

Supplementary Information: Survey of hyperfine structure measurements in alkali atoms

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(Dated: 8 September 2022)

I. INTRODUCTION

This supplementary information (SI) material to the Allegrini, Arimondo, and Orozco (2022) “Survey of hyperfine structure measurements in alkali atoms” presents a comparison of the weighted error (w.e.) and the weighted enhanced error (w.e.e.) reported in our main text with the values we get by using the cluster maximum likelihood estimator (CMLE) introduced by Rukhin (2009, 2019).

In Sec. IV of the main text we have calculate the weighted average (w.a.) of a data set containing a certain number of entries $m > 1$ and the degrees of freedom $\text{DOF}=m - 1$. We have further calculated the reduced χ_{red}^2 squared (rcs) and the associated standard deviation $\sigma_{\text{rcs}} = \sqrt{2/\text{DOF}}$. Here we focus on the data groups having $\chi_{\text{red}}^2 > 1 + \sigma_{\text{rcs}}$. This inequality implies that the distribution of values for a particular hyperfine constant is not purely random and shows a large data scattering. Following the approach by the Particle Data Group in Zyla *et al.* (2020) and the CODATA group in Tiesinga *et al.* (2021) we treat these discording cases by enhancing the w.e. to w.e.e. by the $(\chi_{\text{red}}^2)^{1/2}$ factor.

Aware of other approaches, we present also an analysis based on the algorithm of Rukhin (2009, 2019) called the cluster maximum likelihood estimator (CMLE). This produces a weighted average (w.a._{CMLE}) and a weighted error (w.e._{CMLE}) not identical to those of the χ_{red}^2 method.

We report a detailed comparison between the two methods for all cases of Allegrini, Arimondo, and Orozco (2022) where a Table recommended value includes a w.e.e. derived from the χ_{red}^2 analysis. The comparison is based on the Δ separation between the output of the two analyses defined as

$$\Delta = \frac{\text{w.a.} - \text{w.a.}_{\text{CMLE}}}{\text{w.e.e.}}. \quad (1)$$

Δ gives the normalized distance in units of w.e.e. between the two ways of evaluating the mean value.

II. COMPARISON RESULTS

The comparison for discording cases is illustrated through figures and tables. In each figure the blue dots represent all available experimental data with their uncertainties (in black), in chronological order from the top as in the main text. On the bottom each figure plots also the w.a. (red triangle) and the w.e.e. (in red) as well as the w.a._{CMLE} (green square) and w.e.e._{CMLE} (in green). All the error bars are symmetric, but to facilitate viewing all of them on a single plot we have truncated one side of the largest one keeping complete the remaining ones. The not-visible errors are smaller than the black, red and green dots.

The table that accompanies each plot reports the χ_{red}^2 , its associated standard deviation σ_{rcs} , and the square root of the χ_{red}^2 that enter in w.e.e. evaluation. We then list the w.a._{CMLE} and w.e._{CLME} for the same data set. Finally, the table includes the Δ normalized separation. All hyperfine constant values are in MHz units.

The following comparison between the recommended values obtained by these two approaches shows that in almost all the 28 cases the weighted average of the two analyses agrees within two times the w.e.e.. There are only two cases with a greater difference, associated with a large $(\chi_{\text{red}}^2)^{1/2}$ value as an indicator of an anomalous scatter of the data. Those are the A constants for ${}^7\text{Li } 2^2P_{1/2}$ in Table I and for ${}^{87}\text{Rb } 5^2P_{1/2}$ in Table XV.

TABLE I. ${}^7\text{Li } 2^2P_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
83.134	0.535	9.118
w.a.	w.e.	w.e.e.
46.005	0.0017	0.016
CMLE method		
w.a. _{CMLE}	w.e. _{CMLE}	
45.943	0.003	
Δ		
3.875		

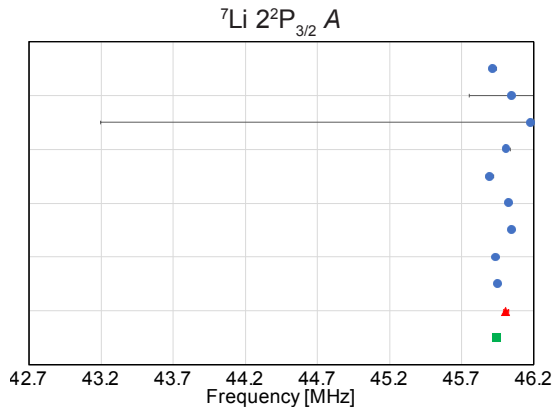


FIG. 1. ${}^7\text{Li } 2^2P_{1/2}$ state: A constant.

