Supporting Information

Five-to-Six Membered Ring-rearrangements in the Reaction of 5-Perfluoroalkyl-1,2,4-oxadiazoles with Hydrazine and Methylhydrazine

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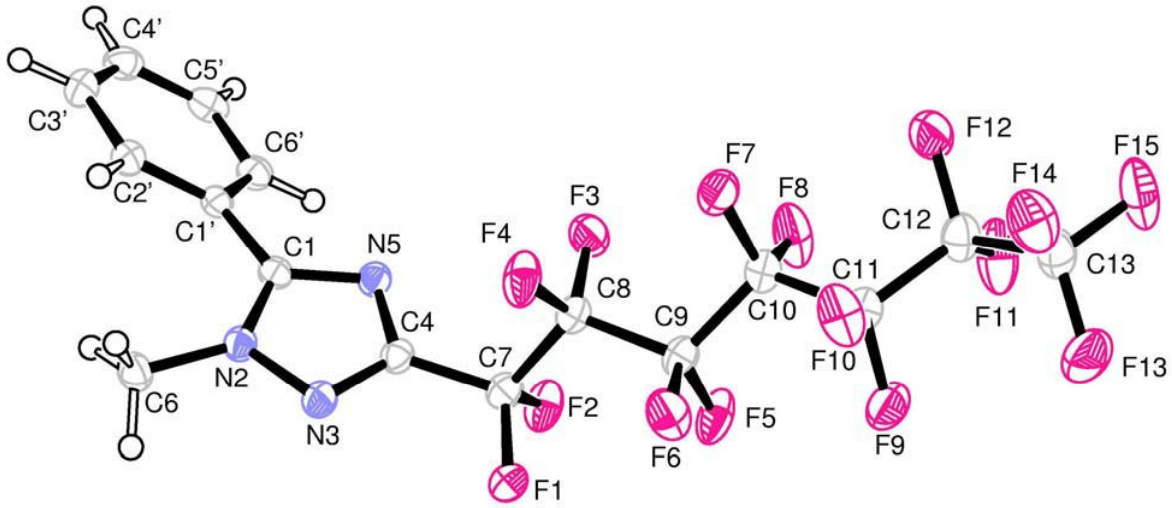
General. Melting points were determined with a hot-stage apparatus and are uncorrected. IR spectra were recorded from Nujol mulls. Flash chromatography (silica gel 0.040-0.063 mm) was performed by using mixtures of ethyl acetate and light petroleum (fraction boiling in the range of 40-60°C) in varying ratios. Compounds **5a-c**,[1] and **15a-c**[2] were prepared as reported.

NMR Measurements. ^{1}H NMR spectra (300 MHz, unless otherwise stated) were taken with TMS as internal standard. The ^{1}H, ^{13}C, ^{19}F ,^{15}N NMR spectra of compounds **9a-c**, **14a-c**, **27c**, **28c** and **30**, were recorded on a spectrometer equipped with a dual switchable PFG direct probe, operating at 599.7, 150.8, 564.2 and 60.8 MHz, respectively. The samples were dissolved in DMSO-d_6. The residual peak of DMSO-d_6 in the ^{1}H spectra and in the ^{13}C spectra (2.50 and 39.5 ppm, respectively), the external standard C_6F_6 (neat, set at –163.0 ppm) in the ^{19}F spectra and the external standard CH_3NO_2 (neat, set at 380.0 ppm) in the ^{15}N spectra were used as references. In the case of the ^{15}N spectra, almost saturated solutions of the compounds were used, in order to have sufficiently high S/N ratio in a reasonable amount of time (10000 scans, 5 s delay). Two dimensional indirect-detected ^{1}H-^{13}C g-HSQC, ^{1}H-^{13}C g-HMBC and ^{1}H-^{15}N g-HMBC[3] were recorded with a triple-resonance indirect detection PFG probe, operating at 599.7, 150.8 and 60.8 MHz for ^{1}H, ^{13}C, and ^{15}N, respectively. In the case of ^{1}H-^{13}C long range correlation spectra, the long-range coupling constant was set to 8 Hz, while in the case of ^{1}H-^{15}N long range correlation spectra, the coupling constant was set to 6 Hz.

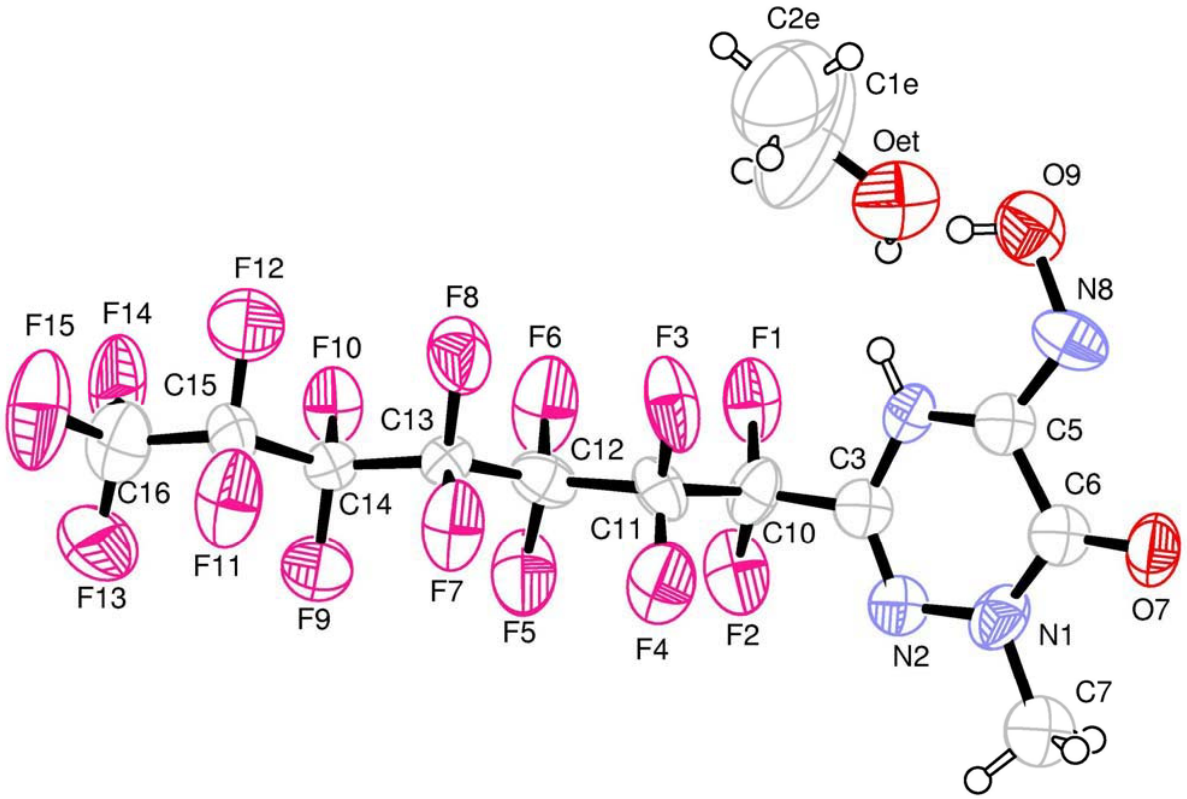
X-Ray Crystallographic Analyses. Single crystals of **9c**, of **28c × C_2H_5OH** and of the dibenzoyl derivative **30**, have been obtained by dissolving few mg of powder of each compound in ethanol and allowing the solution to concentrate at room temperature. A Siemens P4 four-circle (for **28c × C_2H_5OH**) and a Bruker-Nonius FR591 rotating anode diffractometers (for **9c** and for the dibenzoyl derivative **30**) with graphite monochromated Mo-*K*α radiation (λ =0.71073Å) were used for data collections. The structures were solved by direct methods implemented in the SHELXS-97

