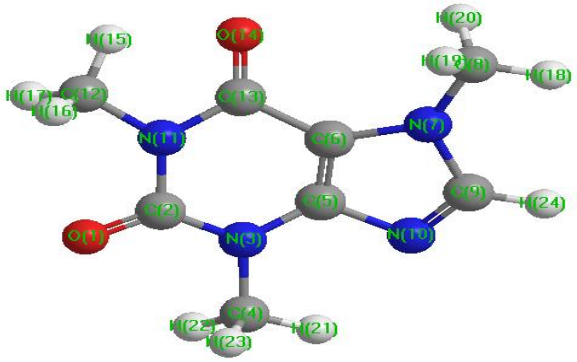
ANNEXES

***Présentation d'un fichier de résultats obtenu avec la méthode DFT (B3LYP/ 6-311G) en utilisant le logiciel Gaussian 03 pour le composé caféine (chapitre* III).**

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 *********************************************
 Gaussian 03:  x86-Win32-G03RevB.04 2-Jun-2003
                 08-Mar-2015
 *********************************************
 -------------------------
 # RB3LYP/6-311G opt=tight
 -------------------------
Charge = 0 Multiplicity = 1
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.105842	-0.290698	0.001970
2	6	0	-1.864978	-0.165871	0.001077
3	7	0	-1.020727	-1.275739	0.000448
4	6	0	-1.619736	-2.618941	0.000521
5	6	0	0.344950	-1.091492	0.000066
6	6	0	0.907868	0.172468	0.000473
7	7	0	2.288938	-0.036383	-0.001831
8	6	0	3.326071	0.999630	0.005732
9	6	0	2.468556	-1.391827	-0.002746
10	7	0	1.308705	-2.071055	-0.002059
11	7	0	-1.255125	1.108304	0.000240
12	6	0	-2.179905	2.257718	-0.000280
13	6	0	0.139610	1.374385	-0.001187
14	8	0	0.594891	2.543119	-0.004161
15	1	0	-0.809072	-3.339947	-0.002222
16	1	0	-2.244297	-2.748472	-0.881069
17	1	0	-2.239972	-2.750494	0.884901
18	1	0	4.298037	0.514692	-0.047254
19	1	0	3.261364	1.592408	0.915071
20	1	0	3.199303	1.662753	-0.845780
21	1	0	3.441611	-1.846582	-0.004345
22	1	0	-1.576423	3.158022	0.000176
23	1	0	-2.815651	2.222761	0.881733
24	1	0	-2.814452	2.223197	-0.883210

```
SCF Done:  E(RB+HF-LYP) =  -680.319580614     A.U. after    5 cycles
             Convg  =    0.3837D-08             -V/T =  2.0030
             S**2   =   0.0000

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               Population analysis using the SCF density.

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

Alpha  occ. eigenvalues -0.30604  -0.29264  -0.29136  -0.27536  -0.26913
Alpha  occ. Eigenvalues -0.23387
Alpha virt. eigenvalues -0.04974   0.00247   0.01664   0.03293   0.05721
Alpha virt. eigenvalues  0.06318   0.07402   0.09324   0.09407   0.10363

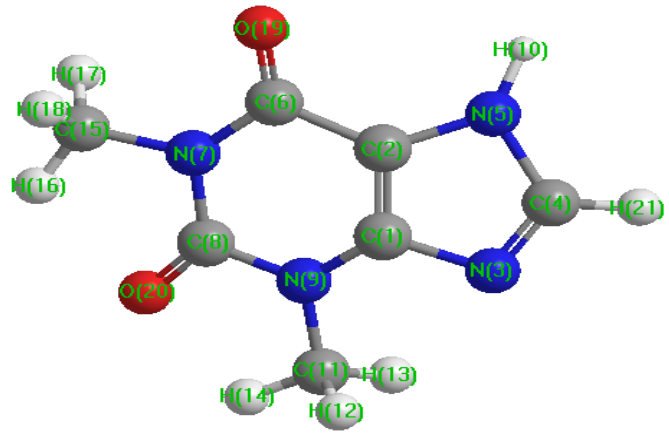
Mulliken atomic charges:
     1 O   -0.423260
     2 C    0.738668
     3 N   -0.674833
     4 C   -0.342007
     5 C    0.339654
     6 C    0.172484
     7 N   -0.688207
     8 C   -0.322087
     9 C    0.233088
    10 N   -0.372553
    11 N   -0.694699
    12 C   -0.343756
    13 C    0.665466
    14 O   -0.414083
    15 H    0.218058
    16 H    0.209525
    17 H    0.209490
    18 H    0.185742
    19 H    0.223646
    20 H    0.226234
    21 H    0.213289
    22 H    0.222443
    23 H    0.208859
    24 H    0.208837

Dipole moment (field-independent basis, Debye):
    X=     4.0725    Y=    -0.8016    Z=     0.0096  Tot=     4.1506

Job cpu time:  0 days 3 hours 43 minutes 45.0 seconds.

Normal termination of Gaussian 03 at Sun Mar 08 23:10:09 2015.
```

