.799300000000      2.798300000000    R=1.30
32 C       1.024800000000      9.749400000000      7.301700000000    R=2.00
33 H       1.316900000000     10.544800000000      7.794300000000    R=1.30
34 H       0.936400000000      8.995300000000      7.921700000000    R=1.30
35 H       0.159400000000      9.927200000000      6.877800000000    R=1.30
36 C       0.725000000000      7.344800000000      5.711000000000    R=2.00
37 H       0.906100000000      6.423500000000      5.397300000000    R=1.30
38 H       0.484300000000      7.301700000000      6.670300000000    R=1.30
39 C      -0.396700000000      7.915400000000      4.945100000000    R=2.00
40 C       3.010000000000      6.369200000000      4.128700000000    R=2.00
41 H       3.846700000000      6.212000000000      3.642900000000    R=1.30
42 H       2.253500000000      6.287100000000      3.511400000000    R=1.30
43 H       2.919500000000      5.707700000000      4.845500000000    R=1.30
44 C       7.908800000000     10.619900000000      6.278400000000    R=2.00
45 H       7.454000000000     10.875900000000      7.106900000000    R=1.30
46 H       8.555700000000     11.314200000000      6.034500000000    R=1.30
47 H       8.377500000000      9.769300000000      6.411400000000    R=1.30
48 C       8.793400000000     10.073700000000      3.572200000000    R=2.00
49 H       9.207400000000      9.622200000000      4.349300000000    R=1.30
50 H       8.896500000000      9.481200000000      2.786100000000    R=1.30
51 C       9.500400000000     11.338600000000      3.317900000000    R=2.00
52 C       6.941900000000     10.314900000000      1.335400000000    R=2.00
53 H       6.197500000000     10.451300000000      0.713100000000    R=1.30
54 H       7.354900000000      9.442800000000      1.164600000000    R=1.30
55 H       7.608300000000     11.021500000000      1.208000000000    R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 11 1.0
8 3 13 1.0
9 4 14 1.0
10 5 16 1.0
```

11 6 17 1.0
12 7 19 1.0
13 8 27 3
14 9 39 3
15 10 51 3
16 11 12 1.0
17 11 20 1
18 12 13 1.0
19 12 24 1
20 13 28 1
21 14 15 1.0
22 14 32 1
23 15 16 1.0
24 15 36 1
25 16 40 1
26 17 18 1.0
27 17 44 1
28 18 19 1.0
29 18 48 1
30 19 52 1
31 20 21 1
32 20 22 1
33 20 23 1
34 24 25 1
35 24 26 1
36 24 27 1
37 28 29 1
38 28 30 1
39 28 31 1
40 32 33 1
41 32 34 1
42 32 35 1
43 36 37 1
44 36 38 1
45 36 39 1
46 40 41 1
47 40 42 1
48 40 43 1
49 44 45 1
50 44 46 1
51 44 47 1
52 48 49 1
53 48 50 1
54 48 51 1
55 52 53 1
56 52 54 1

```
57 52 55 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
```

```
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-XIV

ATOMS
1 Cr     -0.120016780000      0.218683650000      1.214387160000    R=1.875
2 O       1.193496080000      1.347879440000      0.364126030000    R=1.72
3 O      -1.474441120000      0.903353220000      0.026973970000    R=1.72
4 O       0.261330340000     -1.194583320000     -0.041543720000    R=1.72
5 O       2.553447250000      3.015258750000     -1.137606580000    R=1.72
6 O      -3.140199730000      1.493753720000     -1.930889670000    R=1.72
7 O       1.189337320000     -2.793187780000     -1.923574930000    R=1.72
8 C       3.556334750000      1.416935100000      0.267870000000    R=2.00
9 C      -3.296493630000      2.394778600000      0.247488720000    R=2.00
10 C     -0.156948740000     -3.520749630000     -0.123936000000    R=2.00
11 C      2.424070690000      0.923374560000      0.811010000000    R=2.00
12 C     -2.237129450000      1.757969790000      0.786243310000    R=2.00
13 C     -0.303770990000     -2.329422160000      0.489792400000    R=2.00
14 C      3.584611250000      2.444176150000     -0.811959950000    R=2.00
15 C     -3.732293720000      2.238530860000     -1.163801670000    R=2.00
16 C      0.611472470000     -3.722022160000     -1.378565280000    R=2.00
17 H      3.846373480000     -1.409821720000      0.851825660000    R=1.30
```

```
18 C     -1.865844450000     1.973391870000     2.227152680000    R=2.00
19 C     -1.097712830000    -2.218278750000     1.761798420000    R=2.00
20 H      4.186415400000     4.817176270000    -2.009049570000    R=1.30
21 C     -4.920349560000     3.006965790000    -1.655976430000    R=2.00
22 C      0.681446740000    -5.089681990000    -1.985855620000    R=2.00
23 H      4.507371120000     1.071960070000     0.662748100000    R=1.30
24 H     -3.878929780000     3.068480260000     0.870607310000    R=1.30
25 H     -0.622439650000    -4.399940190000     0.313994910000    R=1.30
26 H      1.289545300000    -5.077108680000    -2.915644730000    R=1.30
27 H     -0.342348400000    -5.440686720000    -2.233215500000    R=1.30
28 H      1.145075230000    -5.795033490000    -1.264765080000    R=1.30
29 H     -1.885445140000     1.001538670000     2.763013400000    R=1.30
30 H     -2.562013440000     2.670897240000     2.740244020000    R=1.30
31 H     -0.841770280000     2.397267330000     2.282920220000    R=1.30
32 H     -0.445527320000    -1.836269740000     2.572680120000    R=1.30
33 H     -1.516095210000    -3.196323550000     2.082444950000    R=1.30
34 H     -1.939186590000    -1.510753580000     1.610491910000    R=1.30
35 H      1.256971920000    -0.672227980000     5.020614060000    R=1.30
36 H      2.638405340000    -2.713440920000     4.755721260000    R=1.30
37 H      3.932469360000    -3.073946730000     2.672420510000    R=1.30
38 H     -5.815664230000     2.732150350000    -1.059902470000    R=1.30
39 H     -5.119652990000     2.781256080000    -2.725504190000    R=1.30
40 H     -4.730542620000     4.095597310000    -1.549830840000    R=1.30
41 C      2.496823020000    -0.077201980000     1.900174200000    R=2.00
42 C      1.766702950000     0.118698150000     3.083565060000    R=2.00
43 C      1.821802350000    -0.828439930000     4.110736160000    R=2.00
44 C      2.600662510000    -1.979066820000     3.961655450000    R=2.00
45 C      3.331059460000    -2.181521420000     2.787637780000    R=2.00
46 C      3.283975760000    -1.233935070000     1.760621190000    R=2.00
47 H      1.161081340000     1.006869180000     3.213788320000    R=1.30
48 C      4.858359400000     2.821947160000    -1.481664820000    R=2.00
49 C      5.934540650000     1.917051630000    -1.573484050000    R=2.00
50 C      7.122869560000     2.291814420000    -2.208533470000    R=2.00
51 C      7.250048600000     3.566520980000    -2.764082370000    R=2.00
52 C      6.186623080000     4.468260010000    -2.691511540000    R=2.00
53 C      4.995882120000     4.099285690000    -2.058452290000    R=2.00
54 H      5.855929030000     0.913252580000    -1.178069170000    R=1.30
55 H      7.944335190000     1.590095660000    -2.275190270000    R=1.30
56 H      8.170807690000     3.853796730000    -3.255156970000    R=1.30
57 H      6.284680490000     5.454952650000    -3.125568500000    R=1.30
END

GUIBONDS
1 2 11 1
2 3 12 1
3 4 13 1
```

4 5 14 2
5 6 15 2
6 7 16 2
7 8 11 2
8 8 14 1
9 9 12 2
10 9 15 1
11 10 13 2
12 10 16 1
13 17 46 1.0
14 12 18 1
15 13 19 1
16 20 53 1.0
17 15 21 1
18 16 22 1
19 2 1 1.0
20 3 1 1.0
21 4 1 1.0
22 23 8 1.0
23 24 9 1.0
24 25 10 1.0
25 26 22 1.0
26 27 22 1.0
27 28 22 1.0
28 29 18 1.0
29 30 18 1.0
30 31 18 1.0
31 32 19 1.0
32 33 19 1.0
33 34 19 1.0
34 36 44 1.0
35 37 45 1.0
36 41 11 1
37 38 21 1.0
38 39 21 1.0
39 40 21 1.0
40 41 42 1.5
41 42 43 1.5
42 43 44 1.5
43 44 45 1.5
44 45 46 1.5
45 46 41 1.5
46 47 42 1.0
47 35 43 1.0
48 48 49 1.5
49 49 50 1.5

```
50 50 51 1.5
51 51 52 1.5
52 52 53 1.5
53 53 48 1.5
54 54 49 1.0
55 55 50 1.0
56 56 51 1.0
57 57 52 1.0
58 48 14 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
```

```
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-XIV

ATOMS
1 Cr     -0.120016780000      0.218683650000      1.214387160000     R=1.875
```

2 O	1.193496080000	1.347879440000	0.364126030000	R=1.72
3 O	-1.474441120000	0.903353220000	0.026973970000	R=1.72
4 O	0.261330340000	-1.194583320000	-0.041543720000	R=1.72
5 O	2.553447250000	3.015258750000	-1.137606580000	R=1.72
6 O	-3.140199730000	1.493753720000	-1.930889670000	R=1.72
7 O	1.189337320000	-2.793187780000	-1.923574930000	R=1.72
8 C	3.556334750000	1.416935100000	0.267870000000	R=2.00
9 C	-3.296493630000	2.394778600000	0.247488720000	R=2.00
10 C	-0.156948740000	-3.520749630000	-0.123936000000	R=2.00
11 C	2.424070690000	0.923374560000	0.811010000000	R=2.00
12 C	-2.237129450000	1.757969790000	0.786243310000	R=2.00
13 C	-0.303770990000	-2.329422160000	0.489792400000	R=2.00
14 C	3.584611250000	2.444176150000	-0.811959950000	R=2.00
15 C	-3.732293720000	2.238530860000	-1.163801670000	R=2.00
16 C	0.611472470000	-3.722022160000	-1.378565280000	R=2.00
17 H	3.846373480000	-1.409821720000	0.851825660000	R=1.30
18 C	-1.865844450000	1.973391870000	2.227152680000	R=2.00
19 C	-1.097712830000	-2.218278750000	1.761798420000	R=2.00
20 H	4.186415400000	4.817176270000	-2.009049570000	R=1.30
21 C	-4.920349560000	3.006965790000	-1.655976430000	R=2.00
22 C	0.681446740000	-5.089681990000	-1.985855620000	R=2.00
23 H	4.507371120000	1.071960070000	0.662748100000	R=1.30
24 H	-3.878929780000	3.068480260000	0.870607310000	R=1.30
25 H	-0.622439650000	-4.399940190000	0.313994910000	R=1.30
26 H	1.289545300000	-5.077108680000	-2.915644730000	R=1.30
27 H	-0.342348400000	-5.440686720000	-2.233215500000	R=1.30
28 H	1.145075230000	-5.795033490000	-1.264765080000	R=1.30
29 H	-1.885445140000	1.001538670000	2.763013400000	R=1.30
30 H	-2.562013440000	2.670897240000	2.740244020000	R=1.30
31 H	-0.841770280000	2.397267330000	2.282920220000	R=1.30
32 H	-0.445527320000	-1.836269740000	2.572680120000	R=1.30
33 H	-1.516095210000	-3.196323550000	2.082444950000	R=1.30
34 H	-1.939186590000	-1.510753580000	1.610491910000	R=1.30
35 H	1.256971920000	-0.672227980000	5.020614060000	R=1.30
36 H	2.638405340000	-2.713440920000	4.755721260000	R=1.30
37 H	3.932469360000	-3.073946730000	2.672420510000	R=1.30
38 H	-5.815664230000	2.732150350000	-1.059902470000	R=1.30
39 H	-5.119652990000	2.781256080000	-2.725504190000	R=1.30
40 H	-4.730542620000	4.095597310000	-1.549830840000	R=1.30
41 C	2.496823020000	-0.077201980000	1.900174200000	R=2.00
42 C	1.766702950000	0.118698150000	3.083565060000	R=2.00
43 C	1.821802350000	-0.828439930000	4.110736160000	R=2.00
44 C	2.600662510000	-1.979066820000	3.961655450000	R=2.00
45 C	3.331059460000	-2.181521420000	2.787637780000	R=2.00
46 C	3.283975760000	-1.233935070000	1.760621190000	R=2.00
47 H	1.161081340000	1.006869180000	3.213788320000	R=1.30

48 C 4.858359400000 2.821947160000 -1.481664820000 R=2.00
49 C 5.934540650000 1.917051630000 -1.573484050000 R=2.00
50 C 7.122869560000 2.291814420000 -2.208533470000 R=2.00
51 C 7.250048600000 3.566520980000 -2.764082370000 R=2.00
52 C 6.186623080000 4.468260010000 -2.691511540000 R=2.00
53 C 4.995882120000 4.099285690000 -2.058452290000 R=2.00
54 H 5.855929030000 0.913252580000 -1.178069170000 R=1.30
55 H 7.944335190000 1.590095660000 -2.275190270000 R=1.30
56 H 8.170807690000 3.853796730000 -3.255156970000 R=1.30
57 H 6.284680490000 5.454952650000 -3.125568500000 R=1.30
END

GUIBONDS
1 2 11 1
2 3 12 1
3 4 13 1
4 5 14 2
5 6 15 2
6 7 16 2
7 8 11 2
8 8 14 1
9 9 12 2
10 9 15 1
11 10 13 2
12 10 16 1
13 17 46 1.0
14 12 18 1
15 13 19 1
16 20 53 1.0
17 15 21 1
18 16 22 1
19 2 1 1.0
20 3 1 1.0
21 4 1 1.0
22 23 8 1.0
23 24 9 1.0
24 25 10 1.0
25 26 22 1.0
26 27 22 1.0
27 28 22 1.0
28 29 18 1.0
29 30 18 1.0
30 31 18 1.0
31 32 19 1.0
32 33 19 1.0
33 34 19 1.0