program.[4] The refinements were carried out by full-matrix anisotropic least-squares on F^2 for all reflections for non-H atoms by using the SHELXL-97 program.[5]

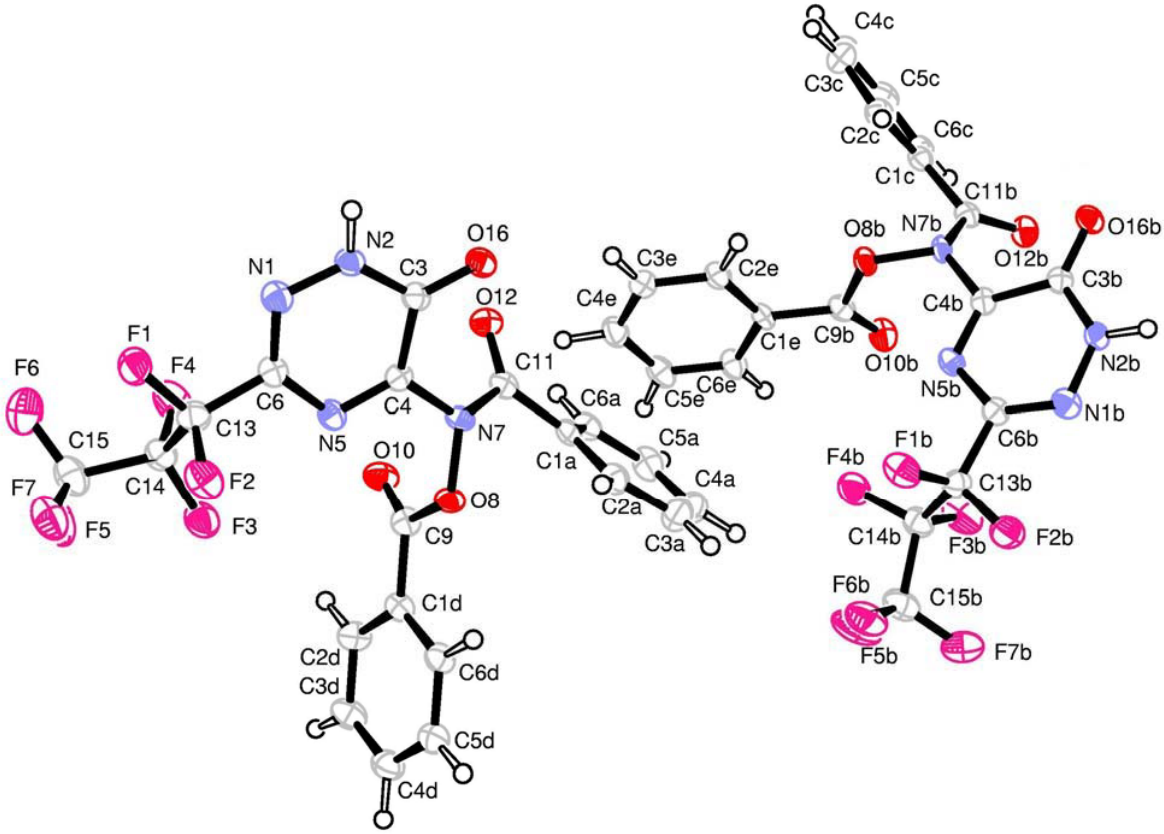
Computational Details. Ab initio calculations were obtained by means of the Gaussian 03 series of programs.[6] The geometry optimization was obtained at the B3LYP/6-311G(d) level (standard Berny algorithm, for each optimized ground state, the vibrational analysis show the absence of imaginary frequencies). Values reported are not ZPE corrected. On the geometry optimized structures, chemical shift calculation were obtained with the GIAO approach at the B3LYP/6-311++G(2d,p) level. NH_3, calculated at the same level of theory (B3LYP/6-311++G(2d,p)// B3LYP/6-311G(d)) was used as reference to scale the absolute shielding value.



