

# Supporting Information

for

## Structure of 1,5-benzodiazepinones in the solid state and in solution: Effect of the fluorination in the six-membered ring

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### Additional material

**Figure S1:** <sup>1</sup>H NMR spectra at several temperatures of compound **1** in toluene-*d*<sub>8</sub>.

**Figure S2:** <sup>1</sup>H NMR spectra at several temperatures of compound **2** in toluene-*d*<sub>8</sub>.

**Figure S3:** <sup>13</sup>C NMR spectra (CPMAS and NQS sequence) of compound **1**.

**Figure S4:** <sup>15</sup>N CPMAS NMR spectrum of compound **1**.

**Figure S5:** <sup>19</sup>F MAS NMR spectrum of compound **1**.

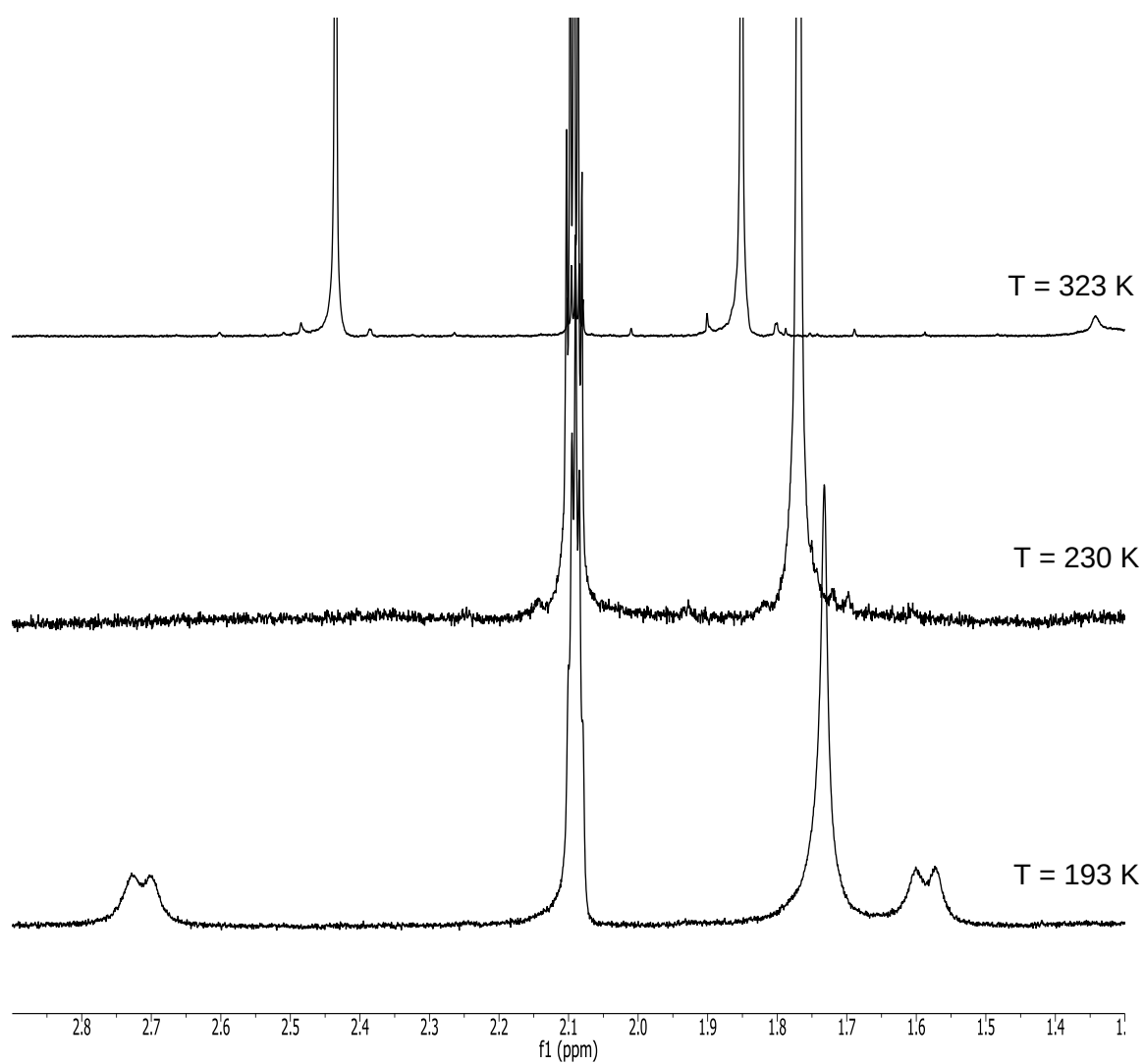
**Figure S6:** <sup>13</sup>C NMR spectra (CPMAS and NQS sequence) of compound **2**.

**Figure S7:** <sup>15</sup>N CPMAS NMR spectrum of compound **2**.

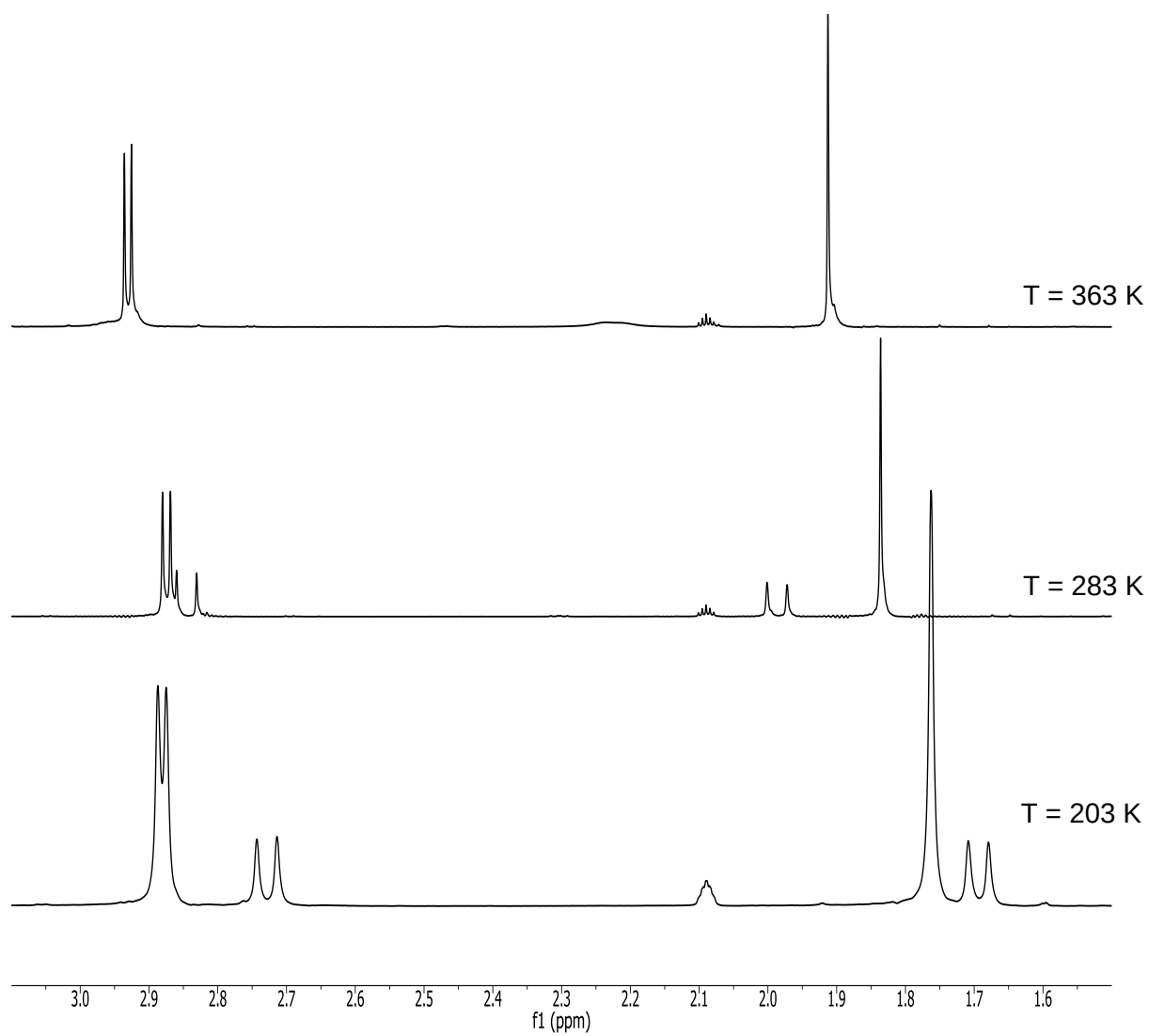
**Figure S8:** <sup>19</sup>F MAS NMR spectrum of compound **2**.

**Table S1:** Calculated and some experimental <sup>1</sup>H, <sup>13</sup>C and <sup>15</sup>N chemical shifts (δ, ppm) of compounds **3a** to **6a**.

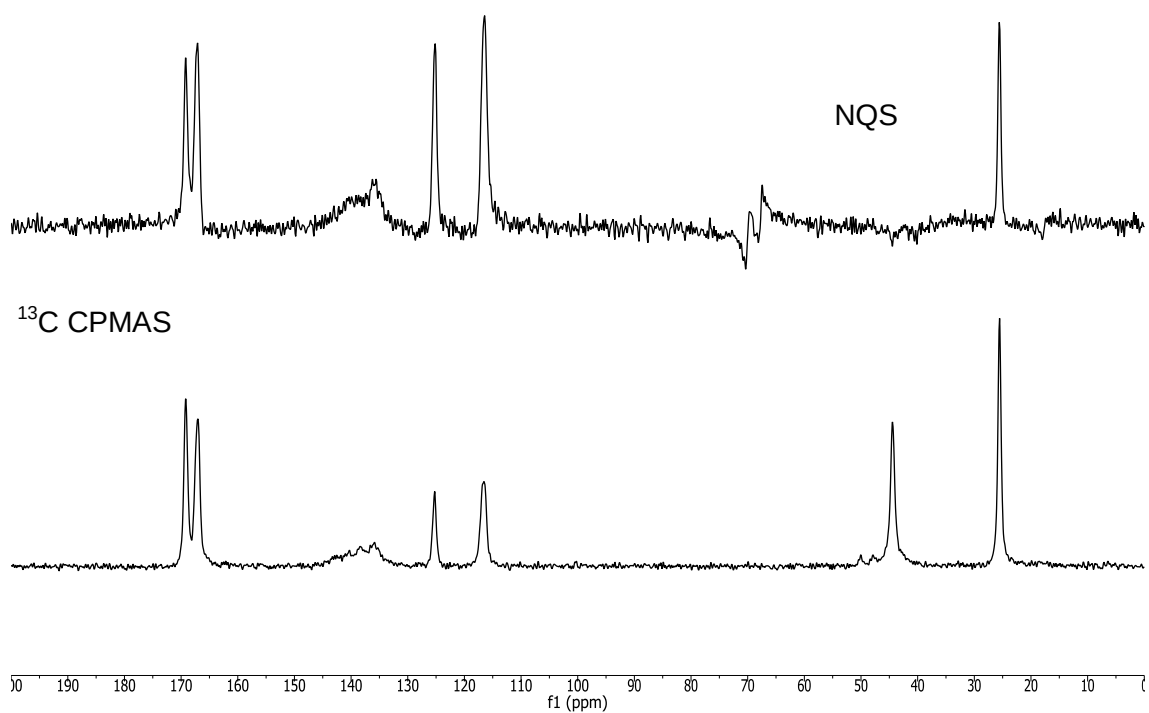
Geometry (Å), energy (hartree) and number of imaginary frequencies of the different tautomers calculated at the B3LYP/6-311++G(d,p) computational level.



