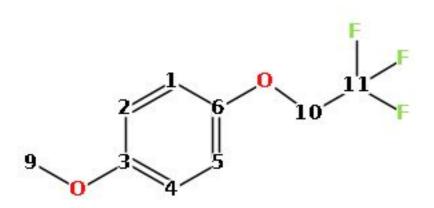
nmrshiftdb2 Quality Report - ¹³C



			Prediction		HOSE
Atom	δ [ppm]	Deviation from prediction	No. Spheres	No. shift values	Code
1	116.2	0.60	4.0	13.0	<u>2D</u>
2	114.7	0.10	5.0	6.0	<u>2D</u>
3	155.0	0.78	6.0	6.0	<u>2D</u>
4	114.7	Symmetric to atom 2	5.0	6.0	<u>2D</u>
5	116.2	Symmetric to atom 1	4.0	13.0	<u>2D</u>
6	151.5	7.16 ⁴	3.0	133.0	<u>2D</u>
9	55.6	0.02	6.0	22.0	<u>2D</u>
10	67.0	4.77 <u></u> 4	2.0	7.0	<u>2D</u>
11	124.0	0.10	3.0	7.0	<u>2D</u>

[D@5ef34cd1

Result: 9/accept

1 yellow shift(s) not taken into account because the underlying prediction was unreliable.

Created Tue Nov 26 17:25:42 CET 2019



 \triangle / \triangle prediction unreliable

Less than 3 spheres used Range > 10 ppm