Electronic Supplementary Information for Dalton Transactions

Supporting Information to Accompany:

Synthesis and Structural Characterization of Group 6 Transition Metal Complexes with Terminal Fluoromethylidyne (CF) Ligands; a DFT/NBO/NRT Comparison of Bonding Characteristics of Terminal NO, CF and CH Ligands.

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Departments of Chemistry, 6128 Burke Laboratories, Dartmouth College, Hanover, New Hampshire 03755, and University of California, San Diego, California 92093

```
Job CrCp_CO_2_CF_REDONE started on n30.bw01.dartmouth.edu at Mon Feb 15
16:14:12 2010
jobid: discovery-0-4b79b73f

  +---------------------------------------------------------------------+
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  +---------------------------------------------------------------------+

  start of program pre

  Job name: CrCp_CO_2_CF_REDONE
  Executables used: /opt/schrodinger/jaguar-v7.6.211/jaguar-v76211/bin/Linux-
x86_64
  Temporary files : /scratch/rhughes/CrCp_CO_2_CF_REDONE
  Maestro file (input):  CrCp_CO_2_CF_REDONE.mae
  Maestro file (output): CrCp_CO_2_CF_REDONE.01.mae


  Dynamic memory assumed available (MB):    3775

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1



  This run will use ECP on 1 atom
  number of basis functions....          313

  final geometry:
                                  angstroms
  atom              x                 y                 z
  Cr1         -0.6866548031      0.9010810761      0.1879482636
  O2          -1.3316286882     -1.0218076469     -2.0382870090
  C3          -1.1071805604     -0.3008359419     -1.1730950366
  O4          -1.4040690354     -1.0831930925      2.3401864497
  C5          -1.1541118447     -0.3353736134      1.5057194221
  F6           2.1253330677     -0.0358833176      0.2273393502
  C7           0.9116321601      0.3827891437      0.2141969761
  C8          -0.8395312465      2.8868939192      1.2274118900
  C9          -2.1548963036      2.3718138111      1.1022561586
  C10         -2.4505677337      2.2301512760     -0.2773946080
  C11         -1.3104112419      2.6670952529     -1.0174444101
  C12         -0.3202746412      3.0729205118     -0.0867479717
  H13         -2.8129070398      2.1133152956      1.9179796318
  H14         -3.3741699479      1.8582977277     -0.6932875206
  H15         -1.2231127698      2.6943534701     -2.0922488691
  H16          0.6573927520      3.4575468915     -0.3313622235
  H17         -0.3254004136      3.0993054169      2.1513204009
```

```
  X18          -1.4955260000      2.8125360000      0.1895340000

SCFE: SCF energy: DFT(b3lyp)      -644.60033377518 hartrees
Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     68.329 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.843      1.481    -10.994   18.55607
    rot.      0.889      2.981     30.708      0.889     -8.267   13.95274
    vib.      4.788     33.007     29.657      4.788     -4.054    6.84272
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      6.566     38.968    102.208      7.158    -23.315   39.35153

  Total internal energy, Utot (SCFE + ZPE + U):    -644.480981 hartrees
             Total enthalpy, Htot (Utot + pV):    -644.480037 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -644.528599 hartrees



Job CrCp_CO_2_NO_ started on andes at Wed Jul  9 11:23:16 2008
jobid: andes-0-4874d7df

  +-------------------------------------------------------------------+
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  +-------------------------------------------------------------------+

  start of program pre
  Job name: CrCp_CO_2_NO_
  Executables used: /usr/local/Jaguar_2007_u1/jaguar-v70207/bin/Linux-x86
  Temporary files : /Not_Backed_Up/scratch2/rhlocal/CrCp_CO_2_NO_
  Maestro file (input):  CrCp_CO_2_NO_.mae
  Maestro file (output): CrCp_CO_2_NO_.01.mae


  Dynamic memory assumed available (MB):     256

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1
```

```
  This run will use ECP on 1 atom
  number of basis functions....          313
 freezing dummy-atom X18

final geometry:
                                  angstroms
  atom              x                   y                   z
  Cr1           0.0730183653     -7.9423911268      0.4580279684
  O2            0.7229975573    -10.8418691553     -0.0869529449
  C3            0.4575386103     -9.7478489925      0.1299784630
  O4           -1.9229168930     -8.6595285846      2.6101471271
  C5           -1.1664911255     -8.4062352884      1.7867418846
  O6            2.2539240930     -7.5363775814      2.2527186682
  N7            1.3514404956     -7.7373688812      1.5395072877
  C8           -0.1117918956     -5.8275266802     -0.2705527009
  C9           -1.3864007949     -6.4385678194     -0.3391147147
  C10          -1.3103685891     -7.5292510945     -1.2529019398
  C11           0.0239648589     -7.5798424526     -1.7517753399
  C12           0.7630894394     -6.5357340291     -1.1467888128
  H13          -2.2642032135     -6.1313671858      0.2083539909
  H14          -2.1196485887     -8.1853782184     -1.5312891978
  H15           0.4072049499     -8.2913804789     -2.4668303685
  H16           1.8081094269     -6.3202746323     -1.3090127043
  H17           0.1547555929     -4.9829689625      0.3461880598
  X18          -0.4732747573     -6.7690669261     -1.0058641104

SCFE: SCF energy: DFT(b3lyp)      -636.66736232069 hartrees
Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     68.995 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.828      1.481    -10.990
    rot.      0.889      2.981     30.618      0.889     -8.240
    vib.      4.731     32.825     28.790      4.731     -3.853
   elec.      0.000      0.000      0.000      0.000      0.000
   total      6.508     38.786    101.236      7.101    -23.083

  Total internal energy, Utot (SCFE + ZPE + U):    -636.547040 hartrees
             Total enthalpy, Htot (Utot + pV):     -636.546096 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -636.594196 hartrees
```

```
Job CrCp_CO_2_CH started on n33.bw01.dartmouth.edu at Sat Jul 10 07:44:13
2010
jobid: discovery-0-4c385d07

  +-------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                  |
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  +-------------------------------------------------------------------+

  start of program pre

  Job name: CrCp_CO_2_CH
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/CrCp_CO_2_CH
  Maestro file (input):  CrCp_CO_2_CH.mae
  Maestro file (output): CrCp_CO_2_CH.01.mae


  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1


 This run will use ECP on 1 atom
  number of basis functions....          298

final geometry:
                                  angstroms
  atom              x                  y                  z
  Cr            0.2398723003     -0.6594772252     -0.1708813266
  O2           -0.5126657974     -1.9335568510     -2.7945227088
  C3           -0.2585644419     -1.4564550303     -1.7819034064
  O4           -0.7595438882     -2.9501779270      1.5109789109
  C5           -0.4089233834     -2.0793052919      0.8507291286
  H6            2.6177421106     -2.0282266583     -0.3674353307
  C7            1.7018150492     -1.4418638328     -0.2758586478
  C8            0.0550018873      0.9517948019      1.3791034680
  C9           -1.2533973152      0.7828659431      0.8397673339
  C10          -1.2086212257      1.1008233298     -0.5345570995
  C11           0.1290791890      1.4699064349     -0.8617296195
  C12           0.9034864157      1.3923963986      0.3274206800
  H13          -2.1229980717      0.4465216412      1.3836906989
  H14          -2.0368619737      1.0509782829     -1.2249324921
  H15           0.4827617177      1.7743792370     -1.8341828089
  H16           1.9536844015      1.6204846979      0.4141011581
  H17           0.3429660076      0.7915875775      2.4061159480
  X18          -0.2973860000      1.2909710000      0.2943200000

SCFE: SCF energy: DFT(b3lyp)      -545.31389908797 hartrees
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Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     72.202 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.568      1.481    -10.912   18.41756
    rot.      0.889      2.981     30.047      0.889     -8.070   13.62023
    vib.      4.949     33.269     33.140      4.949     -4.932    8.32346
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      6.727     39.231    104.755      7.319    -23.913   40.36125

  Total internal energy, Utot (SCFE + ZPE + U):    -545.188118 hartrees
             Total enthalpy, Htot (Utot + pV):    -545.187174 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -545.236946 hartrees



Job MoCp_CO_2_CF_REDONE started on n01.bw01.dartmouth.edu at Tue Feb 16
10:24:26 2010
jobid: discovery-0-4b7ab8b3

  +-----------------------------------------------------------------+
  |  Jaguar version 7.6, release 211                                |
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  +-----------------------------------------------------------------+

  start of program pre

  Job name: MoCp_CO_2_CF_REDONE
  Executables used: /opt/schrodinger/jaguar-v7.6.211/jaguar-v76211/bin/Linux-
x86_64
  Temporary files : /scratch/rhughes/MoCp_CO_2_CF_REDONE
  Maestro file (input):  MoCp_CO_2_CF_REDONE.mae
  Maestro file (output): MoCp_CO_2_CF_REDONE.01.mae


  Dynamic memory assumed available (MB):    3775

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1
```

```
  This run will use ECP on 1 atom
  number of basis functions....          313

final geometry:
                                  angstroms
  atom              x                   y                   z
  Mo1          0.0919100000     -0.6970590000     -0.4229950000
  O2          -1.8403340000     -1.2208930000     -2.8648820000
  C3          -1.1436260000     -1.0583400000     -1.9662310000
  O4          -0.7288160000     -3.4263120000      0.9429890000
  C5          -0.4460570000     -2.4415570000      0.4242340000
  F6           2.4394880000     -2.0786820000     -1.9070810000
  C7           1.4562760000     -1.5211720000     -1.2934080000
  C8           0.8901170000      0.7270390000      1.3793110000
  C9          -0.5090190000      0.5911690000      1.5865990000
  C10         -1.1834490000      1.1866350000      0.4926000000
  C11         -0.1977490000      1.6982150000     -0.4073640000
  C12          1.0797360000      1.4178710000      0.1469430000
  H13         -0.9777800000      0.1147510000      2.4347500000
  H14         -2.2535390000      1.2569100000      0.3688990000
  H15         -0.3910450000      2.2392950000     -1.3205990000
  H16          2.0304280000      1.6946540000     -0.2824600000
  H17          1.6675300000      0.3932910000      2.0490790000
  X18          0.0159280000      1.1241860000      0.6396180000