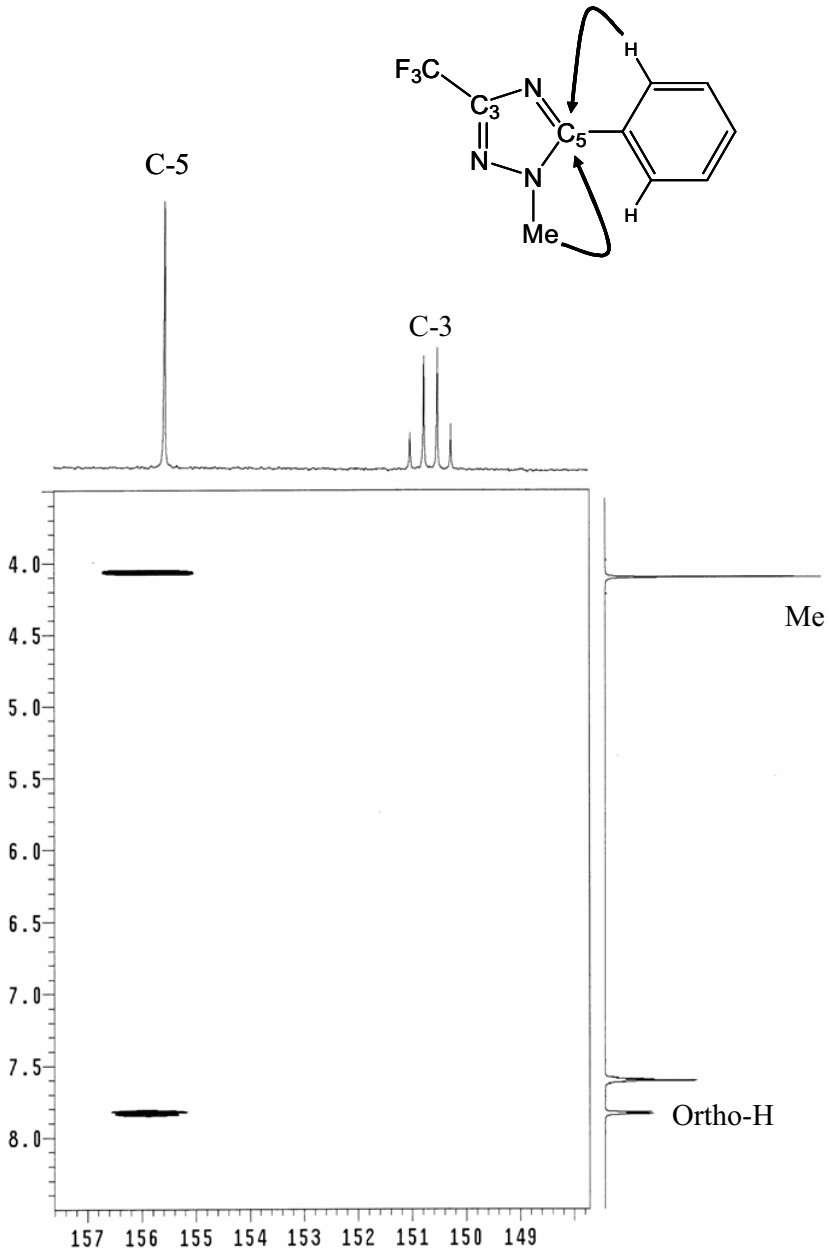
ORTEP drawing of compound **9c**. Thermal ellipsoids enclose 50% probability.



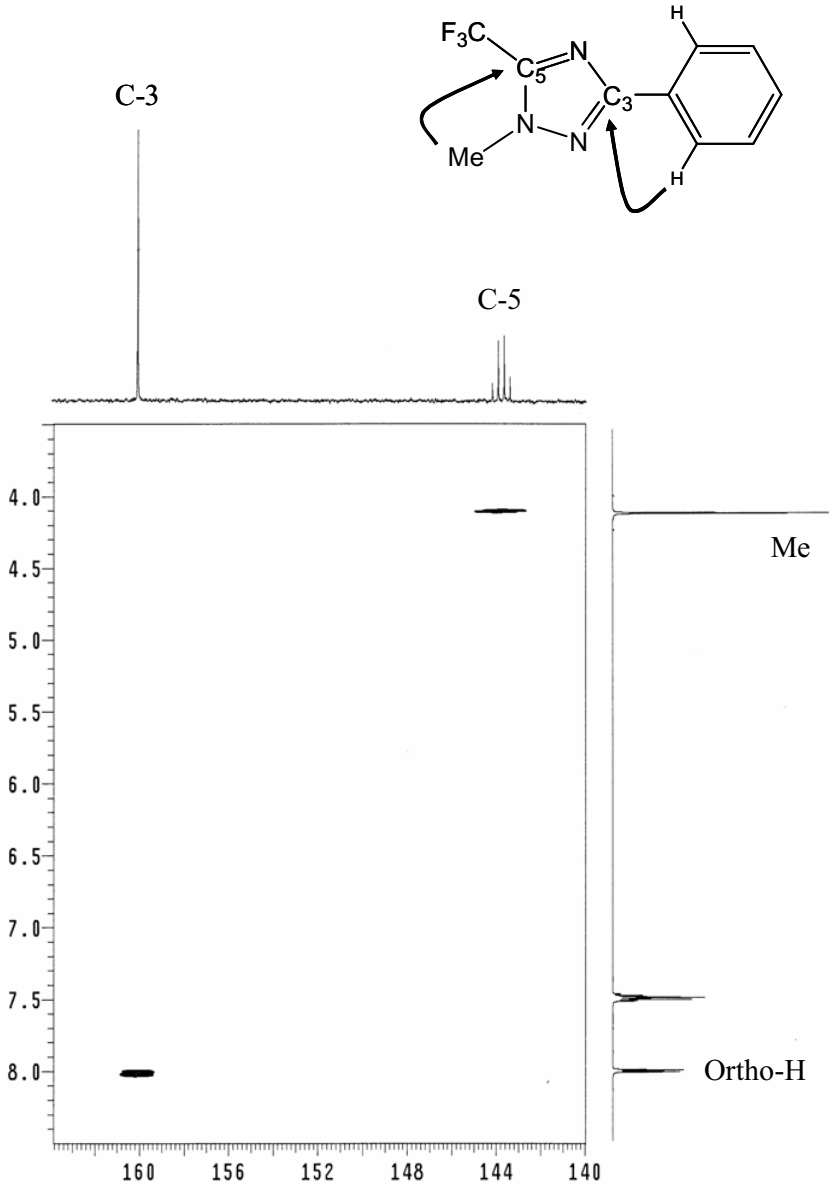
ORTEP drawing of compound **28c**. Thermal ellipsoids enclose 50% probability.