```
34 36 44 1.0
35 37 45 1.0
36 41 11 1
37 38 21 1.0
38 39 21 1.0
39 40 21 1.0
40 41 42 1.5
41 42 43 1.5
42 43 44 1.5
43 44 45 1.5
44 45 46 1.5
45 46 41 1.5
46 47 42 1.0
47 35 43 1.0
48 48 49 1.5
49 49 50 1.5
50 50 51 1.5
51 51 52 1.5
52 52 53 1.5
53 53 48 1.5
54 54 49 1.0
55 55 50 1.0
56 56 51 1.0
57 57 52 1.0
58 48 14 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END
```

```
XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
```

TITLE metalcomplex-XV

ATOMS

1 Cr	5.442700000000	5.213800000000	4.321900000000	R=1.875
2 O	6.472800000000	6.691800000000	5.092500000000	R=1.72
3 O	3.948700000000	6.424900000000	3.985400000000	R=1.72
4 O	6.222300000000	5.717500000000	2.607400000000	R=1.72
5 O	4.421400000000	3.805200000000	3.447800000000	R=1.72
6 O	6.930900000000	3.973200000000	4.635000000000	R=1.72
7 O	4.666100000000	4.764800000000	6.065100000000	R=1.72
8 C	6.240800000000	7.937700000000	4.896800000000	R=2.00
9 C	5.094700000000	8.470700000000	4.296700000000	R=2.00
10 H	5.057100000000	9.410400000000	4.159700000000	R=1.30
11 C	3.996100000000	7.697700000000	3.885600000000	R=2.00
12 C	5.780300000000	5.429800000000	1.442200000000	R=2.00
13 C	4.688300000000	4.571500000000	1.207500000000	R=2.00
14 H	4.328200000000	4.531300000000	0.329400000000	R=1.30
15 C	4.105700000000	3.774700000000	2.199800000000	R=2.00
16 C	7.086800000000	3.197400000000	5.628800000000	R=2.00
17 C	6.241600000000	3.131300000000	6.743000000000	R=2.00
18 H	6.464200000000	2.514600000000	7.431200000000	R=1.30
19 C	5.098000000000	3.907200000000	6.912900000000	R=2.00
20 C	7.326000000000	8.854000000000	5.347800000000	R=2.00
21 C	8.656400000000	8.489200000000	5.111000000000	R=2.00
22 H	8.852100000000	7.662700000000	4.685000000000	R=1.30
23 C	9.692200000000	9.333400000000	5.496900000000	R=2.00
24 H	10.593500000000	9.092800000000	5.316000000000	R=1.30
25 C	9.409600000000	10.530700000000	6.147900000000	R=2.00
26 H	10.119000000000	11.103000000000	6.415300000000	R=1.30
27 C	8.090100000000	10.892800000000	6.407500000000	R=2.00
28 H	7.898700000000	11.703000000000	6.865600000000	R=1.30
29 C	7.054200000000	10.063800000000	5.994100000000	R=2.00
30 H	6.153000000000	10.321600000000	6.151200000000	R=1.30
31 C	2.782400000000	8.329600000000	3.286600000000	R=2.00
32 C	2.651700000000	9.710500000000	3.104000000000	R=2.00
33 H	3.350500000000	10.290300000000	3.384200000000	R=1.30
34 C	1.509600000000	10.244000000000	2.515500000000	R=2.00
35 H	1.430800000000	11.184000000000	2.398800000000	R=1.30
36 C	0.486200000000	9.408600000000	2.099700000000	R=2.00
37 H	-0.291200000000	9.772600000000	1.694200000000	R=1.30
38 C	0.601500000000	8.033700000000	2.278900000000	R=2.00
39 H	-0.100300000000	7.459100000000	1.997100000000	R=1.30
40 C	1.737900000000	7.496700000000	2.867800000000	R=2.00
41 H	1.807000000000	6.556800000000	2.988100000000	R=1.30
42 C	6.536300000000	6.028800000000	0.310500000000	R=2.00

```
43 C      7.421700000000      7.082000000000      0.570000000000    R=2.00
44 H      7.482600000000      7.443600000000      1.446800000000    R=1.30
45 C      8.210400000000      7.600800000000     -0.448800000000    R=2.00
46 H      8.798100000000      8.325700000000     -0.271000000000    R=1.30
47 C      8.141300000000      7.061600000000     -1.729900000000    R=2.00
48 H      8.703800000000      7.398700000000     -2.416900000000    R=1.30
49 C      7.250800000000      6.031000000000     -2.004200000000    R=2.00
50 H      7.193800000000      5.672300000000     -2.882400000000    R=1.30
51 C      6.442700000000      5.525200000000     -0.991100000000    R=2.00
52 H      5.822000000000      4.832200000000     -1.184100000000    R=1.30
53 C      3.057000000000      2.774600000000      1.845700000000    R=2.00
54 C      2.813300000000      2.361400000000      0.531200000000    R=2.00
55 H      3.323000000000      2.729700000000     -0.180700000000    R=1.30
56 C      1.833500000000      1.418900000000      0.259300000000    R=2.00
57 H      1.676700000000      1.144300000000     -0.636500000000    R=1.30
58 C      1.078000000000      0.873700000000      1.295700000000    R=2.00
59 H      0.404400000000      0.230400000000      1.107700000000    R=1.30
60 C      1.314400000000      1.275600000000      2.605700000000    R=2.00
61 H      0.797400000000      0.909300000000      3.313300000000    R=1.30
62 C      2.302600000000      2.210800000000      2.882600000000    R=2.00
63 H      2.467900000000      2.470300000000      3.781600000000    R=1.30
64 C      8.275500000000      2.275700000000      5.583800000000    R=2.00
65 H      8.791300000000      2.448400000000      4.768400000000    R=1.30
66 H      7.967700000000      1.345200000000      5.585600000000    R=1.30
67 H      8.840800000000      2.433500000000      6.368000000000    R=1.30
68 C      4.295600000000      3.779300000000      8.176900000000    R=2.00
69 H      4.418300000000      4.582600000000      8.723800000000    R=1.30
70 H      4.598000000000      2.993500000000      8.677900000000    R=1.30
71 H      3.347300000000      3.678100000000      7.952400000000    R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 12 1.0
10 5 15 1.0
11 6 16 1.0
12 7 19 1.0
13 8 9 1.0
14 8 20 1
```

15 9 10 1
16 9 11 1.0
17 11 31 1
18 12 13 1.0
19 12 42 1
20 13 14 1
21 13 15 1.0
22 15 53 1
23 16 17 1.0
24 16 64 1
25 17 18 1
26 17 19 1.0
27 19 68 1
28 20 21 1.5
29 20 29 1.5
30 21 22 1
31 21 23 1.5
32 23 24 1
33 23 25 1.5
34 25 26 1
35 25 27 1.5
36 27 28 1
37 27 29 1.5
38 29 30 1
39 31 32 1.5
40 31 40 1.5
41 32 33 1
42 32 34 1.5
43 34 35 1
44 34 36 1.5
45 36 37 1
46 36 38 1.5
47 38 39 1
48 38 40 1.5
49 40 41 1
50 42 43 1.5
51 42 51 1.5
52 43 44 1
53 43 45 1.5
54 45 46 1
55 45 47 1.5
56 47 48 1
57 47 49 1.5
58 49 50 1
59 49 51 1.5
60 51 52 1

```
61 53 54 1.5
62 53 62 1.5
63 54 55 1
64 54 56 1.5
65 56 57 1
66 56 58 1.5
67 58 59 1
68 58 60 1.5
69 60 61 1
70 60 62 1.5
71 62 63 1
72 64 65 1
73 64 66 1
74 64 67 1
75 68 69 1
76 68 70 1
77 68 71 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
```