***Présentation d'un fichier de résultats obtenu avec la méthode DFT, utilisant la chaine de programme Gaussian 03, pour le composé théophylline (chapitre* III).**

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*********************************************
 Gaussian 03:  x86-Win32-G03RevB.04 2-Jun-2003
                06-Mar-2015
 *********************************************
 ---------------------------
 # RB3LYP/6-311G opt=tight
 ---------------------------
Charge = 0 Multiplicity = 1
```
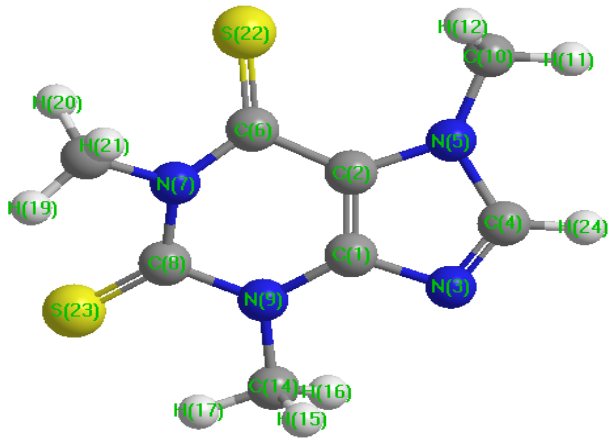

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.202384	-1.322456	0.000000
2	6	0	3.042929	-0.242418	0.000002
3	7	0	2.371655	0.919500	0.000001
4	6	0	1.043398	0.547270	0.000000
5	7	0	-0.047484	1.386655	-0.000002
6	6	0	0.130339	2.846417	-0.000001
7	6	0	-1.335021	0.838741	0.000000
8	8	0	-2.358412	1.550869	0.000003
9	7	0	-1.433461	-0.571182	-0.000002
10	6	0	-2.805568	-1.114285	-0.000001
11	6	0	-0.354363	-1.493897	-0.000001
12	8	0	-0.526071	-2.733893	0.000001
13	6	0	0.904542	-0.825556	-0.000001
14	1	0	2.447314	-2.297584	-0.000002
15	1	0	4.112864	-0.328963	0.000000
16	1	0	-0.856159	3.295752	-0.000017
17	1	0	0.684087	3.153223	-0.885537
18	1	0	0.684057	3.153227	0.885552
19	1	0	-2.724298	-2.195167	0.000005
20	1	0	-3.340605	-0.770779	-0.882518
21	1	0	-3.340607	-0.770770	0.882513

```
SCF Done:  E(RB+HF-LYP) =  -641.010978950     A.U. after    4 cycles
             Convg  =    0.6092D-08             -V/T =  2.0030
             S**2   =   0.0000

         Item               Value     Threshold  Converged?
 Maximum Force            0.000000     0.000015     YES
 RMS     Force            0.000000     0.000010     YES
 Maximum Displacement     0.000019     0.000060     YES
 RMS     Displacement     0.000004     0.000040     YES
 Predicted change in Energy=-2.156433D-12
 Optimization completed.

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

            Population analysis using the SCF density.

 ***********************************************************************
Alpha  occ. eigenvalues -0.34712  -0.31185  -0.30081  -0.29618  -0.27884
Alpha  occ. eigenvalues -0.27240  -0.23894
Alpha virt. eigenvalues -0.05491   0.00051   0.01328   0.02470   0.05684
Alpha virt. eigenvalues  0.06449   0.07150   0.09997   0.10426   0.11925

Mulliken atomic charges:

     1 N   -0.754802
     2 C    0.234959
     3 N   -0.365631
     4 C    0.321940
     5 N   -0.678161
     6 C   -0.346308
     7 C    0.729606
     8 O   -0.417763
     9 N   -0.689368
    10 C   -0.341592
    11 C    0.654528
    12 O   -0.405811
    13 C    0.182165
    14 H    0.370220
    15 H    0.218427
    16 H    0.226781
    17 H    0.208757
    18 H    0.208757
    19 H    0.223204
    20 H    0.210045
    21 H    0.210045

Dipole moment (field-independent basis, Debye):
    X=     3.6723    Y=    -0.6597    Z=     0.0000 Tot=     3.7311

Job cpu time:  0 days 1 hours 43 minutes 54.0 seconds.