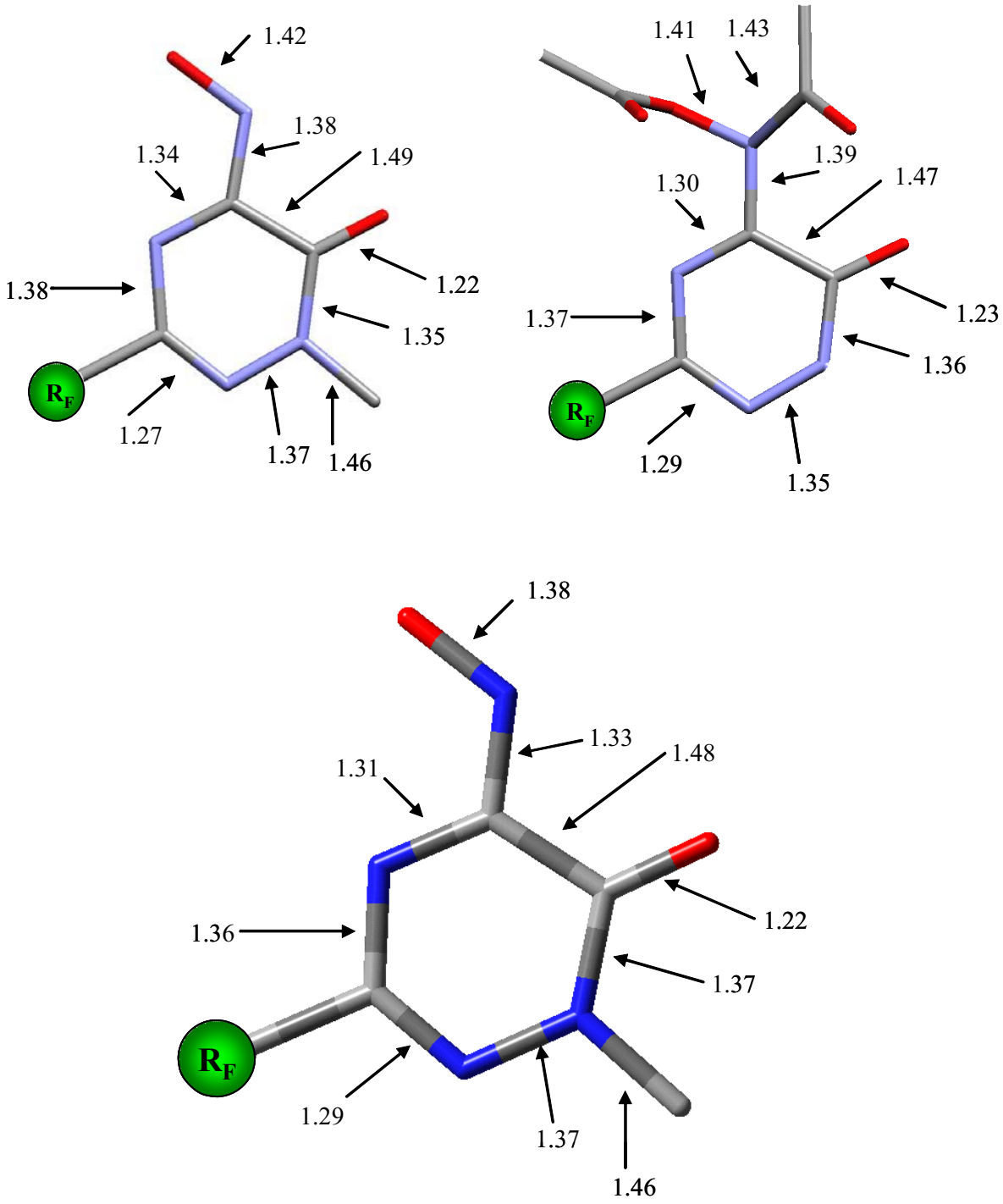
ORTEP drawing of the asymmetric unit of the dibenzoyl derivative **30**. Thermal ellipsoids enclose 50% probability.



^{1}H-^{13}C g-HMBC spectra of compound **9a**



^{1}H-^{13}C g-HMBC spectra of compound **14a**



On the top: X-ray derived bond distances for **28c** (left) and **30** (right); on the bottom: Ab.initio calculated bond distances for **28a** (geometry optimization at the B3LYP/6-311G(d) level)

Ab initio optimized geometry and GIAO chemical shift calculations for the three tautomers of **28a**

Structure **28-NHOH**, optimized geometry, B3LYP/6-311G(d) level.

Total energy: -862.67961906 a.u.
Imaginary frequencies: 0

```
C                 -0.77555600   -0.15787800    0.00287100
 C                 1.91594300   -0.56014300    0.00332500
 N                 0.98751400   -1.57132700    0.00081700
 O                 3.13058200   -0.70435700   -0.00756900
 C                -2.27667600    0.06685000   -0.00028400
 C                 1.27300200    0.77427100    0.01437100
 C                 1.41435100   -2.96851700   -0.00938800
 H                 1.02739100   -3.45723800   -0.90398300
 H                 2.50025400   -2.99157600   -0.00545500
 H                 1.02006200   -3.47134200    0.87399900
 F                -2.65066600    0.77157500    1.08753600
 F                -2.96724600   -1.07691500   -0.00788400
 F                -2.64373600    0.78192600   -1.08386100
 O                 1.60928900    3.10194900   -0.03431900
 H                 0.64038900    2.97663800   -0.02883800
 N                -0.36663200   -1.38678800    0.00296100
 N                -0.02693500    0.97471800    0.00477200
 N                 2.09828500    1.81399900    0.05393000
 H                 3.09576100    1.73180300   -0.06547200
```

Structure **28-NHOH**, Chemical shift calculation GIAO-B3LYP/6-311++G(2d,p) level.
(NH_3 shielding at the same level: +261.7)