SCFE: SCF energy: DFT(b3lyp)      -625.84811894223 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     67.278 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.449      1.481    -11.175   18.86091
    rot.      0.889      2.981     31.065      0.889     -8.373   14.13272
    vib.      5.110     34.268     32.358      5.110     -4.537    7.65759
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      6.888     40.230    105.872      7.480    -24.085   40.65122

  Total internal energy, Utot (SCFE + ZPE + U):    -625.729928 hartrees
             Total enthalpy, Htot (Utot + pV):     -625.728984 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -625.779287 hartrees
```

```
Job MoCp_CO_2_NO_ started on andes at Wed Jul  9 11:20:18 2008
jobid: andes-0-4874d72f

  +-------------------------------------------------------------------+
  |  Jaguar version 7.0, release 207                                  |
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  +-------------------------------------------------------------------+

  start of program pre
  Job name: MoCp_CO_2_NO_
  Executables used: /usr/local/Jaguar_2007_u1/jaguar-v70207/bin/Linux-x86
  Temporary files : /Not_Backed_Up/scratch2/rhlocal/MoCp_CO_2_NO_
  Maestro file (input):  MoCp_CO_2_NO_.mae
  Maestro file (output): MoCp_CO_2_NO_.01.mae


  Dynamic memory assumed available (MB):     256

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1
  This run will use ECP on 1 atom
  number of basis functions....          313

final geometry:
                                  angstroms
  atom              x                 y                 z
  Mo1         -0.0534211142     -0.6257210491     -0.3282819118
  O2          -1.5833255716     -0.9691295171     -3.0705645880
  C3          -1.0298064261     -0.8743878402     -2.0691750437
  O4          -1.4416234185     -3.2091078430      0.8450400337
  C5          -0.9405164135     -2.2816299054      0.3902219668
  O6           2.3851378238     -2.1064121886     -1.2638141729
  N7           1.4049395833     -1.5662657321     -0.9195528340
  C8           0.8955024019      0.8904930832      1.3095631069
  C9          -0.4303119440      0.5988968978      1.7189723769
  C10         -1.3245572154      1.1244732997      0.7398340468
  C11         -0.5379314824      1.7416959156     -0.2764723493
  C12          0.8289846113      1.5989727274      0.0724238811
  H13         -0.7140291216      0.0902401705      2.6277895672
  H14         -2.4024195318      1.0970991840      0.7816618866
  H15         -0.9171343397      2.2513791133     -1.1492074193
  H16          1.6705666327      1.9738469752     -0.4902622861
  H17          1.7964438166      0.6349702990      1.8466577848
  X18         -0.1597788960      1.2303175931      0.7517122375

SCFE: SCF energy: DFT(b3lyp)      -617.90684635506 hartrees

Thermodynamic properties calculated assuming an ideal gas
```

```
  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     67.952 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.437      1.481    -11.171
    rot.      0.889      2.981     30.966      0.889     -8.344
    vib.      5.038     33.996     31.523      5.038     -4.361
   elec.      0.000      0.000      0.000      0.000      0.000
   total      6.815     39.957    104.926      7.408    -23.876

  Total internal energy, Utot (SCFE + ZPE + U):    -617.787698 hartrees
             Total enthalpy, Htot (Utot + pV):    -617.786753 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -617.836607 hartrees



Job MoCp_CO_2_CH started on n34.bw01.dartmouth.edu at Sat Jul 10 07:45:37
2010
jobid: discovery-0-4c385d5b

  +-----------------------------------------------------------------------+
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  +-----------------------------------------------------------------------+

  start of program pre

  Job name: MoCp_CO_2_CH
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/MoCp_CO_2_CH
  Maestro file (input):  MoCp_CO_2_CH.mae
  Maestro file (output): MoCp_CO_2_CH.01.mae


  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          298
```

```
  final geometry:
                                    angstroms
  atom               x                  y                  z
  Mo1          0.0982683531     -0.6832494850     -0.4587168274
  O2          -2.0488637891     -1.3481345548     -2.6843006520
  C3          -1.2785884001     -1.1296795787     -1.8621932691
  O4          -0.3307780870     -3.4505513374      1.0117720403
  C5          -0.1981644174     -2.4520106463      0.4620071379
  H6           2.0628824905     -1.9902976514     -2.1125796800
  C7           1.3408356493     -1.4705880148     -1.4829771169
  C8           0.7461537037      0.6782754829      1.4443188563
  C9          -0.6787680453      0.6516572073      1.5400775310
  C10         -1.2101959510      1.2963153263      0.4067190726
  C11         -0.1237847991      1.7339027187     -0.4109714774
  C12          1.0857055089      1.3700523155      0.2466925582
  H13         -1.2489090723      0.2038769087      2.3407080046
  H14         -2.2592177210      1.4289176226      0.1863741602
  H15         -0.2065220577      2.2974761898     -1.3275164159
  H16          2.0844699821      1.5963360745     -0.0929295510
  H17          1.4390518211      0.3020049010      2.1810813726
  X18          0.0159280000      1.1241860000      0.6396180000

