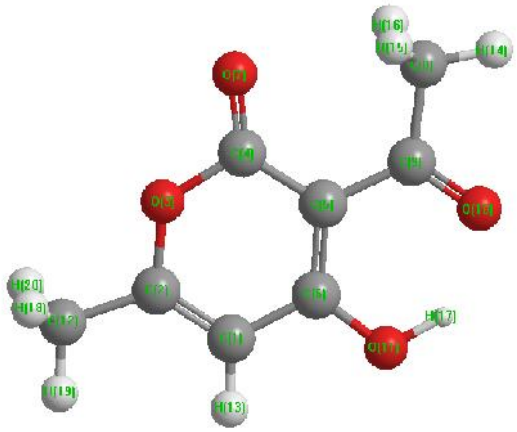
ANNEXE

Présentation d'un fichier de résultat du composé A avec la méthode HF (6-31G) en utilisant le logiciel Gaussian 03 (Chapitre II) :



```
 ******************************************************************
Gaussian 03:  x86-Win32-G03RevB.04 2-Jun-2003
                 04-Mar-2015
******************************************************************
%Chk=Untitled-1.chk
----------------------
# RHF/6-31G opt=tight
----------------------
Charge =  0 Multiplicity = 1
```

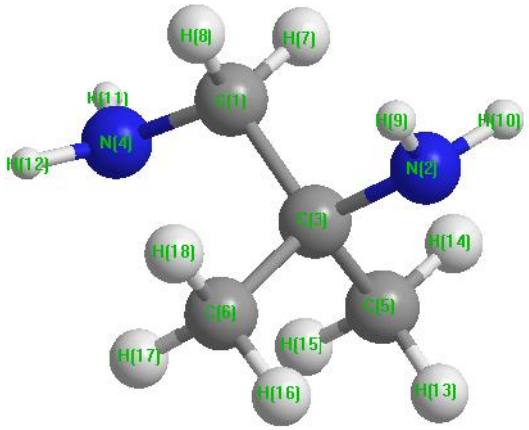
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.537342	1.220689	0.000000
2	6	0	2.195099	0.055770	0.000000
3	8	0	1.503933	-1.112362	-0.000001
4	6	0	0.113754	-1.227317	0.000000
5	6	0	-0.613806	0.021374	-0.000002
6	6	0	0.107444	1.207266	0.000000
7	8	0	-0.332462	-2.351680	0.000001
8	6	0	-2.906068	-1.194811	0.000000
9	6	0	-2.078239	0.053944	-0.000001
10	8	0	-2.655622	1.154481	0.000000
11	8	0	-0.455243	2.405574	0.000001
12	6	0	3.665091	-0.156311	0.000000
13	1	0	2.040023	2.161865	-0.000001
14	1	0	-3.944610	-0.904088	-0.000007
15	1	0	-2.688791	-1.805986	0.864942
16	1	0	-2.688781	-1.805996	-0.864933
17	1	0	-1.424921	2.374667	0.000000
18	1	0	3.952462	-0.728573	0.873231
19	1	0	4.193607	0.784960	0.000001
20	1	0	3.952464	-0.728573	-0.873230

```
SCF Done:  E(RHF) =  -606.800522956     A.U. after    4 cycles
           Convg  =    0.5397D-08             -V/T =  1.9995
```

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000000     0.000015     YES
 RMS     Force            0.000000     0.000010     YES
 Maximum Displacement     0.000361     0.000060     YES
 RMS     Displacement     0.000069     0.000040     YES
 Predicted change in Energy=-2.281504D-10
 Optimization completed.

 ***************************************************************************

            Population analysis using the SCF density.