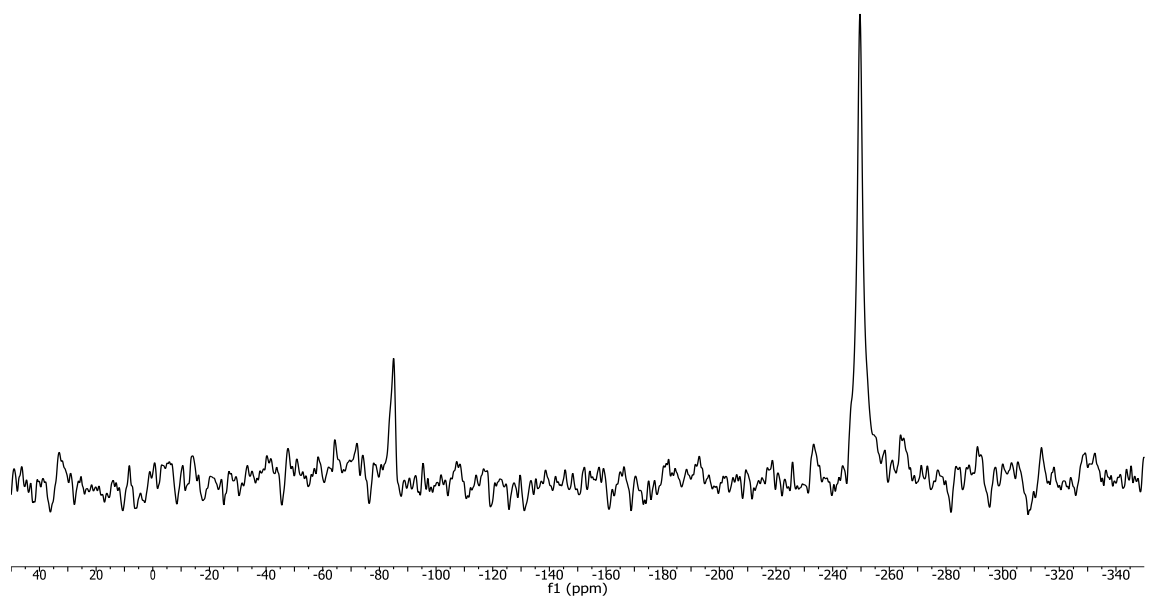
**Figure S1:**  $^1\text{H}$  NMR spectra at several temperatures of compound **1** in  $\text{toluene-}d_8$ .



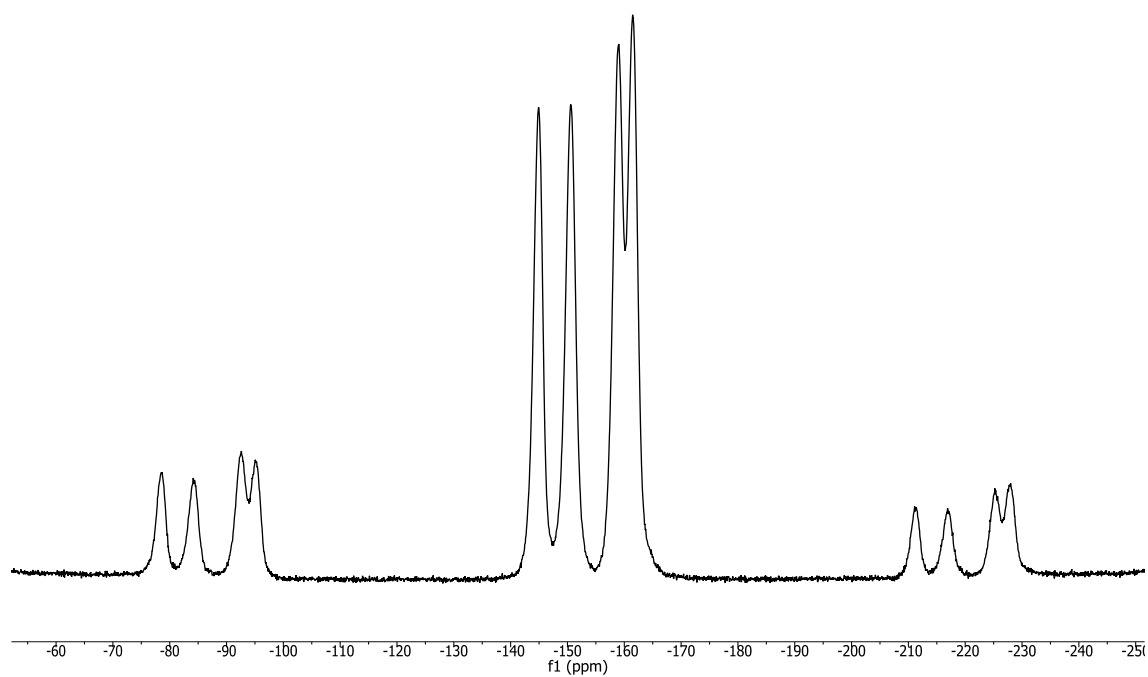
**Figure S2:**  $^1\text{H}$  NMR spectra at several temperatures of compound **2** in  $\text{toluene-}d_8$ .



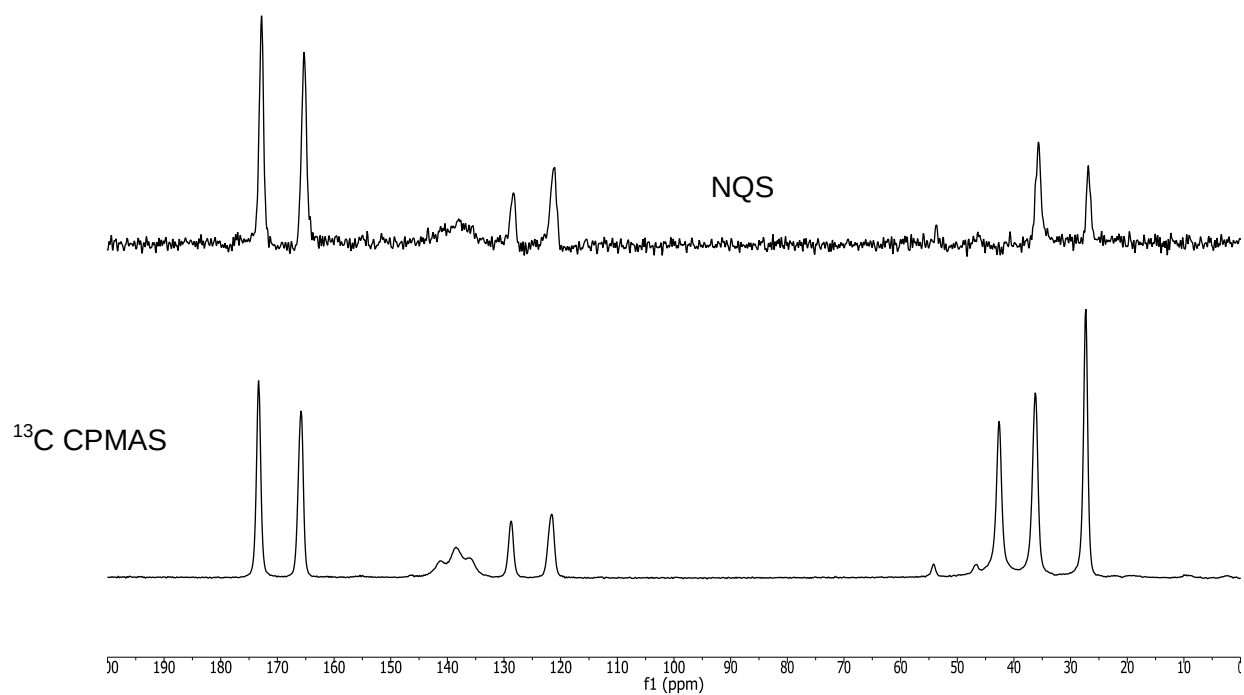
**Figure S3:**  $^{13}\text{C}$  NMR spectra (CPMAS and NQS sequence) of compound **1**.



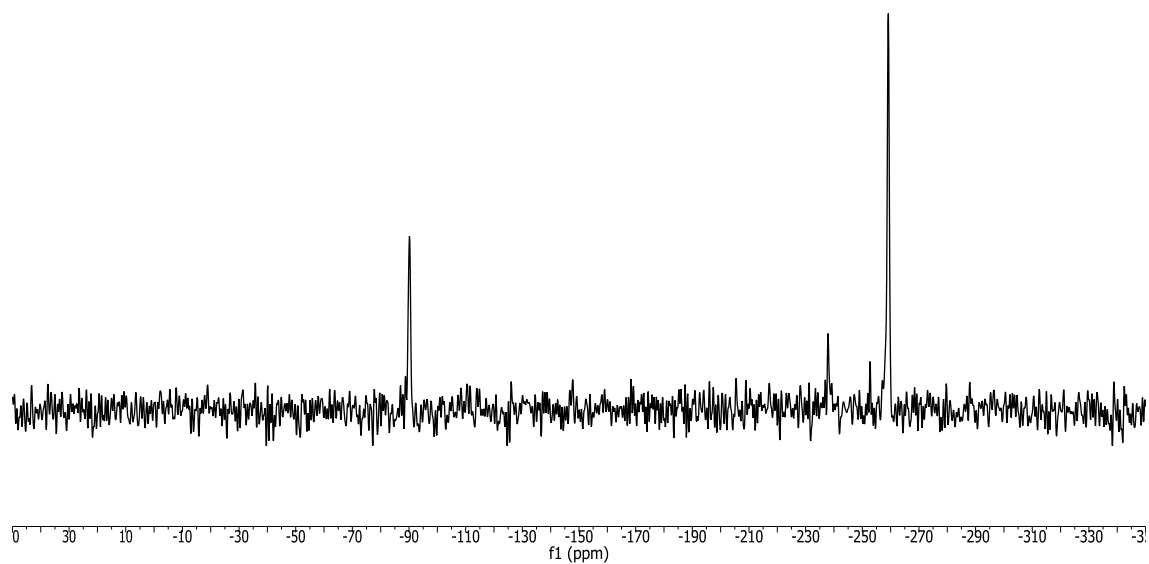
**Figure S4:**  $^{15}\text{N}$  CPMAS NMR spectrum of compound **1**.