SCFE: SCF energy: DFT(b3lyp)      -526.56506855248 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     71.240 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.226      1.481    -11.108   18.74886
    rot.      0.889      2.981     30.437      0.889     -8.186   13.81669
    vib.      5.253     34.395     34.499      5.253     -5.033    8.49454
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      7.031     40.357    107.163      7.623    -24.328   41.06008

  Total internal energy, Utot (SCFE + ZPE + U):    -526.440336 hartrees
              Total enthalpy, Htot (Utot + pV):    -526.439391 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -526.490308 hartrees

Job WCp_CO_2_CF_REDONE started on n109.bw01.dartmouth.edu at Mon Feb 15
16:25:19 2010
jobid: discovery-0-4b79b750

  +-------------------------------------------------------------------+
  |  Jaguar version 7.6, release 211                                  |
  |                                                                   |
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  |  Use of this program should be acknowledged in publications as:     |
  |  Jaguar, version 7.6, Schrodinger, LLC, New York, NY, 2009.         |
  +---------------------------------------------------------------------+

  start of program pre

  Job name: WCp_CO_2_CF_REDONE
  Executables used: /opt/schrodinger/jaguar-v7.6.211/jaguar-v76211/bin/Linux-
x86_64
  Temporary files : /scratch/rhughes/WCp_CO_2_CF_REDONE
  Maestro file (input):  WCp_CO_2_CF_REDONE.mae
  Maestro file (output): WCp_CO_2_CF_REDONE.01.mae


  Dynamic memory assumed available (MB):    3766

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1


  This run will use ECP on 1 atom
  number of basis functions....          313

SCFE: SCF energy: DFT(b3lyp)      -626.14694439909 hartrees


  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     67.462 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     43.330      1.481    -11.438   19.30469
    rot.      0.889      2.981     31.046      0.889     -8.368   14.12290
    vib.      5.036     34.053     31.618      5.036     -4.391    7.41153
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      6.813     40.014    105.995      7.406    -24.197   40.83912

  Total internal energy, Utot (SCFE + ZPE + U):    -626.028580 hartrees
             Total enthalpy, Htot (Utot + pV):    -626.027636 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -626.077997 hartrees
```

```
Job WCp_CO_2_NO_ started on andes at Wed Jul  9 11:21:11 2008
jobid: andes-0-4874d763

  +-----------------------------------------------------------------+
  |  Jaguar version 7.0, release 207                                |
  |                                                                 |
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  |                                                                 |
  |  Use of this program should be acknowledged in publications as: |
  |  Jaguar, version 7.0, Schrodinger, LLC, New York, NY, 2007.     |
  +-----------------------------------------------------------------+

  start of program pre
  Job name: WCp_CO_2_NO_
  Executables used: /usr/local/Jaguar_2007_u1/jaguar-v70207/bin/Linux-x86
  Temporary files : /Not_Backed_Up/scratch2/rhlocal/WCp_CO_2_NO_
  Maestro file (input):  WCp_CO_2_NO_.mae
  Maestro file (output): WCp_CO_2_NO_.01.mae


  Dynamic memory assumed available (MB):     256

  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1


  This run will use ECP on 1 atom
  number of basis functions....          313

SCFE: SCF energy: DFT(b3lyp)      -618.20290412765 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     68.119 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     43.322      1.481    -11.435
    rot.      0.889      2.981     30.941      0.889     -8.336
    vib.      4.953     33.710     30.807      4.953     -4.232
   elec.      0.000      0.000      0.000      0.000      0.000
   total      6.731     39.672    105.069      7.323    -24.003

  Total internal energy, Utot (SCFE + ZPE + U):    -618.083623 hartrees
             Total enthalpy, Htot (Utot + pV):     -618.082679 hartrees
```

```
    Total Gibbs free energy, Gtot (Htot - T*S):    -618.132601 hartrees

Job WCp_CO_2_CH started on n33.bw01.dartmouth.edu at Sat Jul 10 07:44:46 2010
jobid: discovery-0-4c385d28

  +-------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                  |
  |                                                                   |
  |  Copyright (c) 2010 Schrodinger,  LLC.                            |
  |  All Rights Reserved.                                             |
  |                                                                   |
  |  Use of this program should be acknowledged in publications as:   |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.       |
  +-------------------------------------------------------------------+

  start of program pre

  Job name: WCp_CO_2_CH
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/WCp_CO_2_CH
  Maestro file (input):  WCp_CO_2_CH.mae
  Maestro file (output): WCp_CO_2_CH.01.mae


  basis set:             lacv3p**++
  net molecular charge:    0
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          298

SCFE: SCF energy: DFT(b3lyp)      -526.86757865146 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     71.568 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

            U         Cv          S          H          G        ln(Q)
        ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     43.166      1.481    -11.389   19.22214
    rot.      0.889      2.981     30.432      0.889     -8.185   13.81410
    vib.      5.152     34.038     33.459      5.152     -4.824    8.14219
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      6.929     40.000    107.057      7.521    -24.398   41.17843

  Total internal energy, Utot (SCFE + ZPE + U):    -526.742485 hartrees
```

```
            Total enthalpy, Htot (Utot + pV):    -526.741541 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -526.792408 hartrees

Job Cr_CO_2_CF_CATION_OPT_NRTSTR started on n04.bw01.dartmouth.edu at Tue Aug
10 13:28:55 2010
jobid: discovery-0-4c618c4f

  +---------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                    |
  |                                                                     |
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  |  Use of this program should be acknowledged in publications as:     |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.         |
  +---------------------------------------------------------------------+

  start of program pre

  Job name: Cr_CO_2_CF_CATION_OPT_NRTSTR
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Cr_CO_2_CF_CATION_OPT_NRTSTR
  Maestro file (input):  Cr_CO_2_CF_CATION_OPT_NRTSTR.mae
  Maestro file (output): Cr_CO_2_CF_CATION_OPT_NRTSTR.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          168

Final geometry:
                                  angstroms
  atom              x                 y                 z
  Cr            0.2324090000     -0.6427590000     -0.1267170000
  O2           -0.2368370000     -1.8347770000     -2.8922460000
  C3           -0.0774160000     -1.3862200000     -1.8679440000
  O4           -1.0451570000     -3.0017050000      1.3198650000
  C5           -0.5859560000     -2.1205420000      0.7827190000
  F6            2.7546570000     -2.1010790000     -0.0458820000
  C7            1.7080580000     -1.4292550000     -0.0610960000

SCFE: SCF energy: DFT(b3lyp)      -450.66469763378 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.012 kcal/mol
  is not included in U, H, or G in the table below
```

```
  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     40.698      1.481    -10.653   17.98007
    rot.      0.889      2.981     28.657      0.889     -7.655   12.92061
    vib.      2.868     17.659     17.931      2.868     -2.478    4.18292
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.645     23.620     87.286      5.238    -20.787   35.08359

  Total internal energy, Utot (SCFE + ZPE + U):    -450.633371 hartrees
             Total enthalpy, Htot (Utot + pV):    -450.632427 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -450.673899 hartrees


Job Cr_CO_2_NO_CATION_OPT_NRTSTR started on n42.bw01.dartmouth.edu at Fri Aug
6 14:48:10 2010
jobid: discovery-0-4c5c58e4

  +---------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                    |
  |                                                                     |
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  |  Use of this program should be acknowledged in publications as:     |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.         |
  +---------------------------------------------------------------------+

  start of program pre

  Job name: Cr_CO_2_NO_CATION_OPT_NRTSTR
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Cr_CO_2_NO_CATION_OPT_NRTSTR
  Maestro file (input):  Cr_CO_2_NO_CATION_OPT_NRTSTR.mae
  Maestro file (output): Cr_CO_2_NO_CATION_OPT_NRTSTR.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1



  This run will use ECP on 1 atom
  number of basis functions....          168

 Final geometry:
                                  angstroms
  atom              x                  y                  z
  Cr          0.0000000000       0.0000000000       0.0000000000
  O2          0.7349500000      -2.9261950000      -0.5149160000
```

```
  C3            0.4552550000     -1.8483710000     -0.3328720000
  O4           -1.9636860000     -0.6939760000      2.2428210000
  C5           -1.2483280000     -0.4388200000      1.4084150000
  O6            2.1336230000      0.3107620000      1.8354160000
  N             1.2734580000      0.1859760000      1.0952480000


 SCFE: SCF energy: DFT(b3lyp)      -442.72685801255 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.583 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     40.677      1.481    -10.647   17.96923
    rot.      0.889      2.981     28.592      0.889     -7.636   12.88806
    vib.      2.856     17.627     17.659      2.856     -2.409    4.06610
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.633     23.589     86.927      5.226    -20.692   34.92338

  Total internal energy, Utot (SCFE + ZPE + U):    -442.694642 hartrees
             Total enthalpy, Htot (Utot + pV):     -442.693698 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -442.734999 hartrees


Job Cr_CO_2_CH_CATION_OPT started on n41.bw01.dartmouth.edu at Thu Aug  5
14:42:49 2010
jobid: discovery-0-4c5b0623

  +-------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                  |
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  |  Use of this program should be acknowledged in publications as:   |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.       |
  +-------------------------------------------------------------------+

