



Atom number	Shift	Deviation from prediction
1	51.77	0,66
3	51.77	0,66
5	58.33	6,69, prediction not reliable
6	58.33	0,34
7	58.33	6,69, prediction not reliable
8	58.33	0,34
9	170.8	1,56, prediction not reliable
10	170.8	0,70
15	170.8	1,56, prediction not reliable
18	170.8	0,70

Overall mark 4 (out of 1 to 10, 10 being best), recommendation: revision

Mean deviation from prediction: 1,99 ppm -> 0,99 Points

No. of red or missing shifts: 0.0 -> 0.0 Points

No. of yellow shifts: 2.0 -> 5.0 Points

**Result: 4/revision**