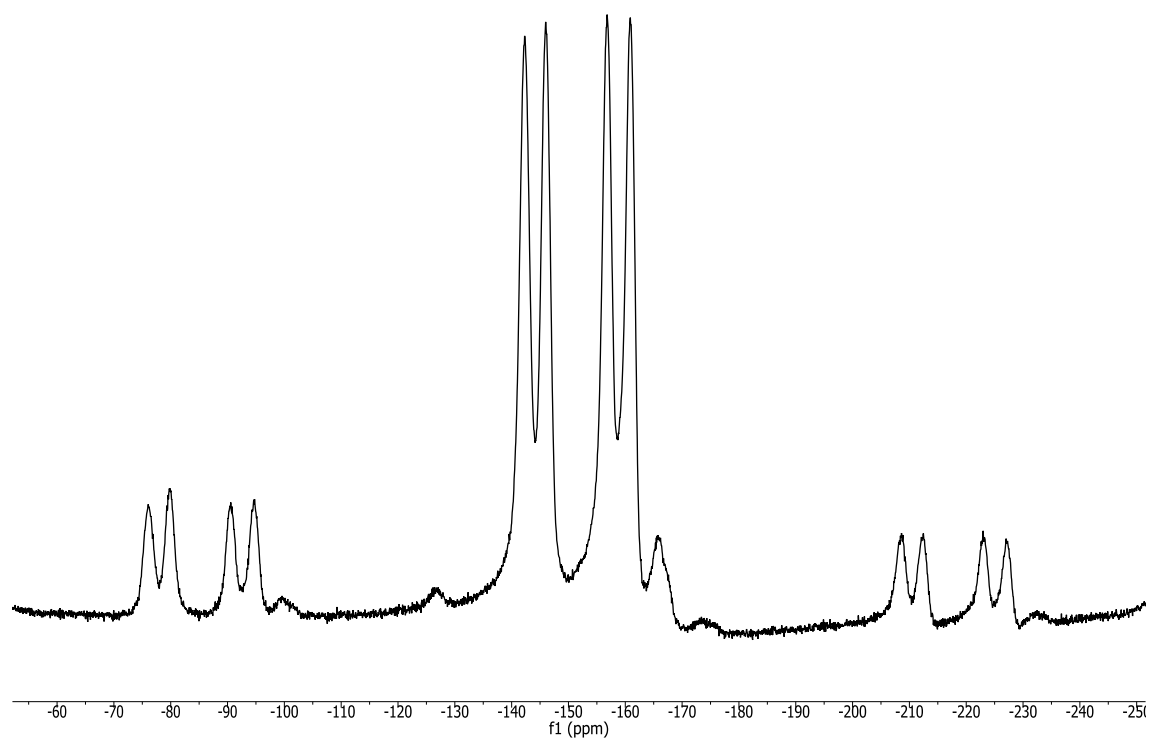
**Figure S5:**  $^{19}\text{F}$  MAS NMR spectrum of compound **1**.



**Figure S6:**  $^{13}\text{C}$  NMR spectra (CPMAS and NQS sequence) of compound **2**.



**Figure S7:**  $^{15}\text{N}$  CPMAS NMR spectrum of compound **2**.



**Figure S8:**  $^{19}\text{F}$  MAS NMR spectrum of compound **2**.

**Table S1:** Calculated and some experimental  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  chemical shifts ( $\delta$ , ppm) of compounds **3a** to **6a**.

| Comp.     | Nucleus                           | Solvent                     | NH               | CH <sub>2</sub>        | 4-CH <sub>3</sub>          | H6                | H7     | H8     | H9    |
|-----------|-----------------------------------|-----------------------------|------------------|------------------------|----------------------------|-------------------|--------|--------|-------|
| <b>3a</b> | $^1\text{H}$                      | (gas)                       | 6.62             | 2.50 (ax)<br>3.12 (eq) | 2.28<br>(CH <sub>3</sub> ) | 7.40              | 7.10   | 7.05   | 6.78  |
| Exp. [1]  |                                   | CDCl <sub>3</sub>           | 9.99             | 3.14 (s)               | 2.38                       | ----              | ----   | ----   | ----  |
| Exp. [2]  |                                   | Acetone                     | ----             | 3.08<br>4.25           | ----                       | ----              | ----   | ----   | ----  |
| Exp. [3]  |                                   | DMSO- <i>d</i> <sub>6</sub> | ----             | 3.87<br>3.42           | ----                       | ----              | ----   | ----   | ----  |
|           | $^{13}\text{C}$                   | (gas)                       | NH               | C2                     | C3                         | C4                | C5a    | C6     | C7    |
|           |                                   |                             | ----             | 162.8                  | 43.4                       | 162.4             | 141.2  | 129.3  | 123.3 |
|           |                                   |                             | C8               | C9                     | C9a                        | 4-CH <sub>3</sub> | N1     | N5     |       |
|           | $^{13}\text{C}$ & $^{15}\text{N}$ |                             | 125.0            | 119.6                  | 130.1                      | 28.1              | -245.0 | -64.4  |       |
| Exp. [4]  | $^{13}\text{C}$                   | CDCl <sub>3</sub>           | NH               | C2                     | C3                         | C4                | C5a    | C6     | C7    |
|           |                                   |                             | ----             | 167.6                  | 43.7                       | 163.1             | 140.0  | 127.9  | 125.2 |
|           | $^{13}\text{C}$ & $^{15}\text{N}$ |                             | C8               | C9                     | C9a                        | 4-CH <sub>3</sub> | N1     | N5     |       |
|           |                                   |                             | 126.4            | 122.1                  | 129.4                      | 27.9              | ----   | ----16 |       |
| <b>4a</b> | $^1\text{H}$                      | (gas)                       | NCH <sub>3</sub> | CH <sub>2</sub>        | 4-CH <sub>3</sub>          | H6                | H7     | H8     | H9    |
|           |                                   |                             | 3.25             | 2.49 (ax)<br>3.14 (eq) | 2.23                       | 7.34              | 7.08   | 7.13   | 7.14  |
|           | $^{13}\text{C}$                   | (gas)                       | NCH <sub>3</sub> | C2                     | C3                         | C4                | C5a    | C6     | C7    |
|           |                                   |                             | 34.2             | 163.6                  | 43.7                       | 164.0             | 143.1  | 128.1  | 123.4 |
|           | $^{13}\text{C}$ & $^{15}\text{N}$ | (gas)                       | C8               | C9                     | C9a                        | 4-CH <sub>3</sub> | N1     | N5     |       |
|           |                                   |                             | 124.4            | 120.0                  | 137.0                      | 27.5              | -248.8 | -66.8  |       |
| Exp. [4]  | $^{13}\text{C}$                   | CDCl <sub>3</sub>           | NCH <sub>3</sub> | C2                     | C3                         | C4                | C5a    | C6     | C7    |

|           |                                   |                   |                  |                        |                                                             |                                                                                      |        |       |       |
|-----------|-----------------------------------|-------------------|------------------|------------------------|-------------------------------------------------------------|--------------------------------------------------------------------------------------|--------|-------|-------|
|           |                                   |                   | 40.0             | 165.7                  | 43.5                                                        | 165.0                                                                                | 141.4  | 126.4 | 125.1 |
|           | <sup>13</sup> C & <sup>15</sup> N |                   | C8               | C9                     | C9a                                                         | 4-CH <sub>3</sub>                                                                    | N1     | N5    |       |
|           |                                   |                   | 125.7            | 121.9                  | 135.3                                                       | 27.4                                                                                 | ----   | ----  |       |
| <b>5a</b> | <sup>1</sup> H                    | (gas)             | NH               | CH <sub>2</sub>        | 4-C <sub>6</sub> H <sub>5</sub>                             | H6                                                                                   | H7     | H8    | H9    |
|           |                                   |                   | 6.73             | 2.58 (ax)<br>3.82 (eq) | 8.30 ( <i>o</i> )<br>7.44 ( <i>m</i> )<br>7.40 ( <i>p</i> ) | 7.47                                                                                 | 7.14   | 7.12  | 6.85  |
|           | <sup>13</sup> C                   | (gas)             | NH               | C2                     | C3                                                          | C4                                                                                   | C5a    | C6    | C7    |
|           |                                   |                   | ----             | 163.8                  | 40.2                                                        | 158.2                                                                                | 141.3  | 129.3 | 123.6 |
|           |                                   |                   |                  |                        |                                                             |                                                                                      |        |       |       |
|           |                                   |                   | C8               | C9                     | C9a                                                         | 4-C <sub>6</sub> H <sub>5</sub>                                                      | N1     | N5    |       |
|           |                                   |                   | 125.1            | 119.7                  | 130.6                                                       | 139.0 ( <i>i</i> )<br>128.4 ( <i>o</i> )<br>127.9 ( <i>m</i> )<br>130.4 ( <i>p</i> ) | −243.5 | −67.7 |       |
| Exp. [4]  | <sup>13</sup> C                   | CDCl <sub>3</sub> | NH               | C2                     | C3                                                          | C4                                                                                   | C5a    | C6    | C7    |
|           |                                   |                   | ----             | 167.8                  | 39.8                                                        | 158.6                                                                                | 139.9  | 128.3 | 126.1 |
|           | <sup>13</sup> C & <sup>15</sup> N |                   | C8               | C9                     | C9a                                                         | 4-C <sub>6</sub> H <sub>5</sub>                                                      | N1     | N5    |       |
|           |                                   |                   | 126.5            | 121.8                  | 129.1                                                       | 137.6 ( <i>i</i> )<br>128.7 ( <i>o</i> )<br>127.7 ( <i>m</i> )<br>130.9 ( <i>p</i> ) |        |       |       |
| <b>6a</b> | <sup>1</sup> H                    | (gas)             | NCH <sub>3</sub> | CH <sub>2</sub>        | 4-C <sub>6</sub> H <sub>5</sub>                             | H6                                                                                   | H7     | H8    | H9    |
|           |                                   |                   | 3.27             | 2.63 (ax)<br>3.86 (eq) | 8.33 ( <i>o</i> )<br>7.42 ( <i>m</i> )<br>7.40 ( <i>p</i> ) | 7.43                                                                                 | 7.18   | 7.19  | 7.13  |
|           | <sup>13</sup> C                   | (gas)             | NCH <sub>3</sub> | C2                     | C3                                                          | C4                                                                                   | C5a    | C6    | C7    |