```
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE metalcomplex-XV

ATOMS
1 Cr      5.442700000000      5.213800000000      4.321900000000    R=1.875
2 O       6.472800000000      6.691800000000      5.092500000000    R=1.72
3 O       3.948700000000      6.424900000000      3.985400000000    R=1.72
4 O       6.222300000000      5.717500000000      2.607400000000    R=1.72
5 O       4.421400000000      3.805200000000      3.447800000000    R=1.72
6 O       6.930900000000      3.973200000000      4.635000000000    R=1.72
7 O       4.666100000000      4.764800000000      6.065100000000    R=1.72
8 C       6.240800000000      7.937700000000      4.896800000000    R=2.00
9 C       5.094700000000      8.470700000000      4.296700000000    R=2.00
10 H      5.057100000000      9.410400000000      4.159700000000    R=1.30
11 C      3.996100000000      7.697700000000      3.885600000000    R=2.00
12 C      5.780300000000      5.429800000000      1.442200000000    R=2.00
13 C      4.688300000000      4.571500000000      1.207500000000    R=2.00
14 H      4.328200000000      4.531300000000      0.329400000000    R=1.30
15 C      4.105700000000      3.774700000000      2.199800000000    R=2.00
16 C      7.086800000000      3.197400000000      5.628800000000    R=2.00
17 C      6.241600000000      3.131300000000      6.743000000000    R=2.00
18 H      6.464200000000      2.514600000000      7.431200000000    R=1.30
19 C      5.098000000000      3.907200000000      6.912900000000    R=2.00
20 C      7.326000000000      8.854000000000      5.347800000000    R=2.00
21 C      8.656400000000      8.489200000000      5.111000000000    R=2.00
22 H      8.852100000000      7.662700000000      4.685000000000    R=1.30
23 C      9.692200000000      9.333400000000      5.496900000000    R=2.00
24 H     10.593500000000      9.092800000000      5.316000000000    R=1.30
25 C      9.409600000000     10.530700000000      6.147900000000    R=2.00
26 H     10.119000000000     11.103000000000      6.415300000000    R=1.30
27 C      8.090100000000     10.892800000000      6.407500000000    R=2.00
28 H      7.898700000000     11.703000000000      6.865600000000    R=1.30
29 C      7.054200000000     10.063800000000      5.994100000000    R=2.00
30 H      6.153000000000     10.321600000000      6.151200000000    R=1.30
31 C      2.782400000000      8.329600000000      3.286600000000    R=2.00
32 C      2.651700000000      9.710500000000      3.104000000000    R=2.00
33 H      3.350500000000     10.290300000000      3.384200000000    R=1.30
34 C      1.509600000000     10.244000000000      2.515500000000    R=2.00
35 H      1.430800000000     11.184000000000      2.398800000000    R=1.30
36 C      0.486200000000      9.408600000000      2.099700000000    R=2.00
37 H     -0.291200000000      9.772600000000      1.694200000000    R=1.30
38 C      0.601500000000      8.033700000000      2.278900000000    R=2.00
39 H     -0.100300000000      7.459100000000      1.997100000000    R=1.30
```

40 C 1.737900000000 7.496700000000 2.867800000000 R=2.00
41 H 1.807000000000 6.556800000000 2.988100000000 R=1.30
42 C 6.536300000000 6.028800000000 0.310500000000 R=2.00
43 C 7.421700000000 7.082000000000 0.570000000000 R=2.00
44 H 7.482600000000 7.443600000000 1.446800000000 R=1.30
45 C 8.210400000000 7.600800000000 -0.448800000000 R=2.00
46 H 8.798100000000 8.325700000000 -0.271000000000 R=1.30
47 C 8.141300000000 7.061600000000 -1.729900000000 R=2.00
48 H 8.703800000000 7.398700000000 -2.416900000000 R=1.30
49 C 7.250800000000 6.031000000000 -2.004200000000 R=2.00
50 H 7.193800000000 5.672300000000 -2.882400000000 R=1.30
51 C 6.442700000000 5.525200000000 -0.991100000000 R=2.00
52 H 5.822000000000 4.832200000000 -1.184100000000 R=1.30
53 C 3.057000000000 2.774600000000 1.845700000000 R=2.00
54 C 2.813300000000 2.361400000000 0.531200000000 R=2.00
55 H 3.323000000000 2.729700000000 -0.180700000000 R=1.30
56 C 1.833500000000 1.418900000000 0.259300000000 R=2.00
57 H 1.676700000000 1.144300000000 -0.636500000000 R=1.30
58 C 1.078000000000 0.873700000000 1.295700000000 R=2.00
59 H 0.404400000000 0.230400000000 1.107700000000 R=1.30
60 C 1.314400000000 1.275600000000 2.605700000000 R=2.00
61 H 0.797400000000 0.909300000000 3.313300000000 R=1.30
62 C 2.302600000000 2.210800000000 2.882600000000 R=2.00
63 H 2.467900000000 2.470300000000 3.781600000000 R=1.30
64 C 8.275500000000 2.275700000000 5.583800000000 R=2.00
65 H 8.791300000000 2.448400000000 4.768400000000 R=1.30
66 H 7.967700000000 1.345200000000 5.585600000000 R=1.30
67 H 8.840800000000 2.433500000000 6.368000000000 R=1.30
68 C 4.295600000000 3.779300000000 8.176900000000 R=2.00
69 H 4.418300000000 4.582600000000 8.723800000000 R=1.30
70 H 4.598000000000 2.993500000000 8.677900000000 R=1.30
71 H 3.347300000000 3.678100000000 7.952400000000 R=1.30
END

GUIBONDS
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 1 6 1
6 1 7 1
7 2 8 1.0
8 3 11 1.0
9 4 12 1.0
10 5 15 1.0
11 6 16 1.0

12 7 19 1.0
13 8 9 1.0
14 8 20 1
15 9 10 1
16 9 11 1.0
17 11 31 1
18 12 13 1.0
19 12 42 1
20 13 14 1
21 13 15 1.0
22 15 53 1
23 16 17 1.0
24 16 64 1
25 17 18 1
26 17 19 1.0
27 19 68 1
28 20 21 1.5
29 20 29 1.5
30 21 22 1
31 21 23 1.5
32 23 24 1
33 23 25 1.5
34 25 26 1
35 25 27 1.5
36 27 28 1
37 27 29 1.5
38 29 30 1
39 31 32 1.5
40 31 40 1.5
41 32 33 1
42 32 34 1.5
43 34 35 1
44 34 36 1.5
45 36 37 1
46 36 38 1.5
47 38 39 1
48 38 40 1.5
49 40 41 1
50 42 43 1.5
51 42 51 1.5
52 43 44 1
53 43 45 1.5
54 45 46 1
55 45 47 1.5
56 47 48 1
57 47 49 1.5

```
58 49 50 1
59 49 51 1.5
60 51 52 1
61 53 54 1.5
62 53 62 1.5
63 54 55 1
64 54 56 1.5
65 56 57 1
66 56 58 1.5
67 58 59 1
68 58 60 1.5
69 60 61 1
70 60 62 1.5
71 62 63 1
72 64 65 1
73 64 66 1
74 64 67 1
75 68 69 1
76 68 70 1
77 68 71 1
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

RELATIVISTIC Scalar ZORA

RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
  Quality Good
End

ZlmFit
  Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

=====
COSKF
=====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO

#! /bin/sh

==============================
The Molecule
==============================

"$ADFBIN/adf" <<eor

TITLE metalcomplex-XVI

ATOMS

1 Cr	5.404708962000	5.317945223000	4.158835943000	R=1.875
2 O	6.515571041000	6.742376401000	4.941486573000	R=1.72
3 O	3.950466140000	6.595765812000	3.794226930000	R=1.72
4 O	6.192674788000	5.707148508000	2.394644695000	R=1.72
5 O	4.296424338000	3.882334046000	3.394787193000	R=1.72
6 O	6.866266740000	4.031103980000	4.495941080000	R=1.72
7 O	4.600993703000	4.950438337000	5.926684360000	R=1.72
8 C	6.263358931000	8.012756006000	4.956415383000	R=2.00
9 C	5.080868090000	8.595615774000	4.464193676000	R=2.00
10 H	5.013515068000	9.679029457000	4.470712599000	R=1.30
11 C	3.990969789000	7.883283349000	3.932291808000	R=2.00
12 C	5.854736940000	5.188290750000	1.256756293000	R=2.00
13 C	4.889295672000	4.177864328000	1.095398301000	R=2.00
14 H	4.649914290000	3.870162415000	0.082062034770	R=1.30
15 C	4.177854913000	3.567095314000	2.144197398000	R=2.00
16 C	7.027778753000	3.304152014000	5.552942636000	R=2.00
17 C	6.175361594000	3.309094683000	6.669859848000	R=2.00
18 H	6.426221607000	2.644450381000	7.494294282000	R=1.30
19 C	5.028454692000	4.108482784000	6.809925215000	R=2.00
20 C	7.341334276000	8.867967860000	5.535577510000	R=2.00
21 C	8.639963691000	8.336734561000	5.660788300000	R=2.00
22 H	8.827404454000	7.317458658000	5.324602839000	R=1.30
23 C	9.673292112000	9.104291134000	6.198190810000	R=2.00
24 H	10.675942990000	8.681930292000	6.280469334000	R=1.30
25 C	9.425652284000	10.412389950000	6.630896717000	R=2.00
26 H	10.232563290000	11.011622070000	7.055469390000	R=1.30
27 C	8.136757702000	10.947013500000	6.521755204000	R=2.00
28 H	7.933471798000	11.961278100000	6.868116561000	R=1.30
29 C	7.102870928000	10.183857030000	5.977051617000	R=2.00
30 H	6.102628343000	10.612700390000	5.921864065000	R=1.30
31 C	2.774661441000	8.609803959000	3.462638938000	R=2.00
32 C	2.448419932000	9.903382138000	3.913197902000	R=2.00
33 H	3.077554257000	10.406581480000	4.647337062000	R=1.30
34 C	1.297206136000	10.543886420000	3.451577000000	R=2.00
35 H	1.051171534000	11.541630870000	3.817745551000	R=1.30
36 C	0.458171350300	9.907820069000	2.529293093000	R=2.00
37 H	-0.438941421200	10.412502990000	2.167480587000	R=1.30
38 C	0.772310319200	8.620782724000	2.076940278000	R=2.00
39 H	0.122933670600	8.120599838000	1.356772705000	R=1.30
40 C	1.916637406000	7.974596225000	2.544319811000	R=2.00
41 H	2.167006168000	6.973266888000	2.195298716000	R=1.30
42 C	6.557140912000	5.752690816000	0.066926822030	R=2.00
43 C	7.155239208000	7.023586042000	0.168543960400	R=2.00
44 H	7.083292522000	7.566286265000	1.110617877000	R=1.30
45 C	7.816628748000	7.586503230000	-0.922896395100	R=2.00
46 H	8.265152986000	8.577018492000	-0.832915530100	R=1.30

47 C 7.903250404000 6.884155895000 -2.130835626000 R=2.00
48 H 8.423987732000 7.322646263000 -2.983573749000 R=1.30
49 C 7.323160420000 5.614985432000 -2.239329752000 R=2.00
50 H 7.398262158000 5.056687045000 -3.173505888000 R=1.30
51 C 6.652173715000 5.053613469000 -1.151727475000 R=2.00
52 H 6.225997722000 4.055352557000 -1.249667758000 R=1.30
53 C 3.190919113000 2.485816818000 1.852937009000 R=2.00
54 C 3.242286643000 1.719217808000 0.672822874600 R=2.00
55 H 4.029993630000 1.888962477000 -0.061148248240 R=1.30
56 C 2.307068695000 0.708356193500 0.444549628800 R=2.00
57 H 2.366281874000 0.114368423600 -0.468602271400 R=1.30
58 C 1.301728688000 0.452952989300 1.384154784000 R=2.00
59 H 0.569615861900 -0.335224010900 1.201568394000 R=1.30
60 C 1.242849943000 1.208588255000 2.561243463000 R=2.00
61 H 0.460589776000 1.014927598000 3.296877656000 R=1.30
62 C 2.183132657000 2.211353051000 2.797333981000 R=2.00
63 H 2.143651169000 2.800943198000 3.712833568000 R=1.30
64 H 9.677709286000 3.984589688000 5.546467141000 R=1.30
65 H 11.649431450000 2.496611783000 5.509208567000 R=1.30
66 H 9.071525899000 -0.918411854700 5.470724263000 R=1.30
67 H 11.346339780000 0.045111133360 5.471337115000 R=1.30
68 H 5.605101256000 2.805273410000 9.145368054000 R=1.30
69 C 8.256884484000 2.376596265000 5.529716887000 R=2.00
70 C 8.085067289000 0.986885485200 5.508248258000 R=2.00
71 C 9.202800440000 0.143378118700 5.487127068000 R=2.00
72 C 10.492350680000 0.689581622400 5.487474488000 R=2.00
73 C 10.664167810000 2.079292371000 5.508943117000 R=2.00
74 C 9.546434710000 2.922799716000 5.530064317000 R=2.00
75 H 7.099803641000 0.569566093200 5.507982798000 R=1.30
76 C 4.181963014000 4.018719150000 8.093277983000 R=2.00
77 C 2.938832982000 4.660324789000 8.158454899000 R=2.00
78 C 2.169044251000 4.578694863000 9.325519612000 R=2.00
79 C 2.642385624000 3.855459286000 10.427407290000 R=2.00
80 C 3.885515629000 3.213853683000 10.362230320000 R=2.00
81 C 4.655304345000 3.295483608000 9.195165659000 R=2.00
82 H 2.577182908000 5.212903219000 7.316572303000 R=1.30
83 H 1.219247347000 5.068905064000 9.375317256000 R=1.30
84 H 2.054238864000 3.793090998000 11.319087500000 R=1.30
85 H 4.247165717000 2.661275241000 11.204112900000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0

