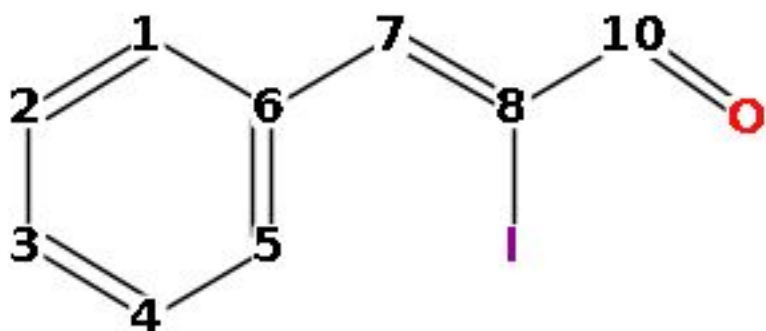


nmrshiftdb2 Quality Report -  $^{13}\text{C}$



Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	130.8	3.34 <sup>2</sup>	3.0	215.0	<u>2D</u>
2	129.0	0.21	4.0	183.0	<u>2D</u>
3	132.9	3.89 <sup>2</sup>	5.0	183.0	<u>2D</u>
4	129.0	Symmetric to atom 2	4.0	183.0	<u>2D</u>
5	130.8	Symmetric to atom 1	3.0	215.0	<u>2D</u>
6	134.5	0.88 <sup>1,2</sup>	2.0	640.0	<u>2D</u>
7	156.2	27.68 <sup>1,2</sup>	1.0	5306.0	<u>2D</u>
8	106.3	6.95 <sup>1,2</sup>	1.0	53.0	<u>2D</u>
10	189.4	1.46 <sup>1,2</sup>	1.0	941.0	<u>2D</u>

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

Mean deviation from prediction: 6.34 ppm  $\rightarrow$  3.17 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

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

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