|          |                                   |                   |                  |       |       |                                                                                      |       |       |       |
|----------|-----------------------------------|-------------------|------------------|-------|-------|--------------------------------------------------------------------------------------|-------|-------|-------|
|          |                                   |                   | 34.3             | 164.6 | 40.4  | 159.8                                                                                | 143.0 | 128.1 | 123.6 |
|          | <sup>13</sup> C & <sup>15</sup> N |                   | C8               | C9    | C9a   | 4-C <sub>6</sub> H <sub>5</sub>                                                      | N1    | N5    |       |
|          |                                   |                   | 124.4            | 120.2 | 137.7 | 137.8 ( <i>i</i> )<br>128.1 ( <i>o</i> )<br>127.9 ( <i>m</i> )<br>130.3 ( <i>p</i> ) |       |       |       |
| Exp. [4] | <sup>13</sup> C                   | CDCl <sub>3</sub> | NCH <sub>3</sub> | C2    | C3    | C4                                                                                   | C5a   | C6    | C7    |
|          |                                   |                   | 35.0             | 166.4 | 39.7  | 160.9                                                                                | 141.9 | 127.5 | 125.2 |
|          | <sup>13</sup> C & <sup>15</sup> N |                   | C8               | C9    | C9a   | 4-C <sub>6</sub> H <sub>5</sub>                                                      | N1    | N5    |       |
|          |                                   |                   | 126.2            | 121.8 | 135.5 | 137.7 ( <i>i</i> )<br>128.8 ( <i>o</i> )<br>127.9 ( <i>m</i> )<br>131.0 ( <i>p</i> ) | ----  | ----  |       |

#### References:

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2. Benasi, R.; Lazzeretti, P.; Taddei, F.; Nardi, D.; Tajana, A. *Org. Magn. Reson.* **1976**, *8*, 387–388. doi:10.1002/mrc.1270080715
3. Chidichimo, G.; Longeri, M.; Menniti, G.; Romeo, G.; Ferlazzo, A. *Org. Magn. Reson.* **1984**, *22*, 52–54. doi:10.1002/mrc.1270220111
4. Bernardini, A.; Viallefont, P.; Essassi, E. M.; Zniber, R. *Org. Magn. Reson.* **1982**, *18*, 134–137. doi:10.1002/mrc.1270180304

Geometry (Å), energy (hartree) and number of imaginary frequencies of the different tautomers calculated at the B3LYP/6-311++G(d,p) computational level.

01\_a, Total Energy= -969.025490094 Hartree, NIMAG= 0

C,-0.3194797381,0.2228050892,-0.6726661843  
C,-0.2098346491,0.2019524789,0.7389418464  
C,0.153030365,1.3983610587,1.3846392312  
C,0.3812150847,2.5728952831,0.6911514029  
C,0.2357135536,2.5924589382,-0.6949006825  
C,-0.1070383204,1.42773057,-1.3539169658  
N,-0.5707146419,-0.8707968744,1.5474680733  
N,-0.7117165322,-0.8897409151,-1.4264625248  
C,-0.3356722304,-2.2106851678,-1.2422233566  
C,-0.3060667168,-2.0811411819,1.2290590575  
C,0.5049391798,-2.4538104055,0.0019479581  
O,-0.6840469792,-3.0818632317,-2.0090214934  
F,-0.2482728107,1.4495343648,-2.6946406387  
F,0.4421883653,3.7232198612,-1.3745643639  
F,0.7326070894,3.6892796416,1.3366248542  
F,0.2757515167,1.4140717756,2.715676302  
C,-0.8243771248,-3.1998935281,2.0816854603  
H,-1.4124079102,-2.806923047,2.9092443948  
H,-1.4413612225,-3.8770387307,1.4808707169  
H,0.0075468724,-3.7953580915,2.4732532524  
H,-1.1510839373,-0.7083673971,-2.3208981873  
H,1.4029815962,-1.8274171805,-0.0436158448  
H,0.7954893645,-3.5019026121,0.0072934253

01\_b, Total Energy= -969.022080828 Hartree, NIMAG= 0

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C,-0.4060942491,0.2083906012,0.6522884727  
C,-0.127257612,1.3739977228,1.3701652762  
C,0.2114673906,2.5715578018,0.760707792  
C,0.3043620682,2.6109774772,-0.6231030138  
C,0.0557571006,1.4544716837,-1.3469367584  
N,-0.7976576388,-0.9244109416,1.3820941102  
N,-0.6413805271,-0.8260620791,-1.5863848362  
C,-0.3349394946,-2.1870645563,-1.4267807775  
C,-0.4484487098,-2.2407594636,1.1185891479  
C,-0.1612436071,-2.7639176224,-0.0943179968  
O,-0.2879310558,-2.881550215,-2.4281451161  
F,0.1341939149,1.5080193321,-2.6915065649  
F,0.6300603904,3.7458951196,-1.2485229443  
F,0.4515806573,3.6643553713,1.4924170679  
F,-0.2204993113,1.3342867941,2.7181205076  
C,-0.4397486366,-3.101221436,2.3541477713  
H,0.3091325855,-2.7465968849,3.0702285876

H,-1.4161791691,-3.0666966512,2.8493604305  
H,-0.2221691078,-4.1382932608,2.1066225591  
H,-0.6997940669,-0.5909844093,-2.5697087665  
H,0.1059571339,-3.8103680276,-0.1364539191  
H,-0.9569070008,-0.7247199116,2.3587814736

01\_c, Total Energy= -968.991195094 Hartree, NIMAG= 0

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C,-0.2955088181,0.1725614387,0.7218158366  
C,0.1360294907,1.3449294964,1.3616423505  
C,0.4021290438,2.5213649558,0.6705088506  
C,0.2417717615,2.557855367,-0.7061071534  
C,-0.1610279842,1.4037900635,-1.3630645182  
N,-0.6300118571,-0.8969847254,1.5567837734  
N,-0.8630587484,-0.8964638478,-1.4313985928  
C,-0.3070283041,-2.1437850179,-1.2321457782  
C,-0.4611536418,-2.1354955246,1.2448628697  
C,-0.0174794993,-2.6944705377,-0.0296749314  
O,-0.1394479907,-2.7771431221,-2.4178370131  
F,-0.3133211241,1.4342854761,-2.7066654789  
F,0.4732511535,3.6832610759,-1.3901902868  
F,0.7970146541,3.6184420613,1.3274981728  
F,0.2886159345,1.3603168795,2.6899243052  
C,-0.7728247335,-3.1518079695,2.3164914212  
H,-1.0666613049,-2.646862677,3.2348220662  
H,-1.5754489845,-3.8220903721,1.9923246585  
H,0.1069464255,-3.7746479546,2.5126771857  
H,-1.0511481466,-0.6976671115,-2.4052403025  
H,0.4050403999,-3.6931662778,-0.0205265849  
H,0.0843873341,-3.7029555774,-2.2660741873

01\_d, Total Energy= -969.008049064 Hartree, NIMAG= 0

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C,-0.1943447597,0.1919620572,0.7063853871  
C,0.0936591527,1.3988483282,1.3738777984  
C,0.3357158914,2.5736746378,0.6913396817  
C,0.2614429895,2.587834576,-0.7021212082  
C,-0.0441936284,1.4264196331,-1.3828777381  
N,-0.5509944133,-0.8846944405,1.5139403531  
N,-0.6361422612,-0.8723326291,-1.5064486942  
C,-0.3143314535,-2.0661490464,-1.1945405219  
C,-0.283892956,-2.0970716688,1.2111917124  
C,0.5330716109,-2.4605455348,-0.0215860267  
O,-0.7776624806,-3.1012010797,-1.919718346  
F,-0.1170103224,1.4721798366,-2.7202296482  
F,0.4950322924,3.7253054961,-1.365464339

F,0.6403606754,3.6977529406,1.3496805029  
F,0.1511563914,1.4170671466,2.7115238366  
C,-0.8021915977,-3.214912713,2.0659059616  
H,-1.3877574645,-2.8179956841,2.8933498909  
H,-1.4233920818,-3.8932035332,1.4709247982  
H,0.0297027886,-3.8099957349,2.4586572299  
H,1.454032335,-1.8667118981,-0.0323195449  
H,0.7810148887,-3.5198160358,-0.0577934277  
H,-1.3460273066,-2.734319488,-2.614669301

01\_e, Total Energy= -969.004546282 Hartree, NIMAG= 0

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C,-0.4533366085,0.190411577,0.6280430585  
C,-0.1986818391,1.3473554343,1.3592007544  
C,0.2122959309,2.5319289198,0.7630526724  
C,0.3975136294,2.5557726777,-0.6089598265  
C,0.1546969239,1.4047073667,-1.3514532568  
N,-0.9103706346,-0.9428076818,1.3411921825  
N,-0.5669528535,-0.835122335,-1.6545407617  
C,-0.4550647799,-2.0762507216,-1.3564671807  
C,-0.4478991967,-2.2376534244,1.1226540909  
C,-0.1714319498,-2.7483198442,-0.0959133325  
O,-0.6480858428,-2.9678328044,-2.3558562254  
F,0.3373508539,1.4738081757,-2.6756094573  
F,0.7979729126,3.6799895681,-1.2145351103  
F,0.4266567396,3.6257605713,1.5026356995  
F,-0.3766626335,1.3238692189,2.7019745174  
C,-0.3391407572,-3.066166873,2.3712645102  
H,0.4086141198,-2.644703497,3.0512734801  
H,-1.2975941142,-3.0796111083,2.9016936361  
H,-0.0638723967,-4.0937754022,2.1398711582  
H,0.1465234271,-3.778711698,-0.1683170535  
H,-1.0996451405,-0.7344446364,2.3109656057  
H,-0.81155773,-2.4487514653,-3.1581868424