5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 12 1.0
10 5 15 1.0
11 6 16 1.0
12 7 19 1.0
13 8 9 1.0
14 8 20 1.0
15 9 10 1.0
16 9 11 1.0
17 11 31 1.0
18 12 13 1.0
19 12 42 1.0
20 13 14 1.0
21 13 15 1.0
22 15 53 1.0
23 16 17 1.0
24 64 74 1.0
25 17 18 1.0
26 17 19 1.0
27 68 81 1.0
28 20 21 1.5
29 20 29 1.5
30 21 22 1.0
31 21 23 1.5
32 23 24 1.0
33 23 25 1.5
34 25 26 1.0
35 25 27 1.5
36 27 28 1.0
37 27 29 1.5
38 29 30 1.0
39 31 32 1.5
40 31 40 1.5
41 32 33 1.0
42 32 34 1.5
43 34 35 1.0
44 34 36 1.5
45 36 37 1.0
46 36 38 1.5
47 38 39 1.0
48 38 40 1.5
49 40 41 1.0
50 42 43 1.5

51 42 51 1.5
52 43 44 1.0
53 43 45 1.5
54 45 46 1.0
55 45 47 1.5
56 47 48 1.0
57 47 49 1.5
58 49 50 1.0
59 49 51 1.5
60 51 52 1.0
61 53 54 1.5
62 53 62 1.5
63 54 55 1.0
64 54 56 1.5
65 56 57 1.0
66 56 58 1.5
67 58 59 1.0
68 58 60 1.5
69 60 61 1.0
70 60 62 1.5
71 62 63 1.0
72 69 16 1.0
73 67 72 1.0
74 65 73 1.0
75 69 70 1.5
76 70 71 1.5
77 71 72 1.5
78 72 73 1.5
79 73 74 1.5
80 74 69 1.5
81 75 70 1.0
82 66 71 1.0
83 76 77 1.5
84 77 78 1.5
85 78 79 1.5
86 79 80 1.5
87 80 81 1.5
88 81 76 1.5
89 82 77 1.0
90 83 78 1.0
91 84 79 1.0
92 85 80 1.0
93 76 19 1.0
END

SOLVATION

```
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End
```

```
ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"\$ADFBIN/adf" <<eor
TITLE metalcomplex-XVI

ATOMS
1 Cr      5.404708962000      5.317945223000      4.158835943000     R=1.875
2 O       6.515571041000      6.742376401000      4.941486573000     R=1.72
3 O       3.950466140000      6.595765812000      3.794226930000     R=1.72
4 O       6.192674788000      5.707148508000      2.394644695000     R=1.72
5 O       4.296424338000      3.882334046000      3.394787193000     R=1.72
6 O       6.866266740000      4.031103980000      4.495941080000     R=1.72
7 O       4.600993703000      4.950438337000      5.926684360000     R=1.72
8 C       6.263358931000      8.012756006000      4.956415383000     R=2.00
9 C       5.080868090000      8.595615774000      4.464193676000     R=2.00
10 H      5.013515068000      9.679029457000      4.470712599000     R=1.30
11 C      3.990969789000      7.883283349000      3.932291808000     R=2.00
12 C      5.854736940000      5.188290750000      1.256756293000     R=2.00
13 C      4.889295672000      4.177864328000      1.095398301000     R=2.00
```

14 H	4.649914290000	3.870162415000	0.082062034770	R=1.30
15 C	4.177854913000	3.567095314000	2.144197398000	R=2.00
16 C	7.027778753000	3.304152014000	5.552942636000	R=2.00
17 C	6.175361594000	3.309094683000	6.669859848000	R=2.00
18 H	6.426221607000	2.644450381000	7.494294282000	R=1.30
19 C	5.028454692000	4.108482784000	6.809925215000	R=2.00
20 C	7.341334276000	8.867967860000	5.535577510000	R=2.00
21 C	8.639963691000	8.336734561000	5.660788300000	R=2.00
22 H	8.827404454000	7.317458658000	5.324602839000	R=1.30
23 C	9.673292112000	9.104291134000	6.198190810000	R=2.00
24 H	10.675942990000	8.681930292000	6.280469334000	R=1.30
25 C	9.425652284000	10.412389950000	6.630896717000	R=2.00
26 H	10.232563290000	11.011622070000	7.055469390000	R=1.30
27 C	8.136757702000	10.947013500000	6.521755204000	R=2.00
28 H	7.933471798000	11.961278100000	6.868116561000	R=1.30
29 C	7.102870928000	10.183857030000	5.977051617000	R=2.00
30 H	6.102628343000	10.612700390000	5.921864065000	R=1.30
31 C	2.774661441000	8.609803959000	3.462638938000	R=2.00
32 C	2.448419932000	9.903382138000	3.913197902000	R=2.00
33 H	3.077554257000	10.406581480000	4.647337062000	R=1.30
34 C	1.297206136000	10.543886420000	3.451577000000	R=2.00
35 H	1.051171534000	11.541630870000	3.817745551000	R=1.30
36 C	0.458171350300	9.907820069000	2.529293093000	R=2.00
37 H	-0.438941421200	10.412502990000	2.167480587000	R=1.30
38 C	0.772310319200	8.620782724000	2.076940278000	R=2.00
39 H	0.122933670600	8.120599838000	1.356772705000	R=1.30
40 C	1.916637406000	7.974596225000	2.544319811000	R=2.00
41 H	2.167006168000	6.973266888000	2.195298716000	R=1.30
42 C	6.557140912000	5.752690816000	0.066926822030	R=2.00
43 C	7.155239208000	7.023586042000	0.168543960400	R=2.00
44 H	7.083292522000	7.566286265000	1.110617877000	R=1.30
45 C	7.816628748000	7.586503230000	-0.922896395100	R=2.00
46 H	8.265152986000	8.577018492000	-0.832915530100	R=1.30
47 C	7.903250404000	6.884155895000	-2.130835626000	R=2.00
48 H	8.423987732000	7.322646263000	-2.983573749000	R=1.30
49 C	7.323160420000	5.614985432000	-2.239329752000	R=2.00
50 H	7.398262158000	5.056687045000	-3.173505888000	R=1.30
51 C	6.652173715000	5.053613469000	-1.151727475000	R=2.00
52 H	6.225997722000	4.055352557000	-1.249667758000	R=1.30
53 C	3.190919113000	2.485816818000	1.852937009000	R=2.00
54 C	3.242286643000	1.719217808000	0.672822874600	R=2.00
55 H	4.029993630000	1.888962477000	-0.061148248240	R=1.30
56 C	2.307068695000	0.708356193500	0.444549628800	R=2.00
57 H	2.366281874000	0.114368423600	-0.468602271400	R=1.30
58 C	1.301728688000	0.452952989300	1.384154784000	R=2.00
59 H	0.569615861900	-0.335224010900	1.201568394000	R=1.30

60 C 1.242849943000 1.208588255000 2.561243463000 R=2.00
61 H 0.460589776000 1.014927598000 3.296877656000 R=1.30
62 C 2.183132657000 2.211353051000 2.797333981000 R=2.00
63 H 2.143651169000 2.800943198000 3.712833568000 R=1.30
64 H 9.677709286000 3.984589688000 5.546467141000 R=1.30
65 H 11.649431450000 2.496611783000 5.509208567000 R=1.30
66 H 9.071525899000 -0.918411854700 5.470724263000 R=1.30
67 H 11.346339780000 0.045111133360 5.471337115000 R=1.30
68 H 5.605101256000 2.805273410000 9.145368054000 R=1.30
69 C 8.256884484000 2.376596265000 5.529716887000 R=2.00
70 C 8.085067289000 0.986885485200 5.508248258000 R=2.00
71 C 9.202800440000 0.143378118700 5.487127068000 R=2.00
72 C 10.492350680000 0.689581622400 5.487474488000 R=2.00
73 C 10.664167810000 2.079292371000 5.508943117000 R=2.00
74 C 9.546434710000 2.922799716000 5.530064317000 R=2.00
75 H 7.099803641000 0.569566093200 5.507982798000 R=1.30
76 C 4.181963014000 4.018719150000 8.093277983000 R=2.00
77 C 2.938832982000 4.660324789000 8.158454899000 R=2.00
78 C 2.169044251000 4.578694863000 9.325519612000 R=2.00
79 C 2.642385624000 3.855459286000 10.427407290000 R=2.00
80 C 3.885515629000 3.213853683000 10.362230320000 R=2.00
81 C 4.655304345000 3.295483608000 9.195165659000 R=2.00
82 H 2.577182908000 5.212903219000 7.316572303000 R=1.30
83 H 1.219247347000 5.068905064000 9.375317256000 R=1.30
84 H 2.054238864000 3.793090998000 11.319087500000 R=1.30
85 H 4.247165717000 2.661275241000 11.204112900000 R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 1 4 1.0
4 1 5 1.0
5 1 6 1.0
6 1 7 1.0
7 2 8 1.0
8 3 11 1.0
9 4 12 1.0
10 5 15 1.0
11 6 16 1.0
12 7 19 1.0
13 8 9 1.0
14 8 20 1.0
15 9 10 1.0
16 9 11 1.0
17 11 31 1.0

