

SCF GIAO Magnetic shielding
X-Axis: Shift (ppm)
Y-Axis: Degeneracy
Reference: TMS B3LYP/6-31G(d,p) Chloroform
Reference shielding: 192.17 ppm
NMR Degeneracy Tolerance: 0.05

#	X	Y	Degeneracy
4-C	135.1349880457	1.0000000000	1.0000000000
6-C	124.1328622445	1.0000000000	1.0000000000
8-C	123.4151257270	1.0000000000	1.0000000000
9-C	122.9651695894	1.0000000000	2.0000000000
7-C	122.9532464870	2.0000000000	2.0000000000
5-C	118.2680099944	1.0000000000	1.0000000000
2-C	54.0507803829	1.0000000000	1.0000000000
3-C	53.4548396877	1.0000000000	1.0000000000