02\_a, Total Energy= -1008.33819155 Hartree, NIMAG= 0

C,-0.2626495523,0.235267469,-0.725667463  
C,-0.2910134594,0.222415119,0.6937287612  
C,0.0332261367,1.405447227,1.3789172914  
C,0.3840532337,2.5674769607,0.7159160523  
C,0.4202714113,2.5763404079,-0.6748886092  
C,0.113439413,1.421449647,-1.3733793419  
N,-0.7008565473,-0.8593495379,1.467175221  
N,-0.651742922,-0.8800653354,-1.5002363367  
C,-0.2092468118,-2.1706620271,-1.2572271718  
C,-0.3185589706,-2.0466363478,1.1772998156

C,0.6102813274,-2.3413079897,0.0153556245  
O,-0.5212686108,-3.1038140247,-1.9703205818  
F,0.2080148225,1.4567920243,-2.7150745459  
F,0.7799111517,3.6856904878,-1.3277738918  
F,0.6984977635,3.6731379793,1.3969208518  
F,0.0129517484,1.4209501079,2.7162917148  
C,-0.8352459418,-3.2076450442,1.9706683654  
H,-1.5225269595,-2.8658269959,2.7427517751  
H,-1.3453221185,-3.9174025888,1.3101257024  
H,-0.0036533821,-3.7498122735,2.4336440939  
C,-1.5603527869,-0.697968387,-2.6480327068  
H,-2.1416545761,0.2096111777,-2.4976739497  
H,-1.0125631543,-0.6296147668,-3.5884243685  
H,-2.2241495061,-1.5598697608,-2.6912886754  
H,1.4540513896,-1.6440374418,0.0238404576  
H,0.9813334094,-3.3632103273,0.0361755986

O2\_b, Total Energy= -1008.33112530 Hartree, NIMAG= 0

C,-0.3509244931,0.2121411838,-0.7692716756  
C,-0.555886564,0.1856635641,0.621325183  
C,-0.2623446989,1.320644854,1.3786770251  
C,0.2301383251,2.4833494689,0.8097304572  
C,0.4828799573,2.5027885762,-0.5543955342  
C,0.2191552415,1.3710539851,-1.315323617  
N,-1.0275955511,-0.9594314443,1.2824011366  
N,-0.7618680075,-0.8474260871,-1.6084116114  
C,-0.3645723606,-2.1754996674,-1.4336168687  
C,-0.4281893262,-2.2107281639,1.0954991565  
C,0.0032541782,-2.669530343,-0.096358793  
O,-0.4217659229,-2.9519513216,-2.3747417728  
F,0.5115907938,1.4270995367,-2.6249499523  
F,0.9907319788,3.5988296662,-1.1281484922  
F,0.4867661508,3.5561036896,1.5638674018  
F,-0.473900427,1.283202817,2.7129482672  
C,-0.3231068981,-3.0276989114,2.3536815756  
H,0.2994775048,-2.5223294527,3.0997199816  
H,-1.3154070118,-3.1741258336,2.794874806  
H,0.1017021756,-4.0087197259,2.1478371007  
C,-1.4336761447,-0.535342332,-2.8812273843  
H,-1.9703001112,0.4064415384,-2.7704975728  
H,-0.733392584,-0.462145658,-3.7140757268  
H,-2.1412858984,-1.3345911167,-3.0947722063  
H,0.4650506074,-3.646748968,-0.127948534  
H,-1.2872700479,-0.7746889392,2.2411950572

02\_c, Total Energy= -1008.30022956 Hartree, NIMAG= 0

C,-0.3297740505,0.2344278902,-0.7309287411  
C,-0.3618800313,0.2032011308,0.6789403473  
C,0.0238922017,1.3654514285,1.3664853656  
C,0.4280507721,2.516129507,0.7047282939  
C,0.469692442,2.5315575191,-0.681888271  
C,0.1123633579,1.3878264919,-1.3824107037  
N,-0.7714995436,-0.8709226337,1.4679404762  
N,-0.749594011,-0.8902263549,-1.4929365142  
C,-0.1338205025,-2.0981788584,-1.2671562559  
C,-0.4857030994,-2.0967734004,1.1806119579  
C,0.1318911114,-2.6091504758,-0.0361111439  
O,0.1305183958,-2.7623400837,-2.4216565006  
F,0.1972495192,1.4196215917,-2.726814156  
F,0.8598036199,3.6329773607,-1.3351360553  
F,0.7790182598,3.6072535321,1.3948390663  
F,0.0072433877,1.3897449882,2.7043634133  
C,-0.8447064306,-3.1373161951,2.2141273463  
H,-1.2727131452,-2.657594231,3.0926404367  
H,-1.5570853039,-3.8614933946,1.8063043425  
H,0.0492050405,-3.6975156258,2.5099489448  
C,-1.648966344,-0.7255130784,-2.6435256254  
H,-2.308263483,0.1184715615,-2.4407344618  
H,-1.1151687158,-0.5464318456,-3.5780565683  
H,-2.2587728587,-1.6237903482,-2.7465003133  
H,0.6705258679,-3.5488179458,0.0259780357  
H,0.3894109995,-3.6691902742,-2.2180232432

03\_a, Total Energy= -571.984544062 Hartree, NIMAG= 0

C,-0.3196635463,0.2349820746,-0.6786252296  
C,-0.2331221217,0.216374162,0.7340609317  
C,0.1154457965,1.409494063,1.3931096271  
C,0.3854541743,2.5756658609,0.6970288761  
C,0.2784373076,2.5895104284,-0.6969810199  
C,-0.0716821216,1.4301422983,-1.3709352826  
N,-0.5829711517,-0.8715310627,1.5414480589  
N,-0.7227888828,-0.8912235401,-1.4260764747  
C,-0.3583684726,-2.2077695238,-1.2449172106  
C,-0.3060205491,-2.0783295178,1.2242181769  
C,0.4960043638,-2.4483538833,-0.0102956726  
O,-0.7189257789,-3.0865960509,-2.0040430837  
C,-0.7954466478,-3.2046078765,2.0876656367  
H,-1.3811696799,-2.8177295403,2.9201442535  
H,-1.4090492672,-3.894321581,1.4976705361  
H,0.0493418106,-3.7857844156,2.4737970999  
H,-0.1482194846,1.4309650194,-2.4534691015  
H,0.4694931004,3.4990408389,-1.2542252958

H,0.6584676123,3.476536003,1.2337808009  
H,0.1489633355,1.3848971242,2.4757703174  
H,-1.2022494941,-0.7184241837,-2.3005352355  
H,1.388853199,-1.8150788559,-0.0643459067  
H,0.792412484,-3.4950413177,-0.006661741

03\_b, Total Energy= -571.978955327 Hartree, NIMAG= 0

C,-0.3128381923,0.2572007452,-0.7424854492  
C,-0.4187373718,0.2212003025,0.6567126624  
C,-0.1409368213,1.3768691876,1.3932874727  
C,0.2166908668,2.5685760588,0.7720773481  
C,0.3291742684,2.6057144065,-0.6145529565  
C,0.0779415283,1.4548736946,-1.3535834443  
N,-0.8342835542,-0.932758182,1.3610092207  
N,-0.658161964,-0.8325889555,-1.5674828136  
C,-0.3181478012,-2.1804251761,-1.42435468  
C,-0.4524259833,-2.2385923681,1.1119693798  
C,-0.1281181916,-2.7578220148,-0.0949179877  
O,-0.2589361839,-2.874542502,-2.4304842036  
C,-0.4467935553,-3.1011786157,2.3474682692  
H,0.2907041631,-2.7395300084,3.0722769012  
H,-1.4288924518,-3.0788479912,2.8326072795  
H,-0.2152037474,-4.1359600302,2.1020508627  
H,0.1668984655,1.4775769242,-2.4347850824  
H,0.6140619423,3.5196573284,-1.1217254955  
H,0.412477485,3.4514063173,1.3684156305  
H,-0.2205095348,1.3360728412,2.4754839106  
H,-0.7514334061,-0.6036117871,-2.5488873689  
H,0.1668565793,-3.7969847168,-0.133696874  
H,-1.0404314836,-0.7446106247,2.3307815238

03\_c, Total Energy= -571.947775116 Hartree, NIMAG= 0

C,-0.4202340646,0.2344082371,-0.6863824108  
C,-0.3085231064,0.1886541975,0.7166421326  
C,0.1078015378,1.356997014,1.37102365  
C,0.406464004,2.5264658276,0.6792715769  
C,0.2775437187,2.5575046908,-0.7060471894  
C,-0.127861547,1.4079772515,-1.3805678166  
N,-0.6347028159,-0.8955737375,1.5538454167  
N,-0.8750277463,-0.8964470136,-1.4281281068  
C,-0.3303931137,-2.1431202064,-1.2350122314  
C,-0.4594716596,-2.1320867295,1.2428775355  
C,-0.0296933566,-2.6956219853,-0.0355589184  
O,-0.1748361771,-2.7864748139,-2.4231364704  
C,-0.7431303479,-3.152054394,2.3220706767  
H,-1.0342164629,-2.6482309893,3.2422324576

H,-1.5402938498,-3.8354206216,2.0112826503  
H,0.1474392055,-3.7620321216,2.5116610294  
H,-0.2248374145,1.4197028102,-2.4620831395  
H,0.4874420762,3.4632855982,-1.2626825387  
H,0.7191700046,3.4110359784,1.2218196686  
H,0.1687406392,1.3188349448,2.4520821876  
H,-1.0848276021,-0.706412526,-2.3983784648  
H,0.3944493272,-3.6939019442,-0.03025549  
H,0.0321062739,-3.714285242,-2.2615201282

03\_d, Total Energy= -571.966019867 Hartree, NIMAG= 0

C,-0.2719310373,0.2191812405,-0.7179187494  
C,-0.2223350875,0.2051729624,0.7033692912  
C,0.0701752633,1.4061852284,1.3796486899  
C,0.3592074763,2.5730735592,0.6958195017  
C,0.3026485657,2.5870729438,-0.7038895263  
C,-0.0332792465,1.4334379508,-1.3895871739  
N,-0.5712448895,-0.884120405,1.5130082476  
N,-0.6431077472,-0.8697668828,-1.514832054  
C,-0.3207891993,-2.0603798107,-1.2015076398  
C,-0.2943719384,-2.0936448822,1.2116269227  
C,0.5199609624,-2.453786805,-0.0238231097  
O,-0.7687954976,-3.1024980583,-1.9378793691  
C,-0.7874161493,-3.2180562606,2.07611627  
H,-1.3721182089,-2.8263473192,2.9070781286  
H,-1.4049423413,-3.9081675081,1.4907795325  
H,0.0554260743,-3.8002726404,2.4655958529  
H,-0.1146266588,1.4293860368,-2.4702851687  
H,0.5026715008,3.5017710352,-1.2502284278  
H,0.6033905622,3.4762607905,1.2430709237  
H,0.0612520796,1.3802431897,2.4630741048  
H,1.4396831101,-1.8573758904,-0.0323996499  
H,0.7713617322,-3.5125871939,-0.0603016349  
H,-1.3372363027,-2.7325112433,-2.6302871582