18 12 13 1.0
19 12 42 1.0
20 13 14 1.0
21 13 15 1.0
22 15 53 1.0
23 16 17 1.0
24 64 74 1.0
25 17 18 1.0
26 17 19 1.0
27 68 81 1.0
28 20 21 1.5
29 20 29 1.5
30 21 22 1.0
31 21 23 1.5
32 23 24 1.0
33 23 25 1.5
34 25 26 1.0
35 25 27 1.5
36 27 28 1.0
37 27 29 1.5
38 29 30 1.0
39 31 32 1.5
40 31 40 1.5
41 32 33 1.0
42 32 34 1.5
43 34 35 1.0
44 34 36 1.5
45 36 37 1.0
46 36 38 1.5
47 38 39 1.0
48 38 40 1.5
49 40 41 1.0
50 42 43 1.5
51 42 51 1.5
52 43 44 1.0
53 43 45 1.5
54 45 46 1.0
55 45 47 1.5
56 47 48 1.0
57 47 49 1.5
58 49 50 1.0
59 49 51 1.5
60 51 52 1.0
61 53 54 1.5
62 53 62 1.5
63 54 55 1.0

```
64 54 56 1.5
65 56 57 1.0
66 56 58 1.5
67 58 59 1.0
68 58 60 1.5
69 60 61 1.0
70 60 62 1.5
71 62 63 1.0
72 69 16 1.0
73 67 72 1.0
74 65 73 1.0
75 69 70 1.5
76 70 71 1.5
77 71 72 1.5
78 72 73 1.5
79 73 74 1.5
80 74 69 1.5
81 75 70 1.0
82 66 71 1.0
83 76 77 1.5
84 77 78 1.5
85 78 79 1.5
86 79 80 1.5
87 80 81 1.5
88 81 76 1.5
89 82 77 1.0
90 83 78 1.0
91 84 79 1.0
92 85 80 1.0
93 76 19 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

CHARGE 0.0 3.0

UNRESTRICTED
```

```
BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"\$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
#! /bin/sh

# ==============================
# The Molecule
# ==============================


"$ADFBIN/adf" <<eor
TITLE c6h12

ATOMS
1 C     -1.271148401000     -0.733897871500      0.228393178100     R=2.00
2 C      0.000000000000      1.467795743000      0.228393178100     R=2.00
3 C     -1.271148401000      0.733897871500     -0.228393178100     R=2.00
4 C      0.000000000000     -1.467795743000     -0.228393178100     R=2.00
5 C      1.271148401000     -0.733897871500      0.228393178100     R=2.00
6 C      1.271148401000      0.733897871500     -0.228393178100     R=2.00
7 H     -1.331796392000     -0.768913005500      1.330251475000     R=1.30
8 H      0.000000000000      1.537826011000      1.330251475000     R=1.30
9 H      0.000000000000      2.500482470000     -0.154056756700     R=1.30
10 H     -1.331796392000      0.768913005500     -1.330251475000     R=1.30
11 H     -2.165481341000      1.250241235000      0.154056756700     R=1.30
12 H      0.000000000000     -1.537826011000     -1.330251475000     R=1.30
13 H      0.000000000000     -2.500482470000      0.154056756700     R=1.30
14 H      2.165481341000     -1.250241235000     -0.154056756700     R=1.30
15 H      1.331796392000     -0.768913005500      1.330251475000     R=1.30
16 H      1.331796392000      0.768913005500     -1.330251475000     R=1.30
17 H      2.165481341000      1.250241235000      0.154056756700     R=1.30
18 H     -2.165481341000     -1.250241235000     -0.154056756700     R=1.30
END

GUIBONDS
1 2 3 1.0
2 3 1 1.0
3 1 4 1.0
4 4 5 1.0
5 5 6 1.0
6 6 2 1.0
7 7 1 1.0
8 8 2 1.0
9 9 2 1.0
10 10 3 1.0
11 11 3 1.0
12 12 4 1.0
13 13 4 1.0
14 14 5 1.0
```

```
15 15 5 1.0
16 16 6 1.0
17 17 6 1.0
18 18 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End
```

```
ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" -n $NPROC <<eor
TITLE c6h12

ATOMS
1 C     -1.271148401000     -0.733897871500      0.228393178100     R=2.00
2 C      0.000000000000      1.467795743000      0.228393178100     R=2.00
3 C     -1.271148401000      0.733897871500     -0.228393178100     R=2.00
4 C      0.000000000000     -1.467795743000     -0.228393178100     R=2.00
5 C      1.271148401000     -0.733897871500      0.228393178100     R=2.00
6 C      1.271148401000      0.733897871500     -0.228393178100     R=2.00
7 H     -1.331796392000     -0.768913005500      1.330251475000     R=1.30
8 H      0.000000000000      1.537826011000      1.330251475000     R=1.30
9 H      0.000000000000      2.500482470000     -0.154056756700     R=1.30
10 H     -1.331796392000      0.768913005500     -1.330251475000     R=1.30
11 H     -2.165481341000      1.250241235000      0.154056756700     R=1.30
12 H      0.000000000000     -1.537826011000     -1.330251475000     R=1.30
13 H      0.000000000000     -2.500482470000      0.154056756700     R=1.30
14 H      2.165481341000     -1.250241235000     -0.154056756700     R=1.30
15 H      1.331796392000     -0.768913005500      1.330251475000     R=1.30
16 H      1.331796392000      0.768913005500     -1.330251475000     R=1.30
```

```
17 H      2.165481341000      1.250241235000      0.154056756700    R=1.30
18 H     -2.165481341000     -1.250241235000     -0.154056756700    R=1.30
END

GUIBONDS
1 2 3 1.0
2 3 1 1.0
3 1 4 1.0
4 4 5 1.0
5 5 6 1.0
6 6 2 1.0
7 7 1 1.0
8 8 2 1.0
9 9 2 1.0
10 10 3 1.0
11 11 3 1.0
12 12 4 1.0
13 13 4 1.0
14 14 5 1.0
15 15 5 1.0
16 16 6 1.0
17 17 6 1.0
18 18 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE diisoprpylether

ATOMS
1 O       3.422807717000       0.083829617500      -0.563716205700     R=1.72
2 C       2.732659265000       0.194620471000       0.710499924400     R=2.00
```

```
3 C      4.871556336000      0.040509950590     -0.457309842800    R=2.00
4 C      1.384337351000      0.847227703400      0.429201274700    R=2.00
5 C      2.586487974000     -1.178235677000      1.369701997000    R=2.00
6 C      5.448462710000      1.450769287000     -0.317478565600    R=2.00
7 C      5.385819791000     -0.671322315100     -1.702969643000    R=2.00
8 H      3.318930092000      0.854996567100      1.372865071000    R=1.30
9 H      5.141991406000     -0.553645938200      0.432938178000    R=1.30
10 H     5.099682911000     -0.114842691000     -2.607920569000    R=1.30
11 H     4.973358386000     -1.686944501000     -1.771344368000    R=1.30
12 H     6.481996717000     -0.740991540200     -1.676644662000    R=1.30
13 H     6.541502910000      1.406967464000     -0.206592878000    R=1.30
14 H     5.042569704000      1.965964814000      0.563774701300    R=1.30
15 H     5.213570154000      2.048183019000     -1.210718284000    R=1.30
16 H     2.090134478000     -1.081669394000      2.346104681000    R=1.30
17 H     1.980358010000     -1.842525237000      0.736102129500    R=1.30
18 H     3.564500141000     -1.650401376000      1.535666273000    R=1.30
19 H     0.793175968600      0.224402562300     -0.258738120700    R=1.30
20 H     1.517321328000      1.839251153000     -0.022935112620    R=1.30
21 H     0.814571658400      0.962210729700      1.361655238000    R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
3 2 4 1.0
4 2 5 1.0
5 2 8 1.0
6 3 6 1.0
7 3 7 1.0
8 3 9 1.0
9 4 19 1.0
10 4 20 1.0
11 4 21 1.0
12 5 16 1.0
13 5 17 1.0
14 5 18 1.0
15 6 13 1.0
16 6 14 1.0
17 6 15 1.0
18 7 10 1.0
19 7 11 1.0
20 7 12 1.0
END

SOLVATION
   Surf Delley
```

```
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor
```

```
# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE diisoprpylether

ATOMS
1 O      3.422807717000      0.083829617500     -0.563716205700     R=1.72
2 C      2.732659265000      0.194620471000      0.710499924400     R=2.00
3 C      4.871556336000      0.040509950590     -0.457309842800     R=2.00
4 C      1.384337351000      0.847227703400      0.429201274700     R=2.00
5 C      2.586487974000     -1.178235677000      1.369701997000     R=2.00
6 C      5.448462710000      1.450769287000     -0.317478565600     R=2.00
7 C      5.385819791000     -0.671322315100     -1.702969643000     R=2.00
8 H      3.318930092000      0.854996567100      1.372865071000     R=1.30
9 H      5.141991406000     -0.553645938200      0.432938178000     R=1.30
10 H     5.099682911000     -0.114842691000     -2.607920569000     R=1.30
11 H     4.973358386000     -1.686944501000     -1.771344368000     R=1.30
12 H     6.481996717000     -0.740991540200     -1.676644662000     R=1.30
13 H     6.541502910000      1.406967464000     -0.206592878000     R=1.30
14 H     5.042569704000      1.965964814000      0.563774701300     R=1.30
15 H     5.213570154000      2.048183019000     -1.210718284000     R=1.30
16 H     2.090134478000     -1.081669394000      2.346104681000     R=1.30
17 H     1.980358010000     -1.842525237000      0.736102129500     R=1.30
18 H     3.564500141000     -1.650401376000      1.535666273000     R=1.30
19 H     0.793175968600      0.224402562300     -0.258738120700     R=1.30
20 H     1.517321328000      1.839251153000     -0.022935112620     R=1.30
21 H     0.814571658400      0.962210729700      1.361655238000     R=1.30
END

GUIBONDS
1 1 2 1.0
2 1 3 1.0
```

```
3 2 4 1.0
4 2 5 1.0
5 2 8 1.0
6 3 6 1.0
7 3 7 1.0
8 3 9 1.0
9 4 19 1.0
10 4 20 1.0
11 4 21 1.0
12 5 16 1.0
13 5 17 1.0
14 5 18 1.0
15 6 13 1.0
16 6 14 1.0
17 6 15 1.0
18 7 10 1.0
19 7 11 1.0
20 7 12 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
```

```
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE butanol

ATOMS
1 C     -5.941474867000     -1.478416935000      0.000805013136     R=2.00
2 C     -5.263299893000     -0.108195508300     -0.101123190700     R=2.00
3 C     -3.744896828000     -0.177898459400      0.106327319000     R=2.00
4 C     -3.080997500000      1.186628150000      0.000198082432     R=2.00
5 O     -1.654154300000      1.029686025000      0.206016705400     R=1.72
6 H     -1.255332222000      1.917341993000      0.128166403900     R=1.30
7 H     -5.544121890000     -2.173858099000     -0.753652066500     R=1.30
8 H     -7.026717237000     -1.399456259000     -0.154317674200     R=1.30
9 H     -5.775536211000     -1.929943894000      0.990436497300     R=1.30
10 H     -5.701971758000      0.575572099700      0.644145342000     R=1.30
11 H     -5.475880351000      0.334408147200     -1.088205805000     R=1.30
```

```
12 H     -3.298355031000     -0.853235459300     -0.642347609200     R=1.30
13 H     -3.524311048000     -0.608297381900      1.097347409000     R=1.30
14 H     -3.495872178000      1.872943580000      0.758481043300     R=1.30
15 H     -3.269864035000      1.626246569000     -0.994398000700     R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 1.0
3 4 3 1.0
4 5 4 1.0
5 6 5 1.0
6 7 1 1.0
7 8 1 1.0
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
```

```
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE butanol

ATOMS
1 C     -5.941474867000     -1.478416935000      0.000805013136    R=2.00
2 C     -5.263299893000     -0.108195508300     -0.101123190700    R=2.00
3 C     -3.744896828000     -0.177898459400      0.106327319000    R=2.00
4 C     -3.080997500000      1.186628150000      0.000198082432    R=2.00
5 O     -1.654154300000      1.029686025000      0.206016705400    R=1.72
6 H     -1.255332222000      1.917341993000      0.128166403900    R=1.30
7 H     -5.544121890000     -2.173858099000     -0.753652066500    R=1.30
8 H     -7.026717237000     -1.399456259000     -0.154317674200    R=1.30
9 H     -5.775536211000     -1.929943894000      0.990436497300    R=1.30
10 H     -5.701971758000      0.575572099700      0.644145342000    R=1.30
11 H     -5.475880351000      0.334408147200     -1.088205805000    R=1.30
12 H     -3.298355031000     -0.853235459300     -0.642347609200    R=1.30
13 H     -3.524311048000     -0.608297381900      1.097347409000    R=1.30
14 H     -3.495872178000      1.872943580000      0.758481043300    R=1.30
15 H     -3.269864035000      1.626246569000     -0.994398000700    R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 1.0
3 4 3 1.0
4 5 4 1.0
5 6 5 1.0
6 7 1 1.0
7 8 1 1.0
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
```

```
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
```

```
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" -n $NPROC <<eor
TITLE hexanol

ATOMS
1 C     -5.670791575000     -1.719860405000     -0.011842237510     R=2.00
2 C     -5.223069292000     -0.256850641300     -0.098243203220     R=2.00
3 C     -3.707354100000     -0.080266045650      0.054211073150     R=2.00
4 C     -3.251322741000      1.380836295000     -0.035830468820     R=2.00
5 C     -1.734076493000      1.551505889000      0.110947513000     R=2.00
6 C     -1.303585243000      3.007108677000      0.010692093440     R=2.00
7 O      0.137652624700      3.078739740000      0.152616858100     R=1.72
8 H      0.385130008200      4.020483405000      0.081289669990     R=1.30
9 H     -5.197199079000     -2.325740657000     -0.799160952300     R=1.30
10 H     -6.760158493000     -1.815375264000     -0.125936138500     R=1.30
11 H     -5.395380459000     -2.161292156000      0.957994734700     R=1.30
12 H     -5.736048449000      0.332570338000      0.680212878400     R=1.30
13 H     -5.540950113000      0.169550520100     -1.064498994000     R=1.30
14 H     -3.193075063000     -0.670964024900     -0.723831966400     R=1.30
15 H     -3.387458222000     -0.503615385300      1.022267974000     R=1.30
16 H     -3.763673919000      1.969955603000      0.744103704100     R=1.30
17 H     -3.574763515000      1.802307685000     -1.003093290000     R=1.30
18 H     -1.216683643000      0.970945936800     -0.670749578900     R=1.30
19 H     -1.404979426000      1.146133014000      1.082081452000     R=1.30
20 H     -1.788637792000      3.604159574000      0.802211896100     R=1.30
21 H     -1.605387201000      3.427558232000     -0.964138612900     R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 1.0
3 4 3 1.0
4 5 4 1.0
5 6 5 1.0
6 7 6 1.0
7 8 7 1.0
8 9 1 1.0
```

```
9 10 1 1.0
10 11 1 1.0
11 12 2 1.0
12 13 2 1.0
13 14 3 1.0
14 15 3 1.0
15 16 4 1.0
16 17 4 1.0
17 18 5 1.0
18 19 5 1.0
19 20 6 1.0
20 21 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
```

```
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" -n $NPROC <<eor
TITLE hexanol

ATOMS
1 C     -5.670791575000     -1.719860405000     -0.011842237510     R=2.00
2 C     -5.223069292000     -0.256850641300     -0.098243203220     R=2.00
```

```
3 C     -3.707354100000     -0.080266045650      0.054211073150    R=2.00
4 C     -3.251322741000      1.380836295000     -0.035830468820    R=2.00
5 C     -1.734076493000      1.551505889000      0.110947513000    R=2.00
6 C     -1.303585243000      3.007108677000      0.010692093440    R=2.00
7 O      0.137652624700      3.078739740000      0.152616858100    R=1.72
8 H      0.385130008200      4.020483405000      0.081289669990    R=1.30
9 H     -5.197199079000     -2.325740657000     -0.799160952300    R=1.30
10 H    -6.760158493000     -1.815375264000     -0.125936138500    R=1.30
11 H    -5.395380459000     -2.161292156000      0.957994734700    R=1.30
12 H    -5.736048449000      0.332570338000      0.680212878400    R=1.30
13 H    -5.540950113000      0.169550520100     -1.064498994000    R=1.30
14 H    -3.193075063000     -0.670964024900     -0.723831966400    R=1.30
15 H    -3.387458222000     -0.503615385300      1.022267974000    R=1.30
16 H    -3.763673919000      1.969955603000      0.744103704100    R=1.30
17 H    -3.574763515000      1.802307685000     -1.003093290000    R=1.30
18 H    -1.216683643000      0.970945936800     -0.670749578900    R=1.30
19 H    -1.404979426000      1.146133014000      1.082081452000    R=1.30
20 H    -1.788637792000      3.604159574000      0.802211896100    R=1.30
21 H    -1.605387201000      3.427558232000     -0.964138612900    R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 1.0
3 4 3 1.0
4 5 4 1.0
5 6 5 1.0
6 7 6 1.0
7 8 7 1.0
8 9 1 1.0
9 10 1 1.0
10 11 1 1.0
11 12 2 1.0
12 13 2 1.0
13 14 3 1.0
14 15 3 1.0
15 16 4 1.0
16 17 4 1.0
17 18 5 1.0
18 19 5 1.0
19 20 6 1.0
20 21 6 1.0
END

SOLVATION
  Surf Delley
```

```
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
```

```
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE hexyne

ATOMS
1 C     -1.174607966000     -0.155135832000      0.259467852500    R=2.00
2 C     -0.063497183450     -1.205557288000      0.160638132700    R=2.00
3 C      1.327199567000     -0.583933772600     -0.006316226876    R=2.00
4 C      2.434710176000     -1.654480370000     -0.104216187600    R=2.00