 ***************************************************************************

Alpha  occ. eigenvalues -  -0.57611  -0.56215  -0.55001  -0.52110  -0.51066
Alpha  occ. eigenvalues -  -0.45889  -0.43489  -0.42991  -0.35478
Alpha virt. eigenvalues -   0.05359   0.13504   0.17026   0.22377   0.24957
Alpha virt. eigenvalues -   0.26763   0.28767   0.29046   0.30297   0.31171

Mulliken atomic charges:
              1
     1  C   -0.290215
     2  C    0.477263
     3  O   -0.780831
     4  C    0.841693
     5  C   -0.336385
     6  C    0.496070
     7  O   -0.554957
     8  C   -0.493397
     9  C    0.553476
    10  O   -0.666762
    11  O   -0.770311
    12  C   -0.482861
    13  H    0.260677
    14  H    0.198007
    15  H    0.211993
    16  H    0.211993
    17  H    0.502424
    18  H    0.216019
    19  H    0.190086
    20  H    0.216019

 Dipole moment (field-independent basis, Debye):
    X=     3.8647    Y=     1.5392    Z=     0.0000  Tot=     4.1599

Job cpu time:  0 days  0 hours 11 minutes  6.0 seconds.
Normal termination of Gaussian 03 at Wed Mar 04 17:53:32 2015.
```

Présentation d'un fichier de résultat du composé B avec la méthode HF (6-31G) en utilisant le logiciel Gaussian 03 (Chapitre II) :




```
 ******************************************************************
 Gaussian 03:  x86-Win32-G03RevB.04 2-Jun-2003
                16-Apr-2015
 ******************************************************************
 RHF/6-31G opt=tight
 ---------------------
 Charge =  0 Multiplicity = 1

                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.888815   -0.156074   -0.787275
    2          7             0        1.574812   -0.130151   -0.917518
    3          6             0        0.437256   -0.002756   -0.004551
    4          7             0       -2.080097   -0.011280    0.027938
    5          6             0        0.556837   -1.097831    1.057191
    6          6             0        0.513225    1.381456    0.646634
    7          1             0       -0.898115   -1.144130   -1.236129
    8          1             0       -0.873633    0.558126   -1.611592
    9          1             0        1.690550    0.598750   -1.586882
   10          1             0        1.743398   -1.038530   -1.290275
   11          1             0       -2.788135   -0.700413   -0.062655
   12          1             0       -2.426656    0.906719    0.179819
   13          1             0        1.479888   -0.979279    1.610766
   14          1             0        0.567460   -2.081503    0.594520
   15          1             0       -0.280232   -1.057168    1.739932
   16          1             0        1.458954    1.494487    1.160807
   17          1             0       -0.290399    1.517561    1.359062
   18          1             0        0.442897    2.166623   -0.102314
 ---------------------------------------------------------------------
SCF Done:  E(RHF) =  -267.230716994     A.U. after    6 cycles
             Convg  =    0.4170D-08             -V/T =  1.9986
```

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000001     0.000015     YES
 RMS     Force            0.000000     0.000010     YES
 Maximum Displacement     0.000091     0.000060     YES
 RMS     Displacement     0.000021     0.000040     YES
 Predicted change in Energy=-4.475741D-11
 Optimization completed.

 ***************************************************************************

            Population analysis using the SCF density.

 ***************************************************************************

Alpha  occ. eigenvalues -  -0.60622  -0.57005  -0.55721  -0.51892  -0.50339
Alpha  occ. eigenvalues -  -0.49119  -0.48007  -0.45119  -0.38665  -0.33886
Alpha virt. eigenvalues -   0.21512   0.24181   0.26738   0.28795   0.30157
Alpha virt. eigenvalues -   0.31637   0.31813   0.32701   0.35581   0.36702

Mulliken atomic charges:
              1
     1  C   -0.053886
     2  N   -0.841951
     3  C    0.130377
     4  N   -0.884416
     5  C   -0.418308
     6  C   -0.428990
     7  H    0.145816
     8  H    0.131301
     9  H    0.315811
    10  H    0.316680
    11  H    0.331816
    12  H    0.329580
    13  H    0.161404
    14  H    0.126598
    15  H    0.177574
    16  H    0.170489
    17  H    0.160494
    18  H    0.129612

 Dipole moment (field-independent basis, Debye):
    X=    -1.5982    Y=     0.0260    Z=    -1.5421  Tot=     2.2210


Job cpu time:  0 days  0 hours  1 minutes 58.0 seconds.

Normal termination of Gaussian 03 at Thu Apr 16 20:23:49 2015.
```