03\_e, Total Energy= -571.960184604 Hartree, NIMAG= 0

C,-0.2752118283,0.2202646339,-0.7649938655  
C,-0.4469270845,0.2021916658,0.6344412764  
C,-0.1884732341,1.352512366,1.3807896622  
C,0.2259777977,2.5359335734,0.7725573823  
C,0.404140005,2.565038205,-0.6058261505  
C,0.1520125635,1.4178170857,-1.3531171043  
N,-0.9207048353,-0.9471823888,1.3332565246  
N,-0.5418043967,-0.8367809571,-1.6513873074  
C,-0.4245298411,-2.0747997267,-1.3530807156  
C,-0.4622059094,-2.2388844491,1.1234031326



C,-0.1620162541,-2.7505206217,-0.0904363298  
O,-0.5868119919,-2.9720739339,-2.3626353454  
C,-0.3765058232,-3.0745474075,2.3709177283  
H,0.365989228,-2.6623243401,3.0627784844  
H,-1.3420851105,-3.0840252619,2.8887981086  
H,-0.1054450468,-4.1034603495,2.1395587392  
H,0.2630470251,1.4228205896,-2.4308099167  
H,0.7245998057,3.4739520959,-1.1014084826  
H,0.4051973397,3.4182247626,1.3755974274  
H,-0.3248633723,1.3209140979,2.4580727709  
H,0.1550457242,-3.781587958,-0.1579544718  
H,-1.1354590792,-0.7455221266,2.2987828984  
H,-0.743623588,-2.4468112071,-3.1614555976

04\_a, Total Energy= -611.298907752 Hartree, NIMAG= 0

C,-0.285033527,0.2369460845,-0.7094232047  
C,-0.2800386009,0.2255160664,0.7084312707  
C,0.0528294859,1.4102915366,1.388880094  
C,0.4047707423,2.566004709,0.7124809586  
C,0.4016281216,2.5728459133,-0.6843639985  
C,0.0542140769,1.423996061,-1.3793496644  
N,-0.6674674213,-0.8610677312,1.5004277188  
N,-0.6963383714,-0.8854057605,-1.4795843102  
C,-0.2677922427,-2.1793313721,-1.2504653247  
C,-0.316624259,-2.0536340953,1.2011706747  
C,0.5652894742,-2.3662518158,0.0089677504  
O,-0.5723934209,-3.1083739325,-1.9783382774  
C,-0.8080215479,-3.2073614942,2.0248944369  
H,-1.460495374,-2.8539819579,2.822035451  
H,-1.3523038884,-3.9182428042,1.3934555611  
H,0.0365054556,-3.7540372646,2.4589270227  
C,-1.4945834393,-0.6610925056,-2.6916966639  
H,-2.1510625089,0.1930403367,-2.532280814  
H,-0.8647343221,-0.4795323122,-3.568058405  
H,-2.0838106743,-1.5559375178,-2.8809271636  
H,0.0539169296,1.4358501624,-2.4620940232  
H,0.6675435896,3.4703318008,-1.2305863759  
H,0.6662549547,3.4606653196,1.265352659  
H,0.0147619235,1.385460603,2.4713993343  
H,1.4213056198,-1.6831229262,-0.0050436618  
H,0.9195062661,-3.3946269948,0.0193927381

04\_b, Total Energy= -611.290329196 Hartree, NIMAG= 0

C,-0.3834816186,0.2263962225,-0.7447756947  
C,-0.5196522379,0.1959504343,0.6533503703  
C,-0.1990495726,1.3288742577,1.4071492246

C,0.2536794397,2.4960710926,0.8028628695  
C,0.4233333083,2.5235264843,-0.577734598  
C,0.1155783385,1.396729144,-1.3337402019  
N,-0.9848949839,-0.9561540188,1.3304115926  
N,-0.8093097408,-0.8510477598,-1.5715406119  
C,-0.3805190526,-2.1724726117,-1.4097495344  
C,-0.4468236986,-2.2205152351,1.1238887784  
C,-0.0498541524,-2.6921465512,-0.0769611108  
O,-0.3677879664,-2.9285094425,-2.3739117659  
C,-0.353192217,-3.0581916156,2.3711624453  
H,0.3177554323,-2.5968525583,3.1042446682  
H,-1.3394750535,-3.1548851315,2.8389189342  
H,0.0115000165,-4.0588252975,2.1450491877  
C,-1.3283628919,-0.5243975863,-2.9037210763  
H,-1.9260422168,0.3843491683,-2.8332470527  
H,-0.5338743591,-0.3852692289,-3.6445844585  
H,-1.9506524213,-1.3496011848,-3.242768628  
H,0.2471333272,1.4285550791,-2.407118742  
H,0.79215797,3.4154909321,-1.0701513448  
H,0.4829109983,3.3653125481,1.4076327776  
H,-0.3149904842,1.2874660816,2.4859904607  
H,0.3754179355,-3.6854043031,-0.1175301579  
H,-1.220450476,-0.7701694547,2.2946233526

04\_c, Total Energy= -611.258661817 Hartree, NIMAG= 0

C,-0.3735805546,0.2361930266,-0.7106826469  
C,-0.3437705437,0.1997979236,0.6976437679  
C,0.0651454793,1.3577975174,1.3768046763  
C,0.4509384152,2.5088388801,0.700549495  
C,0.4214104483,2.5307144037,-0.6911031371  
C,0.0151154682,1.3948691365,-1.3876160026  
N,-0.7274280802,-0.8791685243,1.5126150311  
N,-0.8340891662,-0.8987334044,-1.4606862056  
C,-0.2166116908,-2.1084015431,-1.2467332471  
C,-0.4789795005,-2.1081201505,1.2170033426  
C,0.0723929745,-2.6315094385,-0.0270040861  
O,0.0419527849,-2.7724952571,-2.4083511858  
C,-0.7989535506,-3.1448964686,2.2694392517  
H,-1.1747565521,-2.6582688839,3.1681732161  
H,-1.5434495785,-3.8582008588,1.9010437214  
H,0.0994973394,-3.71971265,2.521223966  
C,-1.5507228256,-0.6761412365,-2.7171209568  
H,-2.2388025836,0.1569154569,-2.5724225565  
H,-0.8891160023,-0.4527142834,-3.5610834759  
H,-2.1260429246,-1.5674886265,-2.9651730342  
H,-0.0067501976,1.4134280546,-2.4702176781  
H,0.705422559,3.4231287528,-1.2367114498

H,0.7568079154,3.3870882407,1.2574872425  
H,0.0536543731,1.3238191381,2.4596934763  
H,0.5991281231,-3.5795024751,0.0103272184  
H,0.3126786315,-3.6744956578,-2.2007251579

05\_a, Total Energy= -763.767296058 Hartree, NIMAG= 0

C,-0.134183485,0.3693052351,-0.4356126979  
C,0.0342411033,0.2390396108,0.966278475  
C,0.5229716415,1.3517829034,1.679002863  
C,0.8516992574,2.538239649,1.0468648291  
C,0.6635369404,2.6623259714,-0.3334001072  
C,0.1739430589,1.5879717041,-1.0590177289  
N,-0.3626250026,-0.8646547456,1.7169311398  
N,-0.6788750968,-0.6595284104,-1.2313282387  
C,-0.4146790815,-2.0103239124,-1.1653980994  
C,-0.2370523808,-2.074507835,1.3046278449  
C,0.4725231964,-2.4021259957,0.0033892737  
O,-0.8778468716,-2.799778639,-1.9660143407  
H,1.2339158963,3.3719436676,1.6239939404  
H,0.620011366,1.2469547473,2.7529617432  
H,0.8993948552,3.591052981,-0.8393891399  
H,0.0323528657,1.6743796703,-2.1315037788  
C,-0.794033068,-3.1731004002,2.1330257826  
C,-1.0648262871,-4.438211849,1.5909649995  
C,-1.085038434,-2.9436575611,3.4881739481  
C,-1.6139113138,-5.4450089593,2.3826510103  
H,-0.8816344843,-4.6380150518,0.5423316767  
C,-1.6173602827,-3.9540762129,4.2777262994  
H,-0.8842775127,-1.9640643284,3.9021317383  
C,-1.8851882276,-5.2096506691,3.7278021147  
H,-1.8304425949,-6.4124935108,1.9443092819  
H,-1.8262641749,-3.7649772547,5.3247667018  
H,-2.3039527751,-5.996636021,4.3449400919  
H,-1.1835864806,-0.3822383394,-2.0637600396  
H,1.3937874868,-1.8105645131,-0.0376254493  
H,0.7262275371,-3.4529602337,-0.09193956

05\_b, Total Energy= -763.760975552 Hartree, NIMAG= 0

C,-0.0008333123,0.4157699804,-0.5302505153  
C,-0.338764048,0.2448547341,0.8210835909  
C,-0.0791196819,1.2772267518,1.7278561082  
C,0.4920572185,2.4775096499,1.3187251811  
C,0.8402077168,2.6449815508,-0.0184969174  
C,0.6044964105,1.6155369543,-0.923314745  
N,-0.9744662138,-0.9220118747,1.3023478435  
N,-0.3192918305,-0.5321752223,-1.5245216626

C,-0.139060496,-1.9175510755,-1.4994568892  
C,-0.688421144,-2.2293758429,0.961750983  
C,-0.2075836243,-2.6488553113,-0.2365804077  
O,0.0076007632,-2.5046662686,-2.563533609  
H,0.6691261137,3.2655656062,2.0405630629  
H,-0.3443723669,1.1334189381,2.7707369924  
H,1.2946730102,3.5675061153,-0.359325331  
H,0.8735566168,1.7413210524,-1.9669401882  
C,-0.9600997509,-3.2184659875,2.0430919309  
C,-1.6140509636,-4.4237256612,1.7547227476  
C,-0.5629685523,-2.9659699102,3.3643939972  
C,-1.8592449678,-5.3537887094,2.7608839015  
H,-1.9435920019,-4.6185047193,0.7412189579  
C,-0.8043498671,-3.8999013974,4.3685751667  
H,-0.0272046944,-2.0533465491,3.6023578675  
C,-1.4554516024,-5.0956124119,4.0700417204  
H,-2.3736179979,-6.2779909632,2.5231987329  
H,-0.4752842761,-3.6975541607,5.3815351921  
H,-1.6467068353,-5.8212783099,4.8522940948  
H,-0.237487562,-0.1904187819,-2.4736363962  
H,0.0396388249,-3.6949791785,-0.3442354606  
H,-1.4154328161,-0.809986683,2.2023843788