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =    34.8776   Anisotropy =   117.1776
   XX=   -56.5370   YX=   -18.3870   ZX=    -0.3892
   XY=     9.7741   YY=    48.1771   ZY=    -0.1367
   XZ=    -0.8526   YZ=     0.6364   ZZ=   112.9926
   Eigenvalues:   -56.7160    48.3527   112.9960
  2  C    Isotropic =    31.0533   Anisotropy =    97.2712
   XX=    50.6722   YX=    -2.2727   ZX=     0.1296
   XY=     4.0083   YY=   -53.3946   ZY=    -1.4896
   XZ=    -0.6124   YZ=    -1.7072   ZZ=    95.8823
   Eigenvalues:   -53.4189    50.6780    95.9008
  3  N    Isotropic =    41.1140   Anisotropy =   147.0643 (220.6 ppm vs NH3)
   XX=    -1.6584   YX=    90.5013   ZX=     0.6216
   XY=    42.3584   YY=   -14.1429   ZY=    -0.5978
   XZ=     1.0655   YZ=    -2.2321   ZZ=   139.1434
   Eigenvalues:   -74.6353    58.8205   139.1569
  4  O    Isotropic =   -10.9145   Anisotropy =   570.9225
   XX=  -294.8128   YX=    -6.6915   ZX=     3.6922
   XY=   -36.6825   YY=  -107.6021   ZY=    -4.1733
   XZ=    -2.1374   YZ=    -3.1022   ZZ=   369.6714
   Eigenvalues:  -297.2925  -105.1516   369.7004
  5  C    Isotropic =    52.6459   Anisotropy =    15.1515
   XX=    41.6915   YX=     4.6684   ZX=    -0.0143
   XY=     4.2280   YY=    61.8072   ZY=     0.0316
   XZ=    -0.0035   YZ=     0.0023   ZZ=    54.4391
   Eigenvalues:    40.7517    54.4391    62.7469
  6  C    Isotropic =    29.8073   Anisotropy =   137.4778
   XX=    13.6001   YX=    -8.2013   ZX=     0.4548
   XY=    17.9677   YY=   -45.6359   ZY=     0.3724
   XZ=    -0.3263   YZ=    -1.3637   ZZ=   121.4577
   Eigenvalues:   -46.0372    14.0000   121.4592
  7  C    Isotropic =   146.7323   Anisotropy =    52.2944
   XX=   128.8366   YX=   -14.8185   ZX=    -0.0579
```