Normal termination of Gaussian 03 at Fri Mar 06 10:38:26 2015.
```

Présentation d'un fichier de résultats obtenu avec la méthode DFT (B3LYP/ 6-311G) en utilisant le logiciel Gaussian 03 pour le composé 2,6 -dithiocaféine.




```
*********************************************
 Gaussian 03:  x86-Win32-G03RevB.04 2-Jun-2003
                08-Mar-2015
 *********************************************
 -------------------------
 # RB3LYP/6-311G opt=tight
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                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         16             0       -3.418335    0.153869    0.000005
    2          6             0       -1.704255   -0.001247   -0.000001
    3          7             0       -1.108830   -1.249111   -0.000003
    4          6             0       -1.921006   -2.481413   -0.000004
    5          6             0        0.261379   -1.354368   -0.000001
    6          6             0        1.082767   -0.231981    0.000000
    7          7             0        2.387645   -0.752757    0.000002
    8          6             0        3.671025   -0.038290    0.000004
    9          6             0        2.256474   -2.113914    0.000001
   10          7             0        0.979305   -2.520995   -0.000001
   11          7             0       -0.846436    1.120491   -0.000002
   12          6             0       -1.520875    2.441218   -0.000002
   13          6             0        0.569337    1.086226   -0.000001
   14         16             0        1.560215    2.497433   -0.000001
   15          1             0       -1.234417   -3.320621   -0.000022
   16          1             0       -2.556021   -2.501641   -0.882227
   17          1             0       -2.555996   -2.501661    0.882236
   18          1             0        4.463814   -0.783729    0.000002
   19          1             0        3.757032    0.590050    0.880933
   20          1             0        3.757032    0.590054   -0.880923
   21          1             0        3.104849   -2.772399    0.000002
   22          1             0       -0.758650    3.206665   -0.000004
   23          1             0       -2.149293    2.525828    0.882366
   24          1             0       -2.149296    2.525826   -0.882370
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```

```
SCF Done:  E(RB+HF-LYP) =  -1326.24271941     A.U. after    4 cycles
             Convg  =    0.4974D-08             -V/T =  2.0021
             S**2   =   0.0000

         Item               Value     Threshold  Converged?
 Maximum Force            0.000001     0.000015     YES
 RMS     Force            0.000000     0.000010     YES
 Maximum Displacement     0.000021     0.000060     YES
 RMS     Displacement     0.000004     0.000040     YES
 Predicted change in Energy=-2.786161D-12
 ***************************************************************************

           Population analysis using the SCF density.
 ***************************************************************************

Alpha  occ. eigenvalues -0.37579  -0.36833  -0.32068  -0.31380  -0.30072
Alpha  occ. eigenvalues -0.24259  -0.23914  -0.22900  -0.22219
Alpha virt. eigenvalues -0.08537  -0.04876  -0.00308   0.02860   0.04274
Alpha virt. Eigenvalues  0.05817   0.06275   0.07457   0.07481   0.07576


Mulliken atomic charges:
     1  S   -0.074272
     2  C    0.191057
     3  N   -0.608600
     4  C   -0.359577
     5  C    0.314330
     6  C    0.352836
     7  N   -0.698417
     8  C   -0.335801
     9  C    0.235662
    10  N   -0.362585
    11  N   -0.610686
    12  C   -0.350789
    13  C    0.053806
    14  S   -0.050927
    15  H    0.222288
    16  H    0.236673
    17  H    0.236672
    18  H    0.182005
    19  H    0.242388
    20  H    0.242389
    21  H    0.221536
    22  H    0.241660
    23  H    0.239176
    24  H    0.239175

Dipole moment (field-independent basis, Debye):
    X=     4.4706    Y=    -2.8049    Z=     0.0000  Tot=     5.2777
Job cpu time:  0 days  4 hours 34 minutes  0.0 seconds.

Normal termination of Gaussian 03 at Mon Mar 09 00:40:49 2015.
```