05\_c, Total Energy= -763.730493019 Hartree, NIMAG= 0

C,-0.214873451,0.393159881,-0.4899750914  
C,-0.1586898612,0.1938736753,0.9036880037  
C,0.3224256141,1.2523381891,1.690076124  
C,0.7413590545,2.4556171862,1.1327021262  
C,0.6681595552,2.6381316744,-0.2453039817  
C,0.1968961774,1.6018499259,-1.0486892959  
N,-0.6088674502,-0.9348858605,1.6021443518  
N,-0.7326812609,-0.6198290875,-1.3523799  
C,-0.2497391448,-1.906192481,-1.2758369495  
C,-0.5256192792,-2.1509459467,1.1771064465  
C,-0.0584885458,-2.6054687971,-0.1325697803  
O,-0.0246199923,-2.4126436456,-2.5175851113  
H,1.1036766759,3.2511275689,1.7733602702  
H,0.3388013061,1.1022901751,2.7629047273  
H,0.9708541957,3.5754258654,-0.6971343893  
H,0.1412163621,1.7325333852,-2.1251759539  
C,-0.9481265584,-3.213915055,2.1428242909  
C,-1.3987500342,-4.4684755082,1.7098500953  
C,-0.9088588398,-2.9574701011,3.521468188  
C,-1.7994775512,-5.4387055248,2.6267217114  
H,-1.4656159424,-4.6806776439,0.6495509276  
C,-1.3001120423,-3.9277686386,4.4363295943  
H,-0.5674725158,-1.9858105722,3.853785943

C,-1.7474002962,-5.1736180115,3.9929959858  
H,-2.1570981847,-6.3990478297,2.2720281802  
H,-1.2555073152,-3.7146265537,5.498717507  
H,-2.0536402685,-5.9297575759,4.7073430668  
H,-0.8877791897,-0.3179198571,-2.3046684816  
H,0.3618992507,-3.6005332602,-0.2099278696  
H,0.143900431,-3.3601771631,-2.4542035742

05\_d, Total Energy= -763.748846940 Hartree, NIMAG= 0

C,-0.0932092208,0.3615389725,-0.4766049973  
C,0.0517941987,0.2252139701,0.9342365919  
C,0.5042288527,1.3389298375,1.6735841473  
C,0.8581751061,2.5250245767,1.0587801533  
C,0.7073117661,2.6585373088,-0.3282113237  
C,0.2145031337,1.6005652008,-1.0704013109  
N,-0.3461406767,-0.8823540407,1.6813697471  
N,-0.6223753809,-0.6175569919,-1.32339512  
C,-0.3987619104,-1.8540219576,-1.1212237424  
C,-0.2334279958,-2.0951639637,1.276987908  
C,0.4722094052,-2.4090109065,-0.0351452466  
O,-0.9873658314,-2.7896026209,-1.8983646416  
H,1.2261588669,3.354438337,1.6516698365  
H,0.5683552918,1.2267159306,2.7495963304  
H,0.9572440816,3.5927188771,-0.8180174168  
H,0.0582215191,1.6924377277,-2.1388730541  
C,-0.7925435247,-3.188631284,2.1115960604  
C,-0.9987322602,-4.4812371137,1.6076434942  
C,-1.1443410162,-2.9265133605,3.4470536629  
C,-1.5395290801,-5.481419056,2.413769695  
H,-0.7664668627,-4.714602784,0.5762219349  
C,-1.6711879126,-3.9279003639,4.2511640432  
H,-0.9933464118,-1.926828254,3.8329274393  
C,-1.8722681551,-5.2113036115,3.7380911697  
H,-1.7011627449,-6.4713731591,2.002509162  
H,-1.9279717844,-3.7096862844,5.2817986009  
H,-2.2864483911,-5.9916600327,4.3665612488  
H,1.4239617824,-1.8665061291,-0.0412812895  
H,0.6678629825,-3.466694874,-0.1843894588  
H,-1.5682500381,-2.319639366,-2.515775959

05\_e, Total Energy= -763.742077162 Hartree, NIMAG= 0

C,0.0407679971,0.3715438245,-0.5482422387  
C,-0.3745403284,0.2206555211,0.790418056  
C,-0.1166443626,1.2316964134,1.7168338323  
C,0.5415212146,2.4034974855,1.3473089079  
C,0.9662868622,2.5590238221,0.0327164967

C,0.7117063431,1.5514932866,-0.8939446527  
N,-1.0997878688,-0.9213292374,1.2368207306  
N,-0.2018987383,-0.5292528317,-1.5993262173  
C,-0.2898326671,-1.797141401,-1.4560276095  
C,-0.7721887744,-2.2340729532,0.9404013005  
C,-0.3203346419,-2.6408084229,-0.2705572278  
O,-0.3872273337,-2.5428152182,-2.5901356513  
H,0.7148344859,3.1797819711,2.0832556435  
H,-0.4487594702,1.1014239636,2.7427481014  
H,1.4794602245,3.4617647343,-0.2774262526  
H,1.0106763602,1.6623461708,-1.9293658761  
C,-0.9865214757,-3.2115212423,2.0413434264  
C,-1.5806943789,-4.4551873476,1.786721795  
C,-0.5970610205,-2.9064204354,3.3540036332  
C,-1.7709556848,-5.3724173283,2.8161581738  
H,-1.9113723577,-4.6893433269,0.7819004261  
C,-0.7830396922,-3.8275169898,4.3812547128  
H,-0.1117804453,-1.959912264,3.5658127417  
C,-1.3723279816,-5.0625741509,4.1157265879  
H,-2.2404252682,-6.3265025752,2.6049073884  
H,-0.4605635917,-3.5835598193,5.387142629  
H,-1.5220240279,-5.7776926396,4.9165472078  
H,-0.064485724,-3.68068297,-0.4130548796  
H,-1.5404006343,-0.7950106299,2.135254236  
H,-0.3407648124,-1.9139402071,-3.3257320019

O6\_a, Total Energy= -803.081735507 Hartree, NIMAG= 0

C,-0.1084098506,0.3672377183,-0.4584868833  
C,0.0073224907,0.2585007471,0.9529359582  
C,0.5045798782,1.3631877663,1.670860303  
C,0.9130072108,2.523516087,1.0369567259  
C,0.8015944159,2.6238951565,-0.3521058175  
C,0.29073186,1.5609320663,-1.0817006336  
N,-0.4221442948,-0.8305984311,1.7074042186  
N,-0.688054675,-0.6550944051,-1.25839997  
C,-0.3704996693,-1.9953375536,-1.1453481635  
C,-0.2434614767,-2.039609335,1.3120165102  
C,0.5189778347,-2.3411300374,0.0368597929  
O,-0.8068299035,-2.8396846486,-1.9087245082  
H,0.5505969679,1.2704732042,2.749338986  
H,1.302545243,3.3513630076,1.6178084805  
H,1.1095650867,3.5276353693,-0.8648445174  
H,0.2058558781,1.6458070201,-2.1577784473  
C,-0.8001503245,-3.1510488603,2.1219690461  
C,-1.008133345,-4.425662356,1.5746371866  
C,-1.1527651744,-2.9261347793,3.4630635948  
C,-1.5552183469,-5.4472631289,2.3486447108

H,-0.7775425153,-4.6202929317,0.5344587742  
C,-1.6838580461,-3.9506179531,4.2352426898  
H,-0.9993842222,-1.9392342557,3.8801343806  
C,-1.8881130698,-5.2161871296,3.6807105651  
H,-1.7223849685,-6.4228905242,1.9066655243  
H,-1.9406785706,-3.7651259875,5.2722458522  
H,-2.3056602027,-6.0144082002,4.2841333413  
C,-1.5479274559,-0.2748321136,-2.3866117678  
H,-2.1060688841,0.6220473026,-2.1220218183  
H,-0.9704553455,-0.0908241106,-3.2978238751  
H,-2.232877973,-1.0970584311,-2.5830809831  
H,1.4193658876,-1.7183773485,0.0175359705  
H,0.8102040871,-3.3830550956,-0.0510137089

06\_b, Total Energy= -803.072449785 Hartree, NIMAG= 0

C,-0.1914102252,0.379409864,-0.5213040848  
C,-0.4931780981,0.2086523126,0.8399028401  
C,-0.1075701874,1.1832434832,1.765083778  
C,0.578077523,2.3253729041,1.3673089553  
C,0.9159015578,2.4824529199,0.0266115136  
C,0.5401373875,1.5140611769,-0.8990790172  
N,-1.1931665374,-0.928683103,1.3035066996  
N,-0.6786753338,-0.5097244835,-1.5209234971  
C,-0.4767625335,-1.8921238774,-1.499055354  
C,-0.8269334759,-2.2294806917,0.9887865323  
C,-0.3566594705,-2.6082340427,-0.223568973  
O,-0.48367499,-2.5250707856,-2.5486996292  
H,-0.358403249,1.0382305993,2.811354381  
H,0.8552426155,3.0735556532,2.1003288079  
H,1.4671255257,3.3548412646,-0.3039475841  
H,0.7997052334,1.6489494246,-1.9407704745  
C,-0.986371352,-3.2193077312,2.0888771409  
C,-1.5239525037,-4.4874519409,1.8289799283  
C,-0.6007992081,-2.9083051396,3.4015175605  
C,-1.6638606668,-5.4208165363,2.8518725461  
H,-1.8483401729,-4.7286911281,0.8238760289  
C,-0.7381685861,-3.8444062486,4.4230396389  
H,-0.1540429544,-1.9443440259,3.6200519775  
C,-1.2717262675,-5.1031385062,4.1515443339  
H,-2.08854224,-6.3944790872,2.635271332  
H,-0.4196347957,-3.5938576137,5.4286011154  
H,-1.3821980775,-5.8308133358,4.9474344842  
C,-1.0019630109,0.0535846807,-2.8357756885  
H,-1.4608692414,1.0319871939,-2.6941266759  
H,-0.122575719,0.1503183528,-3.4814152709  
H,-1.7018889745,-0.6135109161,-3.3340473686  
H,-0.0300440705,-3.6307517262,-0.348294262

