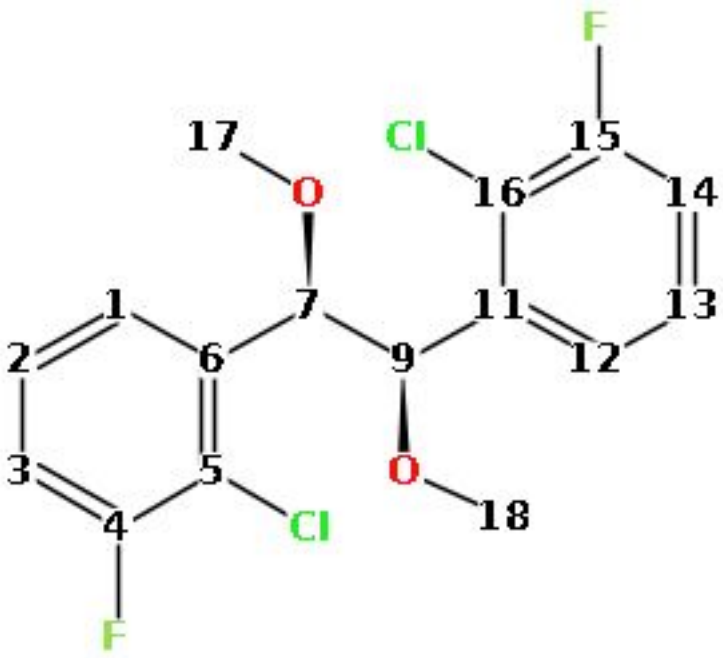
nmrshiftdb2 Quality Report - ^{13}C



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE
			No. Spheres	No. shift values	Code
1	124.9	4.65	3.0	2.0	2D
2	127.3	3.31 [2]	3.0	35.0	2D
3	115.7	0.90	3.0	1.0	2D
4	157.7	1.25	3.0	2.0	2D
5	121.2	1.30 [1]	2.0	2.0	2D
6	138.0	1.30 [1]	2.0	6.0	2D
7	81.0	0.50	3.0	1.0	2D
9	81.0	Symmetric to atom 7	3.0	1.0	2D
11	138.0	Symmetric to atom 6	2.0	6.0	2D
12	124.9	Symmetric to atom 1	3.0	2.0	2D
13	127.3	Symmetric to atom 2	3.0	35.0	2D
14	115.7	Symmetric to atom 3	3.0	1.0	2D
15	157.7	Symmetric to atom 4	3.0	2.0	2D
16	121.2	Symmetric to atom 5	2.0	2.0	2D
17	57.7	0.10	5.0	1.0	2D
18	57.7	Symmetric to atom 17	5.0	1.0	2D

Overall mark 9 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 1.66 ppm → 0.83 Points

No. of red or missing shifts: 0.0 → 0.0 Points

No. of yellow shifts: 0.0 → 0.0 Points

Result: 9/accept

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