5 C      3.774308776000     -1.094454437000     -0.266365295000    R=2.00
6 C      4.880509329000     -0.614511272500     -0.401064223500    R=2.00
7 H     -1.014883429000      0.510341468100      1.120917310000    R=1.30
8 H     -2.159872130000     -0.627393653700      0.378607598700    R=1.30
9 H     -1.209211036000      0.470547108600     -0.644844347900    R=1.30
10 H     -0.264041406700     -1.877447334000     -0.690142033600    R=1.30
11 H     -0.071003997230     -1.838168591000      1.063507727000    R=1.30
12 H      1.543321889000      0.081218287180      0.844564846100    R=1.30
13 H      1.349863055000      0.041663297840     -0.912492415900    R=1.30
14 H      2.224175426000     -2.326431764000     -0.952635356300    R=1.30
15 H      2.418913690000     -2.285179863000      0.799930847800    R=1.30
16 H      5.859171417000     -0.190781594900     -0.520304466600    R=1.30
END

GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 3.0
6 7 1 1.0
7 8 1 1.0
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
```

```
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
15 16 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End
```

```
ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE hexyne

ATOMS
1 C     -1.174607966000     -0.155135832000      0.259467852500    R=2.00
2 C     -0.063497183450     -1.205557288000      0.160638132700    R=2.00
3 C      1.327199567000     -0.583933772600     -0.006316226876    R=2.00
4 C      2.434710176000     -1.654480370000     -0.104216187600    R=2.00
5 C      3.774308776000     -1.094454437000     -0.266365295000    R=2.00
6 C      4.880509329000     -0.614511272500     -0.401064223500    R=2.00
7 H     -1.014883429000      0.510341468100      1.120917310000    R=1.30
8 H     -2.159872130000     -0.627393653700      0.378607598700    R=1.30
9 H     -1.209211036000      0.470547108600     -0.644844347900    R=1.30
10 H     -0.264041406700     -1.877447334000     -0.690142033600    R=1.30
```

```
11 H     -0.071003997230     -1.838168591000      1.063507727000    R=1.30
12 H      1.543321889000      0.081218287180      0.844564846100    R=1.30
13 H      1.349863055000      0.041663297840     -0.912492415900    R=1.30
14 H      2.224175426000     -2.326431764000     -0.952635356300    R=1.30
15 H      2.418913690000     -2.285179863000      0.799930847800    R=1.30
16 H      5.859171417000     -0.190781594900     -0.520304466600    R=1.30
END

GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 3.0
6 7 1 1.0
7 8 1 1.0
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
15 16 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO



#! /bin/sh

# ==============================
# The Molecule
# ==============================


"$ADFBIN/adf" <<eor
TITLE heptyne

ATOMS
```

```
1 C      0.379243629900     -1.644062082000     -0.184305161100     R=2.00
2 C      1.753595595000     -0.966284537500     -0.146741638500     R=2.00
3 C      2.910685339000     -1.964751612000     -0.018476038480     R=2.00
4 C      4.287020308000     -1.292096411000      0.018598061920     R=2.00
5 C      5.432117005000     -2.319388786000      0.147804122800     R=2.00
6 C      6.759465752000     -1.710144086000      0.184524988700     R=2.00
7 C      7.854711961000     -1.188714508000      0.212995146000     R=2.00
8 H      0.301899401500     -2.334420013000     -1.037854942000     R=1.30
9 H     -0.429641285100     -0.905213049700     -0.276323870900     R=1.30
10 H     0.199762167600     -2.225793388000      0.732437385800     R=1.30
11 H     1.792320364000     -0.257381060400      0.696947493500     R=1.30
12 H     1.893466517000     -0.365608217100     -1.060891649000     R=1.30
13 H     2.874465823000     -2.674473316000     -0.862922562600     R=1.30
14 H     2.773742897000     -2.565575266000      0.897217850500     R=1.30
15 H     4.337554426000     -0.589494518100      0.865170956600     R=1.30
16 H     4.438073947000     -0.698661391900     -0.896853628300     R=1.30
17 H     5.388373010000     -3.028546577000     -0.695268948900     R=1.30
18 H     5.289202479000     -2.918424691000      1.062414454000     R=1.30
19 H     8.823475569000     -0.727802672400      0.238413868800     R=1.30
END

GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 1.0
6 6 7 3.0
7 8 1 1.0
8 9 1 1.0
9 10 1 1.0
10 11 2 1.0
11 12 2 1.0
12 13 3 1.0
13 14 3 1.0
14 15 4 1.0
15 16 4 1.0
16 17 5 1.0
17 18 5 1.0
18 19 7 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
```

```
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
```

```
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE heptyne

ATOMS
1 C      0.379243629900     -1.644062082000     -0.184305161100     R=2.00
2 C      1.753595595000     -0.966284537500     -0.146741638500     R=2.00
3 C      2.910685339000     -1.964751612000     -0.018476038480     R=2.00
4 C      4.287020308000     -1.292096411000      0.018598061920     R=2.00
5 C      5.432117005000     -2.319388786000      0.147804122800     R=2.00
6 C      6.759465752000     -1.710144086000      0.184524988700     R=2.00
7 C      7.854711961000     -1.188714508000      0.212995146000     R=2.00
8 H      0.301899401500     -2.334420013000     -1.037854942000     R=1.30
9 H     -0.429641285100     -0.905213049700     -0.276323870900     R=1.30
10 H     0.199762167600     -2.225793388000      0.732437385800     R=1.30
11 H     1.792320364000     -0.257381060400      0.696947493500     R=1.30
12 H     1.893466517000     -0.365608217100     -1.060891649000     R=1.30
13 H     2.874465823000     -2.674473316000     -0.862922562600     R=1.30
14 H     2.773742897000     -2.565575266000      0.897217850500     R=1.30
15 H     4.337554426000     -0.589494518100      0.865170956600     R=1.30
16 H     4.438073947000     -0.698661391900     -0.896853628300     R=1.30
17 H     5.388373010000     -3.028546577000     -0.695268948900     R=1.30
18 H     5.289202479000     -2.918424691000      1.062414454000     R=1.30
19 H     8.823475569000     -0.727802672400      0.238413868800     R=1.30
END
```

```
GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 1.0
6 6 7 3.0
7 8 1 1.0
8 9 1 1.0
9 10 1 1.0
10 11 2 1.0
11 12 2 1.0
12 13 3 1.0
13 14 3 1.0
14 15 4 1.0
15 16 4 1.0
16 17 5 1.0
17 18 5 1.0
18 19 7 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE 1-hexene

ATOMS
1 C     -1.374095589000      0.559723525900     -0.448497628900     R=2.00
2 C     -0.150187230800      1.427627727000     -0.138684702100     R=2.00
3 C      1.139962172000      0.613535959200      0.016972549460     R=2.00
4 C      2.368458580000      1.484690311000      0.339810370900     R=2.00
5 C      3.622642677000      0.682753033700      0.542547645700     R=2.00
6 C      4.750062976000      0.813494625500     -0.166811921500     R=2.00
```

```
7 H     -1.235202117000     -0.001340868748     -1.385118568000     R=1.30
8 H     -2.282272703000      1.170127385000     -0.555580781100     R=1.30
9 H     -1.554195220000     -0.171614750900      0.353983558100     R=1.30
10 H     -0.327899482700      2.000969370000      0.786549479200     R=1.30
11 H     -0.013379574740      2.172545114000     -0.940191916300     R=1.30
12 H      1.330904006000      0.045555539060     -0.909183191400     R=1.30
13 H      1.005943487000     -0.134343611300      0.817066009600     R=1.30
14 H      2.154094991000      2.052543358000      1.263463923000     R=1.30
15 H      2.526008538000      2.225483161000     -0.460732232100     R=1.30
16 H      3.583774290000     -0.072122125520      1.337822384000     R=1.30
17 H      4.833272721000      1.550926217000     -0.970256167600     R=1.30
18 H      5.625446614000      0.192105681700      0.032005753750     R=1.30
END

GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 2.0
6 7 1 1.0
7 8 1 1.0
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
15 16 5 1.0
16 17 6 1.0
17 18 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
```

```
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE 1-hexene

ATOMS
1 C     -1.374095589000      0.559723525900     -0.448497628900     R=2.00
2 C     -0.150187230800      1.427627727000     -0.138684702100     R=2.00
3 C      1.139962172000      0.613535959200      0.016972549460     R=2.00
4 C      2.368458580000      1.484690311000      0.339810370900     R=2.00
5 C      3.622642677000      0.682753033700      0.542547645700     R=2.00
6 C      4.750062976000      0.813494625500     -0.166811921500     R=2.00
7 H     -1.235202117000     -0.001340868748     -1.385118568000     R=1.30
8 H     -2.282272703000      1.170127385000     -0.555580781100     R=1.30
9 H     -1.554195220000     -0.171614750900      0.353983558100     R=1.30
10 H     -0.327899482700      2.000969370000      0.786549479200     R=1.30
11 H     -0.013379574740      2.172545114000     -0.940191916300     R=1.30
12 H      1.330904006000      0.045555539060     -0.909183191400     R=1.30
13 H      1.005943487000     -0.134343611300      0.817066009600     R=1.30
14 H      2.154094991000      2.052543358000      1.263463923000     R=1.30
15 H      2.526008538000      2.225483161000     -0.460732232100     R=1.30
16 H      3.583774290000     -0.072122125520      1.337822384000     R=1.30
17 H      4.833272721000      1.550926217000     -0.970256167600     R=1.30
18 H      5.625446614000      0.192105681700      0.032005753750     R=1.30
END

GUIBONDS
1 1 2 1.0
2 2 3 1.0
3 3 4 1.0
4 4 5 1.0
5 5 6 2.0
6 7 1 1.0
7 8 1 1.0
```

```
8 9 1 1.0
9 10 2 1.0
10 11 2 1.0
11 12 3 1.0
12 13 3 1.0
13 14 4 1.0
14 15 4 1.0
15 16 5 1.0
16 17 6 1.0
17 18 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
```

```
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================


"$ADFBIN/adf" <<eor
TITLE benzene

ATOMS
1 C       0.000000000000       1.400070903000       0.000000000000     R=2.00
2 C      -1.212496969000       0.700035451500       0.000000000000     R=2.00
3 C      -1.212496969000      -0.700035451500       0.000000000000     R=2.00
4 C       0.000000000000      -1.400070903000       0.000000000000     R=2.00
5 C       1.212496969000      -0.700035451500       0.000000000000     R=2.00
6 C       1.212496969000       0.700035451500       0.000000000000     R=2.00
7 H      -2.157791421000       1.245801458000       0.000000000000     R=1.30
8 H      -2.157791421000      -1.245801458000       0.000000000000     R=1.30
9 H       0.000000000000      -2.491602916000       0.000000000000     R=1.30
10 H      2.157791421000      -1.245801458000       0.000000000000     R=1.30
11 H      2.157791421000       1.245801458000       0.000000000000     R=1.30
12 H      0.000000000000       2.491602916000       0.000000000000     R=1.30
END

GUIBONDS
```

```
1 1 2 1.5
2 2 3 1.5
3 3 4 1.5
4 4 5 1.5
5 5 6 1.5
6 6 1 1.5
7 7 2 1.0
8 8 3 1.0
9 9 4 1.0
10 10 5 1.0
11 11 6 1.0
12 12 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
```

```
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE benzene

ATOMS
1 C       0.000000000000       1.400070903000       0.000000000000     R=2.00
2 C      -1.212496969000       0.700035451500       0.000000000000     R=2.00
```

```
3 C     -1.212496969000     -0.700035451500      0.000000000000    R=2.00
4 C      0.000000000000     -1.400070903000      0.000000000000    R=2.00
5 C      1.212496969000     -0.700035451500      0.000000000000    R=2.00
6 C      1.212496969000      0.700035451500      0.000000000000    R=2.00
7 H     -2.157791421000      1.245801458000      0.000000000000    R=1.30
8 H     -2.157791421000     -1.245801458000      0.000000000000    R=1.30
9 H      0.000000000000     -2.491602916000      0.000000000000    R=1.30
10 H     2.157791421000     -1.245801458000      0.000000000000    R=1.30
11 H     2.157791421000      1.245801458000      0.000000000000    R=1.30
12 H     0.000000000000      2.491602916000      0.000000000000    R=1.30
END

GUIBONDS
1 1 2 1.5
2 2 3 1.5
3 3 4 1.5
4 4 5 1.5
5 5 6 1.5
6 6 1 1.5
7 7 2 1.0
8 8 3 1.0
9 9 4 1.0
10 10 5 1.0
11 11 6 1.0
12 12 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE 13do

ATOMS
1 O      1.160635966000     -0.383470227700      0.053626243520     R=1.72
```

```
2 O      -1.160822831000      -0.383040108400      -0.053162533770     R=1.72
3 C       0.707211567400       0.953599319200      -0.277027689600     R=2.00
4 C      -0.706748287100       0.954063847500       0.276511741400     R=2.00
5 C      -0.000176788131      -1.228281444000      -0.000357813516     R=2.00
6 H       0.714744043500       1.107750041000      -1.368475718000     R=1.30
7 H       1.380066578000       1.666352770000       0.213030098800     R=1.30
8 H      -0.714191957900       1.108982936000       1.367846711000     R=1.30
9 H      -1.379287453000       1.666797804000      -0.214021742900     R=1.30
10 H      -0.001513548581      -1.850882471000      -0.910106775300     R=1.30
11 H       0.000975040414      -1.852104075000       0.908525682400     R=1.30
END

GUIBONDS
1 1 3 1.0
2 1 5 1.0
3 2 4 1.0
4 2 5 1.0
5 3 4 1.0
6 3 6 1.0
7 3 7 1.0
8 4 8 1.0
9 4 9 1.0
10 5 10 1.0
11 5 11 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21
```

```
# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE 13do

ATOMS
1 O       1.160635966000     -0.383470227700      0.053626243520     R=1.72
2 O      -1.160822831000     -0.383040108400     -0.053162533770     R=1.72
3 C       0.707211567400      0.953599319200     -0.277027689600     R=2.00
4 C      -0.706748287100      0.954063847500      0.276511741400     R=2.00
5 C      -0.000176788131     -1.228281444000     -0.000357813516     R=2.00
6 H       0.714744043500      1.107750041000     -1.368475718000     R=1.30
7 H       1.380066578000      1.666352770000      0.213030098800     R=1.30
8 H      -0.714191957900      1.108982936000      1.367846711000     R=1.30
9 H      -1.379287453000      1.666797804000     -0.214021742900     R=1.30
10 H     -0.001513548581     -1.850882471000     -0.910106775300     R=1.30
11 H      0.000975040414     -1.852104075000      0.908525682400     R=1.30
END

GUIBONDS
1 1 3 1.0
2 1 5 1.0
3 2 4 1.0
4 2 5 1.0
5 3 4 1.0
6 3 6 1.0
7 3 7 1.0
8 4 8 1.0
9 4 9 1.0
10 5 10 1.0
11 5 11 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END
```

```
BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE acn

ATOMS
1 C       0.000000000000       0.000000000000      -3.847553338000     R=2.00
2 C       0.000000000000       0.000000000000      -2.394526590000     R=2.00
3 N       0.000000000000       0.000000000000      -1.230767850000     R=1.83
4 H      -0.516688183000       0.894930184600      -4.217198118000     R=1.30
5 H      -0.516688183000      -0.894930184600      -4.217198118000     R=1.30
6 H       1.033376366000       0.000000000000      -4.217198118000     R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 3.0
3 4 1 1.0
4 5 1 1.0
5 6 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21
```

```
# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE acn

ATOMS
1 C      0.000000000000      0.000000000000     -3.847553338000     R=2.00
2 C      0.000000000000      0.000000000000     -2.394526590000     R=2.00
3 N      0.000000000000      0.000000000000     -1.230767850000     R=1.83
4 H     -0.516688183000      0.894930184600     -4.217198118000     R=1.30
5 H     -0.516688183000     -0.894930184600     -4.217198118000     R=1.30
6 H      1.033376366000      0.000000000000     -4.217198118000     R=1.30
END

GUIBONDS
1 2 1 1.0
2 3 2 3.0
3 4 1 1.0
4 5 1 1.0
5 6 1 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END
```

```
RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


#! /bin/sh

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE dmpu

ATOMS
1 O      2.628583077000     -3.428601648000      0.000079817254     R=1.72
2 C      2.007857721000     -2.338003994000     -0.058365939340     R=2.00
```