```
  XY=   -22.0290   YY=   175.1605   ZY=     0.1812
  XZ=    -0.2525   YZ=     0.1564   ZZ=   136.2000
  Eigenvalues:   122.4022   136.1996   181.5953
 8  H    Isotropic =    28.8094   Anisotropy =     8.0258
  XX=    26.2184   YX=    -0.6095   ZX=     0.9331
  XY=     0.4105   YY=    31.1033   ZY=     3.5936
  XZ=     1.6134   YZ=     4.1367   ZZ=    29.1064
  Eigenvalues:    25.0705    27.1977    34.1599
 9  H    Isotropic =    27.2659   Anisotropy =     5.8700
  XX=    30.5105   YX=    -0.0077   ZX=     0.0121
  XY=    -2.2725   YY=    29.2355   ZY=     0.0180
  XZ=    -0.0152   YZ=     0.0197   ZZ=    22.0517
  Eigenvalues:    22.0516    28.5668    31.1792
10  H    Isotropic =    28.8032   Anisotropy =     8.0138
  XX=    26.2321   YX=    -0.5854   ZX=    -0.9589
  XY=     0.4639   YY=    31.1994   ZY=    -3.5731
  XZ=    -1.6475   YZ=    -4.0866   ZZ=    28.9782
  Eigenvalues:    25.0577    27.2062    34.1457
11  F    Isotropic =   241.2215   Anisotropy =   143.6458
  XX=   181.9713   YX=   -31.1472   ZX=   -63.2016
  XY=   -20.9242   YY=   252.7423   ZY=    36.1683
  XZ=   -51.1987   YZ=    37.3688   ZZ=   288.9511
  Eigenvalues:   156.1332   230.5460   336.9854
12  F    Isotropic =   256.9736   Anisotropy =   111.8741
  XX=   228.5814   YX=    84.7476   ZX=     0.3137
  XY=    63.8046   YY=   277.9756   ZY=     0.4251
  XZ=     0.0902   YZ=     0.4656   ZZ=   264.3639
  Eigenvalues:   175.0040   264.3606   331.5564
13  F    Isotropic =   241.4877   Anisotropy =   143.6101
  XX=   181.3579   YX=   -31.3945   ZX=    62.1234
  XY=   -20.9825   YY=   253.5152   ZY=   -36.6212
  XZ=    50.0696   YZ=   -37.8463   ZZ=   289.5902
  Eigenvalues:   156.4500   230.7854   337.2278
14  O    Isotropic =   196.3815   Anisotropy =    86.1074
  XX=   138.1267   YX=   -62.9653   ZX=     6.1813
  XY=   -39.3888   YY=   223.0211   ZY=    -9.9734
  XZ=     8.1843   YZ=   -12.3618   ZZ=   227.9966
  Eigenvalues:   114.0571   221.3009   253.7864
15  H    Isotropic =    25.1478   Anisotropy =    11.7197
  XX=    32.9551   YX=     1.5873   ZX=     0.0643
  XY=    -1.2322   YY=    27.2027   ZY=    -0.2085
  XZ=     0.1009   YZ=     0.1054   ZZ=    15.2857
  Eigenvalues:    15.2851    27.1974    32.9610
16  N    Isotropic =   -49.3580   Anisotropy =   317.0525 (311.1 ppm vs NH3)
  XX=  -219.9119   YX=    43.0630   ZX=     0.5815
  XY=    37.0832   YY=   -90.1634   ZY=    -0.2920
  XZ=    -0.0766   YZ=    -2.7443   ZZ=   162.0012
  Eigenvalues:  -231.2917   -78.7927   162.0103
17  N    Isotropic =    36.0408   Anisotropy =   329.8195 (225.7 ppm vs NH3)
  XX=   -77.9150   YX=   -20.7605   ZX=    -2.8235
  XY=   -72.3153   YY=   -69.8761   ZY=    -1.5367
  XZ=     0.5523   YZ=    -0.8083   ZZ=   255.9133
  Eigenvalues:  -120.6137   -27.1844   255.9204
18  N    Isotropic =    77.0337   Anisotropy =    79.6182 (184.7 ppm vs NH3)
  XX=   -12.3115   YX=    13.5491   ZX=     4.0366
  XY=    -3.2203   YY=   127.4522   ZY=    -2.4470
  XZ=     3.4673   YZ=    -9.6155   ZZ=   115.9603
  Eigenvalues:   -12.6250   113.6135   130.1125
19  H    Isotropic =    23.5442   Anisotropy =     7.9687
  XX=    25.6438   YX=    -0.3212   ZX=    -0.3909
  XY=    -3.6117   YY=    27.6372   ZY=    -0.0243
  XZ=    -1.0750   YZ=    -0.0271   ZZ=    17.3514
  Eigenvalues:    17.2832    24.4926    28.8566
```

Structure **28-4NH**, optimized geometry, B3LYP/6-311G(d) level.
Total energy: -862.67666032 a.u.
Imaginary frequencies: 0

C	0.76844600	-0.19710900	-0.04492600
C	-1.98933200	-0.49730900	0.01763800
N	-1.06068900	-1.53204200	-0.01707400
O	-3.18508600	-0.68281900	0.04858200
C	2.26868800	-0.00658100	0.00423900
N	-2.14573300	1.89429200	0.00751600
C	-1.37613700	0.86829900	0.00332000
C	-1.51114000	-2.92073700	-0.01929200
H	-1.12326300	-3.43285800	0.86266300
H	-2.59669200	-2.92365700	-0.00633600
H	-1.14362000	-3.42194300	-0.91592600
F	2.61550300	1.09139100	-0.71304500
F	2.93043800	-1.05250400	-0.48015800
F	2.68610400	0.20952400	1.26859300
O	-1.35707100	3.06161000	-0.01852100
H	-2.00901800	3.76941800	-0.02033200
N	0.30397100	-1.38826800	-0.03792200
N	0.00764500	0.94072900	-0.02606600
H	0.42194500	1.86064500	-0.09012700

Structure **28-4NH**, Chemical shift calculation GIAO-B3LYP/6-311++G(2d,p) level.
(NH_3 shielding at the same level: +261.7)

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =    48.5751   Anisotropy =    99.2454
   XX=   -33.9811   YX=    45.0713   ZX=    -0.3161
   XY=     6.9613   YY=    65.0081   ZY=    -0.3561
   XZ=     1.3716   YZ=     2.8117   ZZ=   114.6983
   Eigenvalues:   -40.4024    71.3890   114.7387
  2  C    Isotropic =    28.2241   Anisotropy =    88.8241
   XX=    57.3133   YX=    15.4338   ZX=     1.1946
   XY=     7.4285   YY=   -59.9552   ZY=    -1.0209
   XZ=     2.6092   YZ=    -2.2634   ZZ=    87.3142
   Eigenvalues:   -61.0814    58.3135    87.4402
  3  N    Isotropic =    57.3350   Anisotropy =   107.4911 (204.4 ppm vs NH3)
   XX=    27.1556   YX=   -81.2239   ZX=     0.9288
   XY=   -53.1945   YY=    15.8826   ZY=     0.0525
   XZ=     2.3708   YZ=     1.3489   ZZ=   128.9668
   Eigenvalues:   -45.9413    88.9505   128.9957
  4  O    Isotropic =   -72.3627   Anisotropy =   646.4587
   XX=  -411.2390   YX=    -9.9542   ZX=    20.2657
   XY=    37.7264   YY=  -163.6743   ZY=    -4.4927
   XZ=    27.6264   YZ=    -5.4693   ZZ=   357.8253
   Eigenvalues:  -412.7747  -162.9232   358.6098
  5  C    Isotropic =    53.4195   Anisotropy =    13.9578
   XX=    41.2041   YX=     0.2355   ZX=    -3.1168
   XY=    -3.8705   YY=    62.3979   ZY=     0.4046
   XZ=    -2.2412   YZ=     1.1370   ZZ=    56.6566
   Eigenvalues:    40.6252    56.9087    62.7248
  6  N    Isotropic =   -92.9682   Anisotropy =   276.1666 (354.7 ppm vs NH3)
   XX=  -115.6200   YX=   -41.5501   ZX=     3.9546
   XY=   -36.1617   YY=  -254.3827   ZY=     4.4547
   XZ=     1.5969   YZ=    -0.2008   ZZ=    91.0980
   Eigenvalues:  -264.5435  -105.5040    91.1429
  7  C    Isotropic =    40.0519   Anisotropy =   112.6693
   XX=    -7.4171   YX=   -44.8325   ZX=     2.8405
   XY=   -83.5962   YY=    12.4848   ZY=     2.5047
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```
  XZ=     2.5998   YZ=     2.4822   ZZ=   115.0879
  Eigenvalues:   -62.5235    67.5143   115.1648
 8  C    Isotropic =   147.5069   Anisotropy =    51.3394
  XX=   130.1077   YX=    15.4806   ZX=     0.4075
  XY=    22.2586   YY=   174.8358   ZY=    -0.0981
  XZ=     0.2853   YZ=     0.1163   ZZ=   137.5773
  Eigenvalues:   123.2034   137.5841   181.7332
 9  H    Isotropic =    29.0247   Anisotropy =     8.0880
  XX=    26.1262   YX=     0.7860   ZX=     0.8755
  XY=    -0.2682   YY=    31.4652   ZY=    -3.6826
  XZ=     1.5939   YZ=    -3.8729   ZZ=    29.4826
  Eigenvalues:    25.1706    27.4868    34.4167
10  H    Isotropic =    27.2599   Anisotropy =     5.7936
  XX=    30.5803   YX=     0.0501   ZX=    -0.1446
  XY=     2.1448   YY=    28.8977   ZY=     0.0499
  XZ=    -0.0975   YZ=     0.1353   ZZ=    22.3018
  Eigenvalues:    22.2982    28.3593    31.1223
11  H    Isotropic =    29.0297   Anisotropy =     8.0477
  XX=    26.0835   YX=     0.9131   ZX=    -0.7801
  XY=    -0.1628   YY=    31.3677   ZY=     3.6827
  XZ=    -1.5113   YZ=     3.8623   ZZ=    29.6377
  Eigenvalues:    25.1833    27.5109    34.3948
12  F    Isotropic =   248.4036   Anisotropy =   142.9175
  XX=   179.8280   YX=    54.5822   ZX=   -40.6229
  XY=    36.0992   YY=   291.6047   ZY=   -39.1619
  XZ=   -29.7862   YZ=   -40.6394   ZZ=   273.7781
  Eigenvalues:   159.7141   241.8149   343.6820
13  F    Isotropic =   254.1984   Anisotropy =   113.2710
  XX=   226.4252   YX=   -71.1470   ZX=   -34.0326
  XY=   -56.2763   YY=   265.1372   ZY=    15.4475
  XZ=   -25.0799   YZ=    19.3461   ZZ=   271.0326
  Eigenvalues:   177.1245   255.7583   329.7123
14  F    Isotropic =   233.4865   Anisotropy =   150.5042
  XX=   178.9339   YX=    10.1577   ZX=    75.6572
  XY=    11.6572   YY=   222.1689   ZY=    14.8145
  XZ=    64.8829   YZ=     9.1540   ZZ=   299.3568
  Eigenvalues:   146.2853   220.3516   333.8226
15  O    Isotropic =   135.6615   Anisotropy =   112.8690
  XX=    78.4839   YX=   109.0856   ZX=     0.9294
  XY=    98.2633   YY=   129.6909   ZY=    -0.8111
  XZ=     2.0002   YZ=    -3.0359   ZZ=   198.8097
  Eigenvalues:    -2.7289   198.8059   210.9075
16  H    Isotropic =    25.8235   Anisotropy =    10.4651
  XX=    26.1335   YX=    -1.8574   ZX=    -0.0708
  XY=    -3.9291   YY=    31.5431   ZY=    -0.0687
  XZ=     0.0322   YZ=    -0.2240   ZZ=    19.7939
  Eigenvalues:    19.7916    24.8787    32.8002
17  N    Isotropic =   -32.6522   Anisotropy =   307.6642 (294.3 ppm vs NH3)
  XX=  -199.3064   YX=   -25.5362   ZX=     3.5792
  XY=   -35.9309   YY=   -71.0617   ZY=    -0.6283
  XZ=    -4.8916   YZ=    -6.0381   ZZ=   172.4115
  Eigenvalues:  -206.2962   -64.1177   172.4573
18  N    Isotropic =   129.5605   Anisotropy =   110.3137 (132.1 ppm vs NH3)
  XX=   124.5481   YX=   -52.8776   ZX=     2.8334
  XY=   -20.7036   YY=    61.4092   ZY=     4.9909
  XZ=    -6.4049   YZ=     6.3111   ZZ=   202.7242
  Eigenvalues:    44.3783   141.2003   203.1030
19  H    Isotropic =    23.8889   Anisotropy =    10.5367
  XX=    27.8749   YX=    -2.6572   ZX=    -0.6626
  XY=    -3.5946   YY=    27.6973   ZY=    -0.3239
  XZ=    -0.6170   YZ=    -0.8702   ZZ=    16.0945
  Eigenvalues:    16.0061    24.7472    30.9134
```

