



Atom number	Shift	Deviation from prediction
1	56.5	1,13
3	149.9	5,16
4	126.2	3,49
5	123.0	3,11
6	132.5	1,92
7	120.0	1,10
8	145.0	0,47
10	54.7	2,15
11	25.8	1,87
12	130.2	1,16
13	120.9	1,68
14	104.9	1,23
15	147.2	1,81
16	149.3	1,94
18	101.6	0,10
20	107.9	1,32
21	137.0	1,88
22	119.7	4,60
23	143.1	8,47
25	61.4	1,31

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

Mean deviation from prediction: 2,29 ppm -> 1,15 Points

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

No. of yellow shifts: 2.0 -> 5.0 Points

Result: 4/revision