3 N 2.682471777000 -1.133699009000 -0.131087033100 R=1.83
4 C 4.123912702000 -1.124367512000 0.097372243710 R=2.00
5 C 2.010722328000 0.163018139400 0.019391554150 R=2.00
6 C 0.609427776200 0.108332118800 -0.567932849600 R=2.00
7 C -0.143241262600 -1.065866123000 0.036679963800 R=2.00
8 N 0.627679628500 -2.304848214000 -0.123391306200 R=1.83
9 C -0.108978467300 -3.543035078000 0.109266479700 R=2.00
10 H 4.586379638000 -0.364729440000 -0.547661701700 R=1.30
11 H 4.534857192000 -2.107947544000 -0.143798711000 R=1.30
12 H 4.364251976000 -0.883031431200 1.147574769000 R=1.30
13 H 2.620797231000 0.916215427100 -0.499307716900 R=1.30
14 H 1.973314355000 0.448720965900 1.087251297000 R=1.30
15 H 0.666577949200 -0.007722733623 -1.660761741000 R=1.30
16 H 0.077267084840 1.044669548000 -0.354541448000 R=1.30
17 H -1.110717774000 -1.208527160000 -0.465143004900 R=1.30
18 H -0.351896182300 -0.882614952600 1.107234622000 R=1.30
19 H 0.514374233400 -4.395068097000 -0.173486463500 R=1.30
20 H -1.021198361000 -3.536626106000 -0.502226775400 R=1.30
21 H -0.399715508200 -3.649816881000 1.168990208000 R=1.30
END