Structure **28-2NH**, optimized geometry, B3LYP/6-311G(d) level.
Total energy: -862.65062109 a.u.
Imaginary frequencies: 0

```
C                 -0.74343900   -0.05220700   -0.03619000
 C                 2.02095700   -0.40766200   -0.04511400
 N                -0.05662600    1.02547900    0.00794500
 N                 1.14649400   -1.49385600   -0.14619400
 O                 3.21655200   -0.57456800    0.00993400
 C                -2.26479000    0.02656800    0.00852000
 N                 2.08098300    1.97452000   -0.01106400
 C                 1.33527900    0.91985800   -0.02201700
 C                 1.60317400   -2.84845200    0.12264200
 H                 2.68733600   -2.83671100    0.06195900
 H                 1.29100400   -3.17460000    1.11936700
 H                 1.20883900   -3.53801600   -0.62927500
 F                -2.71806700    1.10624400   -0.62195300
 F                -2.70938300    0.05404800    1.27398800
 F                -2.80667600   -1.06925800   -0.58520800
 O                 1.41448900    3.15563900    0.03121600
 H                 0.45268300    2.96695500    0.05022200
 N                -0.24322900   -1.31693300   -0.02389600
 H                -0.78150200   -2.03861000   -0.48749400
```

Structure **28-2NH**, Chemical shift calculation GIAO-B3LYP/6-311++G(2d,p) level.
(NH_3 shielding at the same level: +261.7)

