```
                                 ****************
                                 * O   R   C   A *
                                 ****************

           --- An Ab Initio, DFT and Semiempirical electronic structure package
---

    Benzene


-----------------------
VIBRATIONAL FREQUENCIES
-----------------------

   0:         0.00 cm**-1
   1:         0.00 cm**-1
   2:         0.00 cm**-1
   3:         0.00 cm**-1
   4:         0.00 cm**-1
   5:         0.00 cm**-1
   6:       380.07 cm**-1
   7:       387.04 cm**-1
   8:       602.85 cm**-1
   9:       603.28 cm**-1
  10:       658.78 cm**-1
  11:       670.48 cm**-1
  12:       826.92 cm**-1
  13:       828.24 cm**-1
  14:       915.63 cm**-1
  15:       916.09 cm**-1
  16:       960.99 cm**-1
  17:       993.78 cm**-1
  18:       994.69 cm**-1
  19:      1035.69 cm**-1
  20:      1036.14 cm**-1
  21:      1146.22 cm**-1
  22:      1166.67 cm**-1
  23:      1166.89 cm**-1
  24:      1335.85 cm**-1
  25:      1341.93 cm**-1
  26:      1468.20 cm**-1
  27:      1468.58 cm**-1
  28:      1590.85 cm**-1
  29:      1591.52 cm**-1
  30:      3092.21 cm**-1
  31:      3100.36 cm**-1
  32:      3102.69 cm**-1
  33:      3115.61 cm**-1
  34:      3117.49 cm**-1
  35:      3126.55 cm**-1



-----------
IR SPECTRUM
-----------

 Mode    freq (cm**-1)   T**2         TX         TY         TZ
-------------------------------------------------------------------
   6:       380.07    0.013282  (  0.006584  -0.113694  -0.017677)
   7:       387.04    0.000500  (  0.021792  -0.003709  -0.003389)
   8:       602.85    0.000003  (  0.000353   0.000183   0.001783)
   9:       603.28    0.000003  ( -0.001553  -0.000084   0.000346)
```

```
  10:       658.78  112.564020  (  0.065109 -10.578405   0.810632)
  11:       670.48    0.000937  ( -0.000894  -0.030553   0.001747)
  12:       826.92    0.000017  (  0.001210  -0.003895   0.000619)
  13:       828.24    0.000007  ( -0.001849   0.001546   0.000909)
  14:       915.63    0.012030  (  0.086290  -0.056669  -0.037051)
  15:       916.09    0.023279  ( -0.038367  -0.136055  -0.057410)
  16:       960.99    0.000006  (  0.001635  -0.001661   0.000813)
  17:       993.78    0.001901  (  0.043025  -0.001505  -0.006872)
  18:       994.69    0.000001  (  0.000643  -0.000390  -0.000901)
  19:      1035.69    6.489771  (  2.532432  -0.002884  -0.276676)
  20:      1036.14    6.542476  ( -0.294044  -0.171545  -2.535071)
  21:      1146.22    0.000383  ( -0.005609   0.002640  -0.018570)
  22:      1166.67    0.000001  ( -0.001039   0.000150  -0.000596)
  23:      1166.89    0.000004  ( -0.000230  -0.000340  -0.001886)
  24:      1335.85    0.000001  ( -0.000538  -0.000000  -0.000709)
  25:      1341.93    0.001300  ( -0.000909  -0.000664   0.036032)
  26:      1468.20    7.370322  (  2.710174   0.005939  -0.158887)
  27:      1468.58    7.699302  (  0.153772   0.214842   2.762155)
  28:      1590.85    0.000001  ( -0.000406   0.000507  -0.000580)
  29:      1591.52    0.000000  ( -0.000658  -0.000105   0.000016)
  30:      3092.21    0.126105  (  0.355102   0.001057   0.002571)
  31:      3100.36    0.002187  (  0.039069   0.002290   0.025592)
  32:      3102.69    0.002399  (  0.048848   0.000650   0.003477)
  33:      3115.61   33.517894  (  5.786140   0.023869  -0.194691)
  34:      3117.49   34.673504  (  0.183376   0.406460   5.871513)
  35:      3126.55    0.007445  (  0.029684  -0.005431  -0.080836)

The first frequency considered to be a vibration is 6
The total number of vibrations considered is 30


--------------------------
THERMOCHEMISTRY AT 298.15K
--------------------------

Temperature         ... 298.15 K
Pressure            ... 1.00 atm
Total Mass          ... 78.11 AMU

Throughout the following assumptions are being made:
  (1) The electronic state is orbitally nondegenerate
  (2) There are no thermally accessible electronically excited states
  (3) Hindered rotations indicated by low frequency modes) are not
      treated as such but are treated as vibrations and this may
      case some error
  (4) All equations used are the standard statistical mechanics
      equations for an ideal gas
  (5) All vibrations are strinctly harmonic


------------
INNER ENERGY
------------

The inner energy is: U= E(el) + E(ZPE) + E(vib) + E(rot) + E(trans)
    E(el)   - is the total energy from the electronic structure calculation
              = E(kin-el) + E(nuc-el) + E(el-el) + E(nuc-nuc)
    E(ZPE)  - the the zero temperature vibrational energy from the frequency 
calculation
    E(vib)  - the the finite temperature correction to E(ZPE) due to population
              of excietd vibrational states
    E(rot)  - is the rotational thermal energy
    E(trans)- is the translational thermal energy
```

```
Summary of contributions to the inner energy U:
Electronic energy                ...   -232.01175159 Eh
Zero point energy                ...      0.09737409 Eh      61.10 kcal/mol
Thermal vibrational correction   ...      0.00174527 Eh       1.10 kcal/mol
Thermal rotational correction    ...      0.00141627 Eh       0.89 kcal/mol
Thermal translational correction ...      0.00141627 Eh       0.89 kcal/mol
-----------------------------------------------------------------------
Total thermal energy                   -231.90979968 Eh


Summary of corrections to the electronic energy:
(perhaps to be used in another calculation)
Total thermal correction                  0.00457781 Eh       2.87 kcal/mol
Non-thermal (ZPE) correction              0.09737409 Eh      61.10 kcal/mol
-----------------------------------------------------------------------
Total correction                          0.10195190 Eh      63.98 kcal/mol


--------
ENTHALPY
--------

The enthalpy is H = U + kB*T
                kB is Boltzmann's constant
Total free energy                 ...   -231.90979968 Eh
Thermal Enthalpy correction       ...      0.00094421 Eh       0.59 kcal/mol
-----------------------------------------------------------------------
Total Enthalpy                    ...   -231.90885547 Eh


-------
ENTROPY
-------

The entropy contributions are T*S = T*(S(el)+S(vib)+S(rot)+S(trans)
     S(el)   - electronic entropy
     S(vib)  - vibrational entropy
     S(rot)  - rotational entropy
     S(trans)- translational entropy
The entropies will be listed as mutliplied by the temperature to get
units of energy

Electronic entropy                ...      0.00000000 Eh      0.00 kcal/mol
Vibrational entropy               ...      0.00236338 Eh      1.48 kcal/mol
Rotational entropy                ...      0.01116050 Eh      7.00 kcal/mol
Translational entropy             ...      0.01852142 Eh     11.62 kcal/mol
-----------------------------------------------------------------------
Final entropy term                ...      0.03204531 Eh     20.11 kcal/mol


CAUTION: The rotational entropy is not quite correctly treated here
         because it includes a symmetry number that is not yet correctly
         implemented in ORCA!
For a nonlinear molecule the correct rotational entropy is:
    S(rot) = R*(ln(qrot/sn)+1.5)
    R    = 8.31441 J/mol/K = 1.987191683e-3 kcal/mol/K
    qrot = 91027.2228548
    sn is the rotational symmetry number. We have assumed 3 here
       if it is different for your molecule then you should correct
       the printed rotational entropy by manually evaluating the equation
       as given above

For convenience we print out the resulting values for sn=1 - 12:
 sn= 1  qrot/sn=   91027.2229 T*S(rot)=     7.65 kcal/mol T*S(tot)=    20.76
```

```
kcal/mol
 sn= 2  qrot/sn=   45513.6114 T*S(rot)=     7.24 kcal/mol T*S(tot)=    20.35
kcal/mol
 sn= 3  qrot/sn=   30342.4076 T*S(rot)=     7.00 kcal/mol T*S(tot)=    20.11
kcal/mol
 sn= 4  qrot/sn=   22756.8057 T*S(rot)=     6.83 kcal/mol T*S(tot)=    19.94
kcal/mol
 sn= 5  qrot/sn=   18205.4446 T*S(rot)=     6.70 kcal/mol T*S(tot)=    19.81
kcal/mol
 sn= 6  qrot/sn=   15171.2038 T*S(rot)=     6.59 kcal/mol T*S(tot)=    19.70
kcal/mol
 sn= 7  qrot/sn=   13003.8890 T*S(rot)=     6.50 kcal/mol T*S(tot)=    19.61
kcal/mol
 sn= 8  qrot/sn=   11378.4029 T*S(rot)=     6.42 kcal/mol T*S(tot)=    19.53
kcal/mol
 sn= 9  qrot/sn=   10114.1359 T*S(rot)=     6.35 kcal/mol T*S(tot)=    19.46
kcal/mol
 sn=10  qrot/sn=    9102.7223 T*S(rot)=     6.29 kcal/mol T*S(tot)=    19.40
kcal/mol
 sn=11  qrot/sn=    8275.2021 T*S(rot)=     6.23 kcal/mol T*S(tot)=    19.34
kcal/mol
 sn=12  qrot/sn=    7585.6019 T*S(rot)=     6.18 kcal/mol T*S(tot)=    19.29
kcal/mol


-------------------
GIBBS FREE ENTHALPY
-------------------

The Gibbs free enthalpy is G = H - T*S

Total enthalpy                    ...   -231.90885547 Eh
Total entropy correction          ...     -0.03204531 Eh    -20.11 kcal/mol
-----------------------------------------------------------------------
Final Gibbs free enthalpy         ...   -231.94090078 Eh

For completeness - the Gibbs free enthalpy minus the electronic energy
G-E(el)                           ...      0.07085081 Eh     44.46 kcal/mol


Timings for individual modules:

Sum of individual times         ...      299.514 sec (=   4.992 min)
GTO integral calculation        ...        2.024 sec (=   0.034 min)   0.7 %
SCF iterations                  ...       53.952 sec (=   0.899 min)  18.0 %
SCF Gradient evaluation         ...       34.427 sec (=   0.574 min)  11.5 %
Geometry relaxation             ...        1.168 sec (=   0.019 min)   0.4 %
Analytical frequency calculation...      207.944 sec (=   3.466 min)  69.4 %
                             ****ORCA TERMINATED NORMALLY****
TOTAL RUN TIME: 0 days 0 hours 5 minutes 0 seconds 805 msec
```