GUIBONDS
1 1 2 2.0
2 2 3 1.0
3 2 8 1.0
4 3 4 1.0
5 3 5 1.0
6 5 6 1.0
7 6 7 1.0
8 7 8 1.0
9 8 9 1.0
10 10 4 1.0
11 11 4 1.0
12 12 4 1.0
13 13 5 1.0
14 14 5 1.0
15 15 6 1.0
16 16 6 1.0
17 17 7 1.0
18 18 7 1.0
19 19 9 1.0
20 20 9 1.0
21 21 9 1.0
END

SOLVATION

```
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE
```

```
eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE dmpu

ATOMS
1 O      2.628583077000     -3.428601648000      0.000079817254     R=1.72
2 C      2.007857721000     -2.338003994000     -0.058365939340     R=2.00
3 N      2.682471777000     -1.133699009000     -0.131087033100     R=1.83
4 C      4.123912702000     -1.124367512000      0.097372243710     R=2.00
5 C      2.010722328000      0.163018139400      0.019391554150     R=2.00
6 C      0.609427776200      0.108332118800     -0.567932849600     R=2.00
7 C     -0.143241262600     -1.065866123000      0.036679963800     R=2.00
8 N      0.627679628500     -2.304848214000     -0.123391306200     R=1.83
9 C     -0.108978467300     -3.543035078000      0.109266479700     R=2.00
10 H     4.586379638000     -0.364729440000     -0.547661701700     R=1.30
11 H     4.534857192000     -2.107947544000     -0.143798711000     R=1.30
12 H     4.364251976000     -0.883031431200      1.147574769000     R=1.30
13 H     2.620797231000      0.916215427100     -0.499307716900     R=1.30
14 H     1.973314355000      0.448720965900      1.087251297000     R=1.30
15 H     0.666577949200     -0.007722733623     -1.660761741000     R=1.30
16 H     0.077267084840      1.044669548000     -0.354541448000     R=1.30
17 H    -1.110717774000     -1.208527160000     -0.465143004900     R=1.30
```

```
18 H     -0.351896182300     -0.882614952600      1.107234622000    R=1.30
19 H      0.514374233400     -4.395068097000     -0.173486463500    R=1.30
20 H     -1.021198361000     -3.536626106000     -0.502226775400    R=1.30
21 H     -0.399715508200     -3.649816881000      1.168990208000    R=1.30
END

GUIBONDS
1 1 2 2.0
2 2 3 1.0
3 2 8 1.0
4 3 4 1.0
5 3 5 1.0
6 5 6 1.0
7 6 7 1.0
8 7 8 1.0
9 8 9 1.0
10 10 4 1.0
11 11 4 1.0
12 12 4 1.0
13 13 5 1.0
14 14 5 1.0
15 15 6 1.0
16 16 6 1.0
17 17 7 1.0
18 18 7 1.0
19 19 9 1.0
20 20 9 1.0
21 21 9 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END
```

```
XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO


"$ADFBIN/adf" -n $NPROC <<eor
TITLE gbl

ATOMS
1 O      0.069437547570     -1.120676765000     -0.036426434080     R=1.72
2 O      2.033473021000     -0.016858780270     -0.058001220190     R=1.72
3 C     -1.475791201000      0.691720814200     -0.223558869000     R=2.00
4 C     -0.093991764900      1.227337475000      0.166285076600     R=2.00
```

```
5 C     -1.360372236000     -0.793318481000      0.133206910300    R=2.00
6 C      0.814221753600      0.023432796310      0.012211139530    R=2.00
7 H     -2.299433233000      1.175027545000      0.313260664900    R=1.30
8 H     -1.642078819000      0.811055794000     -1.302144491000    R=1.30
9 H     -0.051380714760      1.533248925000      1.224079480000    R=1.30
10 H     0.272221501100      2.063202860000     -0.439486689100    R=1.30
11 H    -1.614830549000     -0.998705501300      1.181555849000    R=1.30
12 H    -1.919066483000     -1.464944216000     -0.525642300300    R=1.30
END

GUIBONDS
1 1 5 1.0
2 1 6 1.0
3 2 6 2.0
4 3 4 1.0
5 3 5 1.0
6 3 7 1.0
7 3 8 1.0
8 4 6 1.0
9 4 9 1.0
10 4 10 1.0
11 5 11 1.0
12 5 12 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA
```

```
GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation
```

```
# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" -n $NPROC <<eor
TITLE gbl

ATOMS
1 O      0.069437547570     -1.120676765000     -0.036426434080     R=1.72
2 O      2.033473021000     -0.016858780270     -0.058001220190     R=1.72
3 C     -1.475791201000      0.691720814200     -0.223558869000     R=2.00
4 C     -0.093991764900      1.227337475000      0.166285076600     R=2.00
5 C     -1.360372236000     -0.793318481000      0.133206910300     R=2.00
6 C      0.814221753600      0.023432796310      0.012211139530     R=2.00
7 H     -2.299433233000      1.175027545000      0.313260664900     R=1.30
8 H     -1.642078819000      0.811055794000     -1.302144491000     R=1.30
9 H     -0.051380714760      1.533248925000      1.224079480000     R=1.30
10 H     0.272221501100      2.063202860000     -0.439486689100     R=1.30
11 H    -1.614830549000     -0.998705501300      1.181555849000     R=1.30
12 H    -1.919066483000     -1.464944216000     -0.525642300300     R=1.30
END

GUIBONDS
1 1 5 1.0
2 1 6 1.0
3 2 6 2.0
4 3 4 1.0
5 3 5 1.0
6 3 7 1.0
7 3 8 1.0
8 4 6 1.0
9 4 9 1.0
10 4 10 1.0
11 5 11 1.0
12 5 12 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
```

```
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
"$ADFBIN/adf" -n $NPROC <<eor
TITLE ma

ATOMS
1 O     -0.668358451200      0.765086021300     -0.000163659803    R=1.72
2 O      0.341141324400     -1.271276769000      0.000295167158    R=1.72
3 C      1.698786233000      0.746445852200     -0.000233051324    R=2.00
4 C      0.420649512000     -0.048055086290     -0.000000131540    R=2.00
5 C     -1.956895521000      0.082847884640     -0.000172799336    R=2.00
6 H      1.733461609000      1.395459895000      0.885107918300    R=1.30
7 H      1.733822845000      1.394204797000     -0.886484075100    R=1.30
8 H      2.556260324000      0.067778858110      0.000396502370    R=1.30
9 H     -2.054342247000     -0.539638352400     -0.897202345700    R=1.30
10 H    -2.703508622000      0.881170151000     -0.000440698930    R=1.30
11 H    -2.054562486000     -0.539233585900      0.897113209000    R=1.30
END

GUIBONDS
1 1 4 1.0
2 1 5 1.0
3 2 4 2.0
4 3 4 1.0
5 3 6 1.0
6 3 7 1.0
7 3 8 1.0
8 5 9 1.0
9 5 10 1.0
10 5 11 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END
```

```
XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" -n $NPROC <<eor
TITLE ma

ATOMS
1 O      -0.668358451200       0.765086021300      -0.000163659803     R=1.72
2 O       0.341141324400      -1.271276769000       0.000295167158     R=1.72
3 C       1.698786233000       0.746445852200      -0.000233051324     R=2.00
4 C       0.420649512000      -0.048055086290      -0.000000131540     R=2.00
5 C      -1.956895521000       0.082847884640      -0.000172799336     R=2.00
6 H       1.733461609000       1.395459895000       0.885107918300     R=1.30
7 H       1.733822845000       1.394204797000      -0.886484075100     R=1.30
8 H       2.556260324000       0.067778858110       0.000396502370     R=1.30
9 H      -2.054342247000      -0.539638352400      -0.897202345700     R=1.30
10 H     -2.703508622000       0.881170151000      -0.000440698930     R=1.30
11 H     -2.054562486000      -0.539233585900       0.897113209000     R=1.30
END

GUIBONDS
1 1 4 1.0
2 1 5 1.0
3 2 4 2.0
4 3 4 1.0
5 3 6 1.0
6 3 7 1.0
7 3 8 1.0
8 5 9 1.0
9 5 10 1.0
10 5 11 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
```

```
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```

```
#! /bin/sh

# ============================
# The Molecule
# ============================

"$ADFBIN/adf" <<eor
TITLE pc

ATOMS
1 O     -1.380495289000      1.843682694000      0.048231311400    R=1.72
2 C     -2.848514110000      2.014037692000      0.166768492800    R=2.00
3 C     -2.952092331000      3.419929231000      0.761616886300    R=2.00
4 O     -1.650485034000      3.621624948000      1.399142265000    R=1.72
5 C     -0.768516116500      2.737676572000      0.861450333400    R=2.00
6 C     -3.507872580000      1.826522114000     -1.178759454000    R=2.00
7 H     -3.178364353000      1.253442692000      0.887392381700    R=1.30
8 H     -3.726114979000      3.512887891000      1.528788055000    R=1.30
9 H     -3.072925353000      4.194070744000     -0.008116234033    R=1.30
10 O     0.426260877600      2.752359675000      1.087867281000    R=1.72
11 H    -3.128380876000      2.556388236000     -1.906092323000    R=1.30
12 H    -4.591435372000      1.972204234000     -1.067384742000    R=1.30
13 H    -3.338380859000      0.810827011800     -1.556824384000    R=1.30
END

GUIBONDS
1 2 3 1.0
2 3 4 1.0
3 4 5 1.0
4 5 1 1.0
5 1 2 1.0
6 6 2 1.0
7 7 2 1.0
8 8 3 1.0
9 9 3 1.0
10 10 5 2.0
11 11 6 1.0
12 12 6 1.0
13 13 6 1.0
END

SOLVATION
   Surf Delley
```

```
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



GEOMETRY
   branch New
   iterations 100
END

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor
```

```
# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO




mv TAPE21 GASPHASE.t21


# COSMO-RS Solvent calculation

# ==============================
# The Molecule
# ==============================

"$ADFBIN/adf" <<eor
TITLE pc

ATOMS
1 O     -1.380495289000      1.843682694000      0.048231311400    R=1.72
2 C     -2.848514110000      2.014037692000      0.166768492800    R=2.00
3 C     -2.952092331000      3.419929231000      0.761616886300    R=2.00
4 O     -1.650485034000      3.621624948000      1.399142265000    R=1.72
5 C     -0.768516116500      2.737676572000      0.861450333400    R=2.00
6 C     -3.507872580000      1.826522114000     -1.178759454000    R=2.00
7 H     -3.178364353000      1.253442692000      0.887392381700    R=1.30
8 H     -3.726114979000      3.512887891000      1.528788055000    R=1.30
9 H     -3.072925353000      4.194070744000     -0.008116234033    R=1.30
10 O     0.426260877600      2.752359675000      1.087867281000    R=1.72
11 H    -3.128380876000      2.556388236000     -1.906092323000    R=1.30
12 H    -4.591435372000      1.972204234000     -1.067384742000    R=1.30
13 H    -3.338380859000      0.810827011800     -1.556824384000    R=1.30
END

GUIBONDS
1 2 3 1.0
2 3 4 1.0
```

```
3 4 5 1.0
4 5 1 1.0
5 1 2 1.0
6 6 2 1.0
7 7 2 1.0
8 8 3 1.0
9 9 3 1.0
10 10 5 2.0
11 11 6 1.0
12 12 6 1.0
13 13 6 1.0
END

SOLVATION
   Surf Delley
   Div  ndiv=4
   Solvent name=CRS cav0=0.0 cav1=0.0
   Charged method=CONJ conv=1.00E-06 iter=300 corr
   C-Mat EXACT
   SCF VAR ALL
   CSMRSP
END

BASIS
type TZP
core Small
createoutput None
END

XC
GGA Becke Perdew
END

RELATIVISTIC Scalar ZORA



RESTART GASPHASE.t21

SCF
iterations 50
mixing 0.2
diis
END

BeckeGrid
```

```
   Quality Good
End


ZlmFit
   Quality Normal
End

ALLPOINTS
NOPRINT LOGFILE

eor

# =====
# COSKF
# =====

rm -f COSKF
"$ADFBIN/cpkf" TAPE21 COSKF COSMO
```