H,-1.5909716981,-0.8193558268,2.2242788554

06\_c, Total Energy= -803.041705448 Hartree, NIMAG= 0

C,-0.2148794501,0.3857131758,-0.4838195202  
C,-0.1643777529,0.2011250396,0.9134276436  
C,0.354507444,1.2453137108,1.6963356599  
C,0.8310766396,2.4207296103,1.1291990488  
C,0.7805659645,2.5877505438,-0.2521548073  
C,0.2633354924,1.5692536851,-1.0498205771  
N,-0.6389992411,-0.9129824915,1.6146370153  
N,-0.7885709717,-0.6259367701,-1.3256075659  
C,-0.2441620302,-1.8881812522,-1.2517360085  
C,-0.5228108382,-2.1303260506,1.1979952304  
C,-0.0118352899,-2.565097136,-0.0986445211  
O,0.0100415911,-2.4211308913,-2.4799015883  
H,0.3568702642,1.104838263,2.7706387149  
H,1.2228933209,3.2075081038,1.7635723281  
H,1.1329427899,3.5039896704,-0.7115490456  
H,0.2245986633,1.7014259138,-2.1239423339  
C,-0.9470943552,-3.2014043407,2.1530863187  
C,-1.3345716454,-4.4726539737,1.7080928044  
C,-0.9746180444,-2.9383981909,3.5308644637  
C,-1.7379860397,-5.4536498241,2.6121359999  
H,-1.3478935075,-4.6896486589,0.6467451174  
C,-1.371093423,-3.9182698238,4.4332544403  
H,-0.6815025736,-1.9539889409,3.871773472  
C,-1.7541336593,-5.1812024434,3.9779417523  
H,-2.0449305046,-6.4279283273,2.248017288  
H,-1.3800424506,-3.699656081,5.4954598387  
H,-2.0634660401,-5.944962829,4.6828244433  
C,-1.4888506658,-0.2238536672,-2.5458244762  
H,-2.1139961051,0.6377405981,-2.3104125797  
H,-0.8150171056,0.0352014993,-3.3696641036  
H,-2.1292756857,-1.041296678,-2.8760129009  
H,0.4884044753,-3.5245276147,-0.1586232614  
H,0.2394801866,-3.3525071823,-2.3788347072

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01new\_3H\_4Fs\_2oxo\_4me\_giao

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| Atom | Abs.  | Rel.   |
|------|-------|--------|
| 1C   | 61.84 | 116.15 |
| 2C   | 51.06 | 126.53 |
| 3C   | 31.62 | 145.25 |
| 4C   | 37.25 | 139.83 |
| 5C   | 36.35 | 140.70 |



|     |        |         |
|-----|--------|---------|
| 6C  | 38.05  | 139.06  |
| 7N  | -73.99 | -82.01  |
| 8N  | 110.71 | -256.73 |
| 9C  | 14.90  | 161.35  |
| 10C | 10.26  | 165.82  |
| 11C | 136.22 | 44.52   |
| 12H | 28.63  | 3.23    |
| 13H | 29.40  | 2.49    |
| 14O | -89.28 | 330.18  |
| 15H | 25.05  | 6.71    |
| 16F | 334.86 | -159.03 |
| 17F | 335.82 | -159.95 |
| 18F | 338.95 | -162.95 |
| 19F | 317.94 | -142.81 |
| 20C | 153.48 | 27.90   |
| 21H | 29.57  | 2.32    |
| 22H | 29.64  | 2.25    |
| 23H | 29.52  | 2.36    |

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02new\_3H\_4Fs\_1me\_2oxo\_4me\_giao

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| Atom | Abs.   | Rel.    |
|------|--------|---------|
| 1C   | 55.58  | 122.17  |
| 2C   | 47.68  | 129.79  |
| 3C   | 33.08  | 143.85  |
| 4C   | 36.34  | 140.70  |
| 5C   | 36.62  | 140.43  |
| 6C   | 34.20  | 142.77  |
| 7N   | -70.85 | -84.97  |
| 8N   | 110.17 | -256.22 |
| 9C   | 13.90  | 162.32  |
| 10C  | 7.09   | 168.87  |
| 11C  | 136.62 | 44.13   |
| 12H  | 28.66  | 3.20    |
| 13H  | 29.41  | 2.47    |
| 14O  | -88.49 | 329.46  |
| 15F  | 321.38 | -146.10 |
| 16F  | 336.63 | -160.72 |
| 17F  | 336.32 | -160.43 |
| 18F  | 319.52 | -144.32 |
| 19C  | 154.04 | 27.36   |
| 20H  | 29.64  | 2.25    |
| 21H  | 29.65  | 2.24    |
| 22H  | 29.57  | 2.32    |
| 23C  | 144.14 | 36.89   |
| 24H  | 29.55  | 2.34    |

|     |       |      |
|-----|-------|------|
| 25H | 28.44 | 3.41 |
| 26H | 28.20 | 3.65 |

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03new\_3H\_2oxo\_4me\_giao

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| Atom | Abs.   | Rel.    |
|------|--------|---------|
| 1C   | 47.34  | 130.11  |
| 2C   | 35.81  | 141.21  |
| 3C   | 48.21  | 129.28  |
| 4C   | 54.38  | 123.33  |
| 5C   | 52.62  | 125.02  |
| 6C   | 58.27  | 119.59  |
| 7N   | -92.55 | -64.45  |
| 8N   | 98.34  | -245.03 |
| 9C   | 13.37  | 162.83  |
| 10C  | 13.83  | 162.38  |
| 11C  | 137.35 | 43.43   |
| 12H  | 28.74  | 3.12    |
| 13H  | 29.38  | 2.50    |
| 14O  | -75.62 | 317.90  |
| 15H  | 25.14  | 6.62    |
| 16C  | 153.24 | 28.13   |
| 17H  | 29.65  | 2.24    |
| 18H  | 29.62  | 2.26    |
| 19H  | 29.55  | 2.34    |
| 20H  | 24.97  | 6.78    |
| 21H  | 24.69  | 7.05    |
| 22H  | 24.64  | 7.10    |
| 23H  | 24.33  | 7.40    |

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04new\_3H\_1me\_2oxo\_4me\_giao

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| Atom | Abs.   | Rel.    |
|------|--------|---------|
| 1C   | 40.23  | 136.96  |
| 2C   | 33.89  | 143.06  |
| 3C   | 49.45  | 128.08  |
| 4C   | 54.31  | 123.40  |
| 5C   | 53.29  | 124.38  |
| 6C   | 57.85  | 119.99  |
| 7N   | -90.08 | -66.79  |
| 8N   | 102.37 | -248.85 |
| 9C   | 12.52  | 163.65  |
| 10C  | 12.15  | 164.00  |
| 11C  | 137.07 | 43.71   |

|     |        |        |
|-----|--------|--------|
| 12H | 28.72  | 3.14   |
| 13H | 29.39  | 2.49   |
| 14O | -81.97 | 323.60 |
| 15C | 153.92 | 27.48  |
| 16H | 29.73  | 2.16   |
| 17H | 29.64  | 2.25   |
| 18H | 29.59  | 2.29   |
| 19C | 146.96 | 34.18  |
| 20H | 29.41  | 2.48   |
| 21H | 28.69  | 3.17   |
| 22H | 27.72  | 4.11   |
| 23H | 24.60  | 7.14   |
| 24H | 24.61  | 7.13   |
| 25H | 24.66  | 7.08   |
| 26H | 24.39  | 7.34   |

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05new\_3H\_2oxo\_4ph\_giao

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| Atom | Abs.   | Rel.    |
|------|--------|---------|
| 1C   | 46.84  | 130.59  |
| 2C   | 35.68  | 141.34  |
| 3C   | 48.15  | 129.33  |
| 4C   | 54.16  | 123.55  |
| 5C   | 52.50  | 125.14  |
| 6C   | 58.16  | 119.69  |
| 7H   | 24.25  | 7.47    |
| 8H   | 24.60  | 7.14    |
| 9H   | 24.62  | 7.12    |
| 10H  | 24.89  | 6.85    |
| 11N  | -89.09 | -67.72  |
| 12N  | 96.75  | -243.53 |
| 13C  | 12.31  | 163.84  |
| 14C  | 18.12  | 158.25  |
| 15C  | 140.73 | 40.18   |
| 16H  | 28.02  | 3.82    |
| 17H  | 29.30  | 2.58    |
| 18O  | -73.54 | 316.04  |
| 19H  | 25.02  | 6.73    |
| 20C  | 38.06  | 139.05  |
| 21C  | 49.65  | 127.88  |
| 22C  | 48.71  | 128.80  |
| 23C  | 49.73  | 127.81  |
| 24H  | 23.75  | 7.96    |
| 25C  | 49.51  | 128.02  |
| 26H  | 23.06  | 8.64    |
| 27C  | 47.08  | 130.36  |

|     |       |      |
|-----|-------|------|
| 28H | 24.29 | 7.44 |
| 29H | 24.29 | 7.44 |
| 30H | 24.33 | 7.40 |

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06new\_3H\_1me\_2oxo\_4ph\_giao

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| Atom | Abs.   | Rel.    |
|------|--------|---------|
| 1C   | 39.49  | 137.67  |
| 2C   | 33.93  | 143.03  |
| 3C   | 49.45  | 128.08  |
| 4C   | 54.13  | 123.58  |
| 5C   | 53.28  | 124.39  |
| 6C   | 57.64  | 120.19  |
| 7H   | 24.29  | 7.43    |
| 8H   | 24.55  | 7.18    |
| 9H   | 24.55  | 7.19    |
| 10H  | 24.61  | 7.13    |
| 11N  | -86.68 | -70.01  |
| 12N  | 101.01 | -247.55 |
| 13C  | 11.54  | 164.59  |
| 14C  | 16.47  | 159.84  |
| 15C  | 140.51 | 40.39   |
| 16H  | 27.98  | 3.86    |
| 17H  | 29.25  | 2.63    |
| 18O  | -81.97 | 323.61  |
| 19C  | 38.28  | 138.84  |
| 20C  | 49.62  | 127.91  |
| 21C  | 49.24  | 128.28  |
| 22C  | 49.63  | 127.90  |
| 23H  | 23.70  | 8.01    |
| 24C  | 49.68  | 127.85  |
| 25H  | 23.04  | 8.65    |
| 26C  | 47.18  | 130.27  |
| 27H  | 24.28  | 7.45    |
| 28H  | 24.34  | 7.39    |
| 29H  | 24.33  | 7.40    |
| 30C  | 146.87 | 34.27   |
| 31H  | 29.41  | 2.47    |
| 32H  | 28.64  | 3.22    |
| 33H  | 27.72  | 4.12    |