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# 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

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#
#           X           Y           Degeneracy
5-C      135.3877583707    1.0000000000    1.0000000000
4-C      130.3706000896    1.0000000000    1.0000000000
3-C      126.6664764477    1.0000000000    1.0000000000
1-C      123.7910885224    1.0000000000    1.0000000000
6-C      123.5334104391    1.0000000000    1.0000000000
2-C      121.7441914640    1.0000000000    1.0000000000
8-C       52.8211629530    1.0000000000    1.0000000000
7-C       52.1924433869    1.0000000000    1.0000000000
10-C      30.1802812248    1.0000000000    1.0000000000
9-C       29.0634872612    1.0000000000    1.0000000000

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