NMR chemical shift and spin-spin coupling calculation by Gaussian03

Example: B^{11} NMR for BF_4^-, BF_3CN^-, $BF_2CN_2^-$, $BFCN_3^-$, BCN_4^-

1) Optimize the structure of $BF_2CN_2^-$

P B3LYP/6-311+G** SCF=(Tight, MaxCycle=199) Pop=MK Opt=(Tight,GDIIS, Maxcycle=199)

bf2cn2min

-1 1

B	-0.281108	-8.878235	-8.588706
F	0.269686	-7.585737	-8.447505
F	0.501561	-9.659303	-9.466900
C	-0.329405	-9.599356	-7.132849
N	-0.361116	-10.112595	-6.096074
C	-1.788005	-8.753584	-9.185025
N	-2.859956	-8.663638	-9.611815

2) Calculate the NMR properties using the optimized structure and the option below

P B3LYP/6-311+G** SCF=(Tight, MaxCycle=199) Pop=MK NMR=(GIAO, SpinSpin)

3) The results are following. In the case of C13, the isotropic magnetic shielding of CH4(methane) is 199 ppm and that of TMS is 195 ppm. Then the chemical shift is 195(TMS) – 199(CH4) = - 4 ppm. The experimental results are -7 ppm.

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 B Isotropic = 111.8845 Anisotropy = 17.3996

XX= 110.8601 YX= 0.0000 ZX= 0.0000

XY= 0.0000 YY= 101.3091 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 123.4842

Eigenvalues: 101.3091 110.8601 123.4842

2 F Isotropic = 338.0094 Anisotropy = 80.1477

XX= 379.7718 YX= 0.0000 ZX= 11.7205

XY= 0.0000 YY= 276.0073 ZY= 0.0000

XZ= 27.6411 YZ= 0.0000 ZZ= 358.2492

Eigenvalues: 276.0073 346.5798 391.4412

3 F Isotropic = 338.0094 Anisotropy = 80.1477

XX= 379.7718 YX= 0.0000 ZX= -11.7205

XY= 0.0000 YY= 276.0073 ZY= 0.0000

XZ= -27.6411 YZ= 0.0000 ZZ= 358.2492

Eigenvalues: 276.0073 346.5798 391.4412

4 C Isotropic = 47.7357 Anisotropy = 360.9372

XX= 45.7287 YX= 171.3616 ZX= 0.0000

XY= 168.5440 YY= 169.3161 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -71.8378

Eigenvalues: -73.3157 -71.8378 288.3605

5 N Isotropic = -24.8639 Anisotropy = 493.1432

XX= -30.2403 YX= 219.4930 ZX= 0.0000

XY= 236.3706 YY= 148.4151 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -192.7665

Eigenvalues: -192.7665 -185.7234 303.8983

6 C Isotropic = 47.7360 Anisotropy = 360.9366

XX= 45.7293 YX= -171.3614 ZX= 0.0000

XY= -168.5438 YY= 169.3160 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -71.8373

Eigenvalues: -73.3151 -71.8373 288.3604

7 N Isotropic = -24.8630 Anisotropy = 493.1424

XX= -30.2391 YX= -219.4927 ZX= 0.0000

XY= -236.3703 YY= 148.4155 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -192.7654

Eigenvalues: -192.7654 -185.7222 303.8986

The spin-spin coupling and its components such as Fermi Contact (FC) Spin-dipolar (SD), Paramagnetic spin-orbit (PSO), Diamagnetic spin-orbit (DSO) contributions can be calculated by the Gaussian code.

Total nuclear spin-spin coupling J (Hz): B(1)F(2)F(3)C(4)N(5)C(6)N(7)

	1	2	3	4	5
1	**0.000000D+00**				
2	**-0.102371D+03**	0.000000D+00			
3	**-0.102371D+03**	0.120830D+03	0.000000D+00		
4	**0.882216D+02**	0.462624D+02	0.462626D+02	0.000000D+00	
5	**0.154042D+01**	0.324018D+00	0.324002D+00	0.117178D+02	0.000000D+00
6	**0.882215D+02**	0.462625D+02	0.462626D+02	0.134440D+02	0.445445D+00
7	**0.154043D+01**	0.324025D+00	0.324011D+00	0.445443D+00	0.788533D-01

	6	7
6	0.000000D+00	
7	0.117179D+02	0.000000D+00