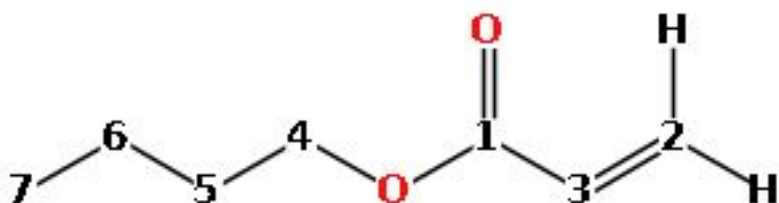


nmrshiftdb2 Quality Report - ^{13}C



| Atom | δ [ppm] | Deviation from prediction | Prediction | | HOSE Code |
|------|----------------|---------------------------|-------------|------------------|-----------|
| | | | No. Spheres | No. shift values | |
| 1 | 165.5 | 0.71 | 5.0 | 3.0 | <u>3D</u> |
| 2 | 129.35 | 1.12 | 6.0 | 3.0 | <u>2D</u> |
| 3 | 127.49 | 1.03 | 6.0 | 3.0 | <u>2D</u> |
| 4 | 63.28 | 1.95 | 3.0 | 24.0 | <u>2D</u> |
| 5 | 29.68 | 0.92 | 4.0 | 14.0 | <u>2D</u> |
| 6 | 18.15 | 0.92 | 5.0 | 14.0 | <u>2D</u> |
| 7 | 12.59 | 1.14 | 6.0 | 14.0 | <u>2D</u> |

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

Mean deviation from prediction: 1.11 ppm \rightarrow 0.56 Points

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

No. of yellow shifts: 0.0 \rightarrow 0.0 Points

Result: 9/accept

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