  start of program pre

  Job name: Cr_CO_2_CH_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Cr_CO_2_CH_CATION_OPT
```

```
  Maestro file (input):  Cr_CO_2_CH_CATION_OPT.mae
  Maestro file (output): Cr_CO_2_CH_CATION_OPT.01.mae


 This run will use ECP on 1 atom
  number of basis functions....          153

final geometry:
                                  angstroms
  atom              x                  y                  z
  Cr            0.2571903873     -0.6446822234     -0.1668689538
  O2           -0.5311148800     -1.9502069702     -2.8100254005
  C3           -0.2582928514     -1.4576502158     -1.8318596467
  O4           -0.7739181000     -2.9724266522      1.5153514154
  C5           -0.4112954059     -2.1021765983      0.8948534970
  H6            2.5745264814     -2.0427249777     -0.3670699622
  C7            1.6763353027     -1.4287685778     -0.2725878893


SCFE: SCF energy: DFT(b3lyp)      -351.38650184039 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     18.815 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     40.285      1.481    -10.530   17.77204
    rot.      0.889      2.981     27.592      0.889     -7.338   12.38465
    vib.      2.408     15.784     14.079      2.408     -1.789    3.01965
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.186     21.746     81.955      4.778    -19.657   33.17634

  Total internal energy, Utot (SCFE + ZPE + U):    -351.349848 hartrees
             Total enthalpy, Htot (Utot + pV):     -351.348904 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -351.387843 hartrees

Job Mo_CO_2_CF_CATION_OPT started on n41.bw01.dartmouth.edu at Thu Aug  5
14:44:08 2010
jobid: discovery-0-4c5b0673

  +-----------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                      |
  |                                                                       |
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  |  All Rights Reserved.                                                 |
  |                                                                       |
```

```
  |  Use of this program should be acknowledged in publications as:    |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.        |
  +--------------------------------------------------------------------+

  start of program pre

  Job name: Mo_CO_2_CF_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Mo_CO_2_CF_CATION_OPT
  Maestro file (input):  Mo_CO_2_CF_CATION_OPT.mae
  Maestro file (output): Mo_CO_2_CF_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          168

final geometry:
                                 angstroms
  atom              x                 y                 z
  Mo1          0.0948870856     -0.6705327875     -0.4070603695
  O2          -1.7555970210     -1.2928233222     -2.8644099432
  C3          -1.0914183488     -1.0645245305     -1.9743385952
  O4          -0.6734990308     -3.4420767833      0.8489472302
  C5          -0.3994215504     -2.4383345153      0.3985386196
  F6           2.2767666350     -2.1470997897     -1.9004226356
  C7           1.4040847643     -1.5094228849     -1.2754337927

SCFE: SCF energy: DFT(b3lyp)      -431.92968677255 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.053 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.550      1.481    -10.907   18.40879
    rot.      0.889      2.981     29.035      0.889     -7.768   13.11088
    vib.      2.797     17.469     17.393      2.797     -2.389    4.03198
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.574     23.431     87.978      5.167    -21.064   35.55166

  Total internal energy, Utot (SCFE + ZPE + U):    -431.898409 hartrees
```

```
            Total enthalpy, Htot (Utot + pV):    -431.897465 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -431.939266 hartrees

Job Mo_CO_2_NO_CATION_OPT started on n41.bw01.dartmouth.edu at Thu Aug  5
14:44:53 2010
jobid: discovery-0-4c5b069f

  +---------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                    |
  |                                                                     |
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  |                                                                     |
  |  Use of this program should be acknowledged in publications as:     |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.         |
  +---------------------------------------------------------------------+

  start of program pre

  Job name: Mo_CO_2_NO_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Mo_CO_2_NO_CATION_OPT
  Maestro file (input):  Mo_CO_2_NO_CATION_OPT.mae
  Maestro file (output): Mo_CO_2_NO_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1


 This run will use ECP on 1 atom
  number of basis functions....          168

final geometry:
                                  angstroms
  atom              x                 y                 z
  Mo1         -0.0572310464     -0.5992602741     -0.3131678179
  O2          -1.5065379523     -1.0448462680     -3.0600188366
  C3          -0.9860682151     -0.8792724647     -2.0668653409
  O4          -1.3672996723     -3.2363204326      0.7702063326
  C5          -0.8970776204     -2.2806698030      0.3825351522
  O6           2.2418628949     -2.1684041320     -1.2935267047
  N            1.3479217840     -1.5595290729     -0.9132478551

SCFE: SCF energy: DFT(b3lyp)      -423.97945503504 hartrees

  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.608 kcal/mol