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =    37.5438   Anisotropy =   101.0080
   XX=   -30.1593   YX=    46.1718   ZX=     3.3970
   XY=    19.1260   YY=    38.2756   ZY=    -3.6194
   XZ=     0.0811   YZ=    -6.2218   ZZ=   104.5152
   Eigenvalues:   -43.3169    51.0658   104.8825
  2  C    Isotropic =    28.3046   Anisotropy =    86.8399
   XX=    59.5123   YX=   -24.1114   ZX=    -1.5626
   XY=    -1.6306   YY=   -60.5561   ZY=    -3.6059
   XZ=    -2.1389   YZ=    -6.1110   ZZ=    85.9577
   Eigenvalues:   -62.0910    60.8070    86.1979
  3  N    Isotropic =    22.5699   Anisotropy =   363.9742 (239.1 ppm vs NH3)
   XX=  -138.8448   YX=    -5.1898   ZX=     4.9652
   XY=   -46.3529   YY=   -58.0704   ZY=   -12.3294
   XZ=    25.7996   YZ=    10.9281   ZZ=   264.6250
   Eigenvalues:  -146.8830   -50.6266   265.2194
  4  N    Isotropic =    94.4434   Anisotropy =    71.2857 (167.3 ppm vs NH3)
   XX=    69.8669   YX=    56.3409   ZX=    -7.3074
   XY=    51.6351   YY=    93.3351   ZY=    -3.9751
   XZ=   -13.5490   YZ=    -6.2414   ZZ=   120.1282
   Eigenvalues:    26.0930   115.2700   141.9672
  5  O    Isotropic =   -64.2600   Anisotropy =   638.3510
   XX=  -381.8601   YX=    18.2501   ZX=   -36.6263
   XY=   -20.9737   YY=  -169.3762   ZY=   -16.7733
   XZ=   -52.9250   YZ=    -1.4265   ZZ=   358.4564
   Eigenvalues:  -384.5753  -169.5120   361.3073
  6  C    Isotropic =    53.8804   Anisotropy =    14.3641
   XX=    41.3635   YX=     5.6141   ZX=     2.8484
   XY=     0.0336   YY=    62.9958   ZY=    -1.1367
   XZ=     1.2413   YZ=    -0.9317   ZZ=    57.2819
   Eigenvalues:    40.7189    57.4659    63.4565
  7  N    Isotropic =  -163.1623   Anisotropy =   425.8338 (424.9 ppm vs NH3)
   XX=  -178.5352   YX=    86.0075   ZX=     8.3541
   XY=    87.1533   YY=  -431.0964   ZY=   -15.1442
```

```
  XZ=    11.6272   YZ=   -13.5285   ZZ=   120.1446
  Eigenvalues:  -458.4060  -151.8078   120.7269
 8  C    Isotropic =    36.6567   Anisotropy =   108.7977
  XX=    -6.5010   YX=    44.2794   ZX=     2.5574
  XY=    96.3242   YY=     7.4268   ZY=    -3.8619
  XZ=     5.4637   YZ=    -2.1212   ZZ=   109.0442
  Eigenvalues:   -70.3213    71.1028   109.1885
 9  C    Isotropic =   150.4314   Anisotropy =    50.1921
  XX=   131.4361   YX=   -14.5979   ZX=     0.6294
  XY=   -22.6387   YY=   175.3377   ZY=    -9.8374
  XZ=     2.2595   YZ=    -6.6390   ZZ=   144.5204
  Eigenvalues:   124.4872   142.9143   183.8928
10  H    Isotropic =    27.0287   Anisotropy =     6.6596
  XX=    30.8025   YX=    -0.4875   ZX=    -0.1006
  XY=    -2.4278   YY=    28.2774   ZY=    -0.1716
  XZ=    -0.1331   YZ=    -0.2807   ZZ=    22.0061
  Eigenvalues:    21.9946    27.6231    31.4684
11  H    Isotropic =    29.2903   Anisotropy =     8.9988
  XX=    25.7291   YX=    -1.1428   ZX=    -0.0933
  XY=    -0.4448   YY=    30.4589   ZY=    -4.4369
  XZ=    -1.0364   YZ=    -3.9093   ZZ=    31.6831
  Eigenvalues:    25.1695    27.4119    35.2896
12  H    Isotropic =    29.5737   Anisotropy =     8.6417
  XX=    26.2333   YX=    -1.0850   ZX=     0.7456
  XY=     0.1420   YY=    33.5169   ZY=     3.5368
  XZ=     1.3547   YZ=     3.2643   ZZ=    28.9710
  Eigenvalues:    25.4559    27.9304    35.3349
13  F    Isotropic =   250.4808   Anisotropy =   117.9217
  XX=   202.1602   YX=   -56.1037   ZX=    39.2823
  XY=   -37.5490   YY=   279.6716   ZY=   -25.5179
  XZ=    32.3453   YZ=   -27.7466   ZZ=   269.6107
  Eigenvalues:   174.7606   247.5865   329.0953
14  F    Isotropic =   235.7198   Anisotropy =   146.2944
  XX=   185.9499   YX=     4.9138   ZX=   -77.3992
  XY=     8.5311   YY=   221.6934   ZY=     1.3603
  XZ=   -63.5502   YZ=     7.6487   ZZ=   299.5162
  Eigenvalues:   151.3175   222.5926   333.2494
15  F    Isotropic =   253.5835   Anisotropy =   140.8428
  XX=   203.5026   YX=    75.5415   ZX=    41.9678
  XY=    54.8996   YY=   285.7053   ZY=    29.7361
  XZ=    31.1181   YZ=    29.8581   ZZ=   271.5426
  Eigenvalues:   164.2571   249.0147   347.4787
16  O    Isotropic =    91.4694   Anisotropy =   216.7576
  XX=    -9.3485   YX=   -69.8495   ZX=     2.0127
  XY=   -57.9450   YY=    47.7995   ZY=    -3.2516
  XZ=     1.0605   YZ=     6.3644   ZZ=   235.9571
  Eigenvalues:   -50.7856    89.2192   235.9745
17  H    Isotropic =    22.8900   Anisotropy =     6.6158
  XX=    27.1040   YX=     1.2900   ZX=    -0.0778
  XY=    -0.2104   YY=    25.8176   ZY=     0.2903
  XZ=    -0.0686   YZ=     0.0694   ZZ=    15.7483
  Eigenvalues:    15.7445    25.6249    27.3005
18  N    Isotropic =   105.0424   Anisotropy =    68.8719 (156.7 ppm vs NH3)
  XX=    96.3660   YX=   -54.6583   ZX=   -19.4645
  XY=   -59.4243   YY=    91.1539   ZY=   -13.7766
  XZ=    -9.4194   YZ=   -12.4349   ZZ=   127.6074
  Eigenvalues:    32.6726   131.4977   150.9570
19  H    Isotropic =    25.3716   Anisotropy =     8.1219
  XX=    30.2273   YX=    -0.7659   ZX=     1.6198
  XY=    -2.0539   YY=    26.0031   ZY=     2.1461
  XZ=     2.3710   YZ=     3.6141   ZZ=    19.8845
  Eigenvalues:    18.2691    27.0596    30.7862
```

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