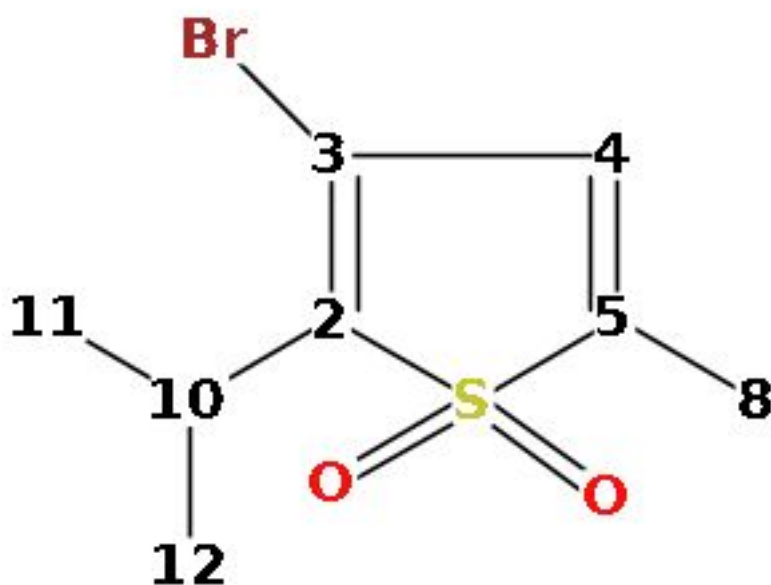


nmrshiftdb2 Quality Report - ^{13}C 

Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
2	143.3	10.91 ^{1, 2}	1.0	61.0	<u>2D</u>
3	119.3	9.92 ^{1, 2}	1.0	42.0	<u>2D</u>
4	126.5	2.87 ^{1, 2}	1.0	1091.0	<u>2D</u>
5	140.6	0.20 ¹	2.0	1.0	<u>2D</u>
8	8.7	5.83 ²	3.0	3.0	<u>3D</u>
10	28.9	6.04 ^{1, 2}	1.0	1717.0	<u>2D</u>
11	19.7	0.03 ^{1, 2}	2.0	2171.0	<u>2D</u>
12	19.7	Symmetric to atom 11	2.0	2171.0	<u>2D</u>

Overall mark 7 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 5.11 ppm \rightarrow 2.56 Points

No. of red or missing shifts: 0.0 \rightarrow 0.0 Points

No. of yellow shifts: 0.0 \rightarrow 0.0 Points

Result: 7/accept

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

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