```

```
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.534      1.481    -10.902   18.40066
    rot.      0.889      2.981     28.930      0.889     -7.737   13.05814
    vib.      2.763     17.348     17.018      2.763     -2.311    3.90059
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.540     23.309     87.482      5.133    -20.950   35.35939

  Total internal energy, Utot (SCFE + ZPE + U):    -423.947347 hartrees
             Total enthalpy, Htot (Utot + pV):    -423.946403 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -423.987968 hartrees

Job Mo_CO_2_CF_CATION_OPT started on n41.bw01.dartmouth.edu at Thu Aug  5
14:44:08 2010
jobid: discovery-0-4c5b0673

  +---------------------------------------------------------------------+
  |  Jaguar version 7.7, release 107                                    |
  |                                                                     |
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  |                                                                     |
  |  Use of this program should be acknowledged in publications as:     |
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.         |
  +---------------------------------------------------------------------+

  start of program pre

  Job name: Mo_CO_2_CF_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Mo_CO_2_CF_CATION_OPT
  Maestro file (input):  Mo_CO_2_CF_CATION_OPT.mae
  Maestro file (output): Mo_CO_2_CF_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

 This run will use ECP on 1 atom
  number of basis functions....          168

final geometry:
                                  angstroms
  atom              x                 y                 z
  Mo1         -0.0572310464     -0.5992602741     -0.3131678179
  O2          -1.5065379523     -1.0448462680     -3.0600188366
  C3          -0.9860682151     -0.8792724647     -2.0668653409
  O4          -1.3672996723     -3.2363204326      0.7702063326
```

```
  C5           -0.8970776204     -2.2806698030      0.3825351522
  O6            2.2418628949     -2.1684041320     -1.2935267047
  N             1.3479217840     -1.5595290729     -0.9132478551

SCFE: SCF energy: DFT(b3lyp)      -423.97945503504 hartrees


  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.608 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.534      1.481    -10.902   18.40066
    rot.      0.889      2.981     28.930      0.889     -7.737   13.05814
    vib.      2.763     17.348     17.018      2.763     -2.311    3.90059
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.540     23.309     87.482      5.133    -20.950   35.35939

  Total internal energy, Utot (SCFE + ZPE + U):    -423.947347 hartrees
             Total enthalpy, Htot (Utot + pV):     -423.946403 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -423.987968 hartrees

Job Mo_CO_2_CH_CATION_OPT started on n41.bw01.dartmouth.edu at Thu Aug  5
14:44:29 2010
jobid: discovery-0-4c5b0687

  +-------------------------------------------------------------------+
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  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.       |
  +-------------------------------------------------------------------+

  start of program pre

  Job name: Mo_CO_2_CH_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/Mo_CO_2_CH_CATION_OPT
  Maestro file (input):  Mo_CO_2_CH_CATION_OPT.mae
  Maestro file (output): Mo_CO_2_CH_CATION_OPT.01.mae
```

```
  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          153

final geometry:
                                  angstroms
  atom              x                 y                 z
  Mo1          0.1124249347     -0.6724909551     -0.4590730472
  O2          -2.0440451073     -1.4081723878     -2.6380726047
  C3          -1.2748940609     -1.1400932966     -1.8515188665
  O4          -0.3771253286     -3.4494324366      0.9510968697
  C5          -0.2061752111     -2.4487941409      0.4494840095
  H6           1.9988059822     -2.0058822153     -2.0935421902
  C7           1.2903850000     -1.4713218164     -1.4605659379

SCFE: SCF energy: DFT(b3lyp)      -332.65772822691 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     18.957 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.245      1.481    -10.816   18.25524
    rot.      0.889      2.981     28.052      0.889     -7.475   12.61612
    vib.      2.349     15.521     13.706      2.349     -1.738    2.93344
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.126     21.483     83.003      4.718    -20.029   33.80480

  Total internal energy, Utot (SCFE + ZPE + U):    -332.620944 hartrees
             Total enthalpy, Htot (Utot + pV):     -332.620000 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -332.659437 hartrees

Job W_CO_2_CF_CATION_OPT started on n45.bw01.dartmouth.edu at Thu Aug  5
15:30:24 2010
jobid: discovery-0-4c5b114b

  +-----------------------------------------------------------------+
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```
  |  Jaguar, version 7.7, Schrodinger, LLC, New York, NY, 2010.        |
  +-------------------------------------------------------------------+

  start of program pre

  Job name: W_CO_2_CF_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/W_CO_2_CF_CATION_OPT
  Maestro file (input):  W_CO_2_CF_CATION_OPT.mae
  Maestro file (output): W_CO_2_CF_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          168

final geometry:
                                  angstroms
  atom              x                  y                  z
  W            7.1546981042     -0.5496098231     -0.2068974496
  O2           6.2670198789     -3.5320758057     -0.3944612508
  C3           6.5886225850     -2.4431165403     -0.3261477762
  O4           9.3657587441     -1.3638220379      1.8348640404
  C5           8.5575596199     -1.0642954131      1.0925574357
  F6           9.1632506739     -1.1448219105     -2.4048238634
  C7           8.3271357968     -0.8735102592     -1.5147431319

SCFE: SCF energy: DFT(b3lyp)      -432.20023945727 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.206 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.689      1.481    -11.247   18.98197
    rot.      0.889      2.981     29.200      0.889     -7.817   13.19384
    vib.      2.710     17.221     16.721      2.710     -2.276    3.84084
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.487     23.183     88.609      5.080    -21.339   36.01664

  Total internal energy, Utot (SCFE + ZPE + U):    -432.168856 hartrees
             Total enthalpy, Htot (Utot + pV):     -432.167912 hartrees
```

```
    Total Gibbs free energy, Gtot (Htot - T*S):    -432.210013 hartrees

Job W_CO_2_NO_CATION_OPT started on n50.bw01.dartmouth.edu at Thu Aug  5
15:31:20 2010
jobid: discovery-0-4c5b1180

  +---------------------------------------------------------------------+
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  +---------------------------------------------------------------------+

  start of program pre

  Job name: W_CO_2_NO_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/W_CO_2_NO_CATION_OPT
  Maestro file (input):  W_CO_2_NO_CATION_OPT.mae
  Maestro file (output): W_CO_2_NO_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1


  This run will use ECP on 1 atom
  number of basis functions....          168

final geometry:
                                  angstroms
  atom              x                 y                 z
  W           -0.2247515649     -0.6623523769     -0.3962529974
  O2          -2.4902995749     -0.4920825193     -2.5272951220
  C3          -1.6634749701     -0.5504934532     -1.7485202223
  O4          -1.8167598757     -2.9002309472      1.0739065361
  C5          -1.2358412226     -2.0802538782      0.5412652242
  O6           1.1418345484     -2.7115851776     -2.0171365890
  N            0.6055264013     -1.9110820039     -1.3843126896

SCFE: SCF energy: DFT(b3lyp)      -424.24587478624 hartrees
Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     15.740 kcal/mol
  is not included in U, H, or G in the table below
```

```
  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.678      1.481    -11.243   18.97642
    rot.      0.889      2.981     29.069      0.889     -7.778   13.12824
    vib.      2.662     17.030     16.295      2.662     -2.197    3.70734
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.439     22.991     88.043      5.032    -21.218   35.81200

  Total internal energy, Utot (SCFE + ZPE + U):    -424.213717 hartrees
             Total enthalpy, Htot (Utot + pV):    -424.212773 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -424.254605 hartrees

Job W_CO_2_CH_CATION_OPT started on n47.bw01.dartmouth.edu at Thu Aug  5
15:30:48 2010
jobid: discovery-0-4c5b1161

  +-------------------------------------------------------------------+
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  +-------------------------------------------------------------------+

  start of program pre

  Job name: W_CO_2_CH_CATION_OPT
  Executables used: /opt/schrodinger/jaguar-v77107.june.2010/jaguar-
v77107/bin/Linux-x86_64
  Temporary files : /scratch/rhughes/W_CO_2_CH_CATION_OPT
  Maestro file (input):  W_CO_2_CH_CATION_OPT.mae
  Maestro file (output): W_CO_2_CH_CATION_OPT.01.mae


  basis set:             lacv3p**++
  net molecular charge:    1
  multiplicity:            1

  This run will use ECP on 1 atom
  number of basis functions....          153

final geometry:
                                  angstroms
  atom              x                 y                 z
  W           7.1489801447     -0.5698248821     -0.2389645975
  O2          6.2947652931     -3.5658880449      0.0081198530
  C3          6.6041491740     -2.4761680049     -0.0805834673
  O4          9.5534758352     -1.1007724295      1.6863770261
  C5          8.6776774597     -0.9065206283      0.9889709907
  H6          8.8603752015     -1.3728577857     -2.3636421465
```

```
  C7            8.1975746297     -1.0453293479     -1.5668974057

SCFE: SCF energy: DFT(b3lyp)      -332.93212435214 hartrees

Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     19.223 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G        ln(Q)
         ---------  ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     42.484      1.481    -11.185   18.87890
    rot.      0.889      2.981     28.203      0.889     -7.520   12.69225
    vib.      2.243     15.134     13.000      2.243     -1.633    2.75603
   elec.      0.000      0.000      0.000      0.000      0.000    0.00000
   total      4.020     21.096     83.687      4.613    -20.338   34.32719

  Total internal energy, Utot (SCFE + ZPE + U):    -332.895083 hartrees
             Total enthalpy, Htot (Utot + pV):     -332.894139 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -332.933901 hartrees
```