TABLE II. ${}^7\text{Li } 3^2P_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
3.911	1	1.977
w.a.	w.e.	w.e.e.
-1.01	0.0012	0.02
CMLE method		
w.a.CMLE	w.e.CMLE	
-1.03	0.002	
Δ		
1.00		

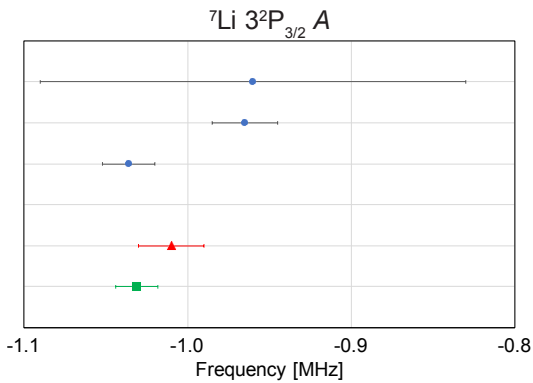


FIG. 2. ${}^7\text{Li } 3^2P_{3/2}$ state: A constant.

TABLE III. ${}^7\text{Li } 3^2P_{3/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
9.632	1.414	3.104
w.a.	w.e.	w.e.e.
-0.081	0.0091	0.028
CMLE method		
w.a.CMLE	w.e.CMLE	
-0.0926	0.0099	
Δ		
0.429		

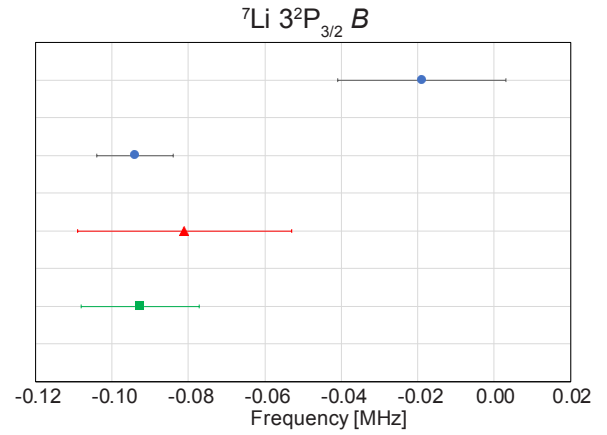


FIG. 3. ${}^7\text{Li } 3^2P_{3/2}$ state: B constant.

TABLE IV. ${}^{23}\text{Na } 3^2P_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
17.432	0.5	4.175
w.a.	w.e.	w.e.e.
94.39	0.006	0.02
CMLE method		
w.a.CMLE	w.e.CMLE	
94.349	0.007	
Δ		
2.00		

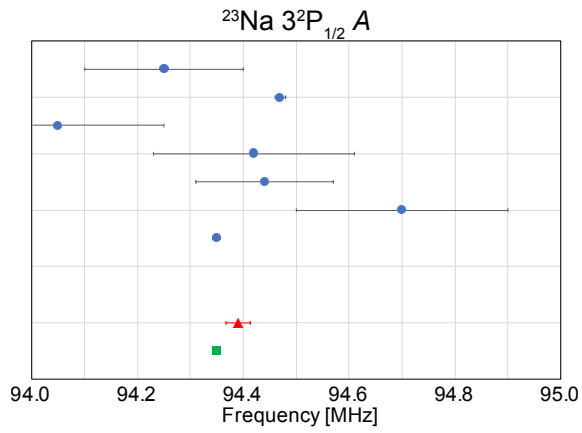


FIG. 4. $^{23}\text{Na } 3^2P_{1/2}$ state: A constant.

TABLE V. $^{23}\text{Na } 3^2P_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
4.375	0.5	2.092
w.a.	w.e.	w.e.e.
18.532	0.003	0.006
CMLE method		
w.a.CMLE	w.e.CMLE	
18.531	0.003	
Δ		
0.167		

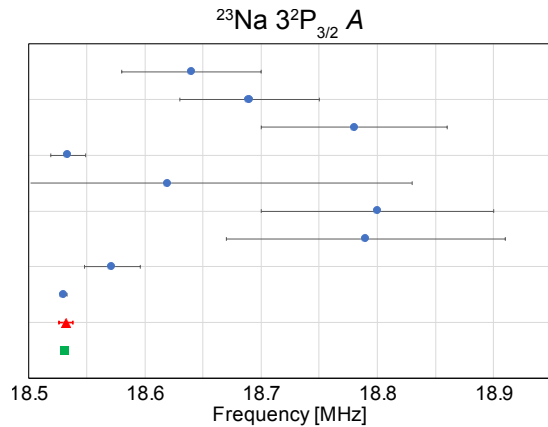


FIG. 5. $^{23}\text{Na } 3^2P_{3/2}$ state: A constant.

TABLE VI. $^{41}\text{K } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
3.453	1.414	1.858
w.a.	w.e.	w.e.e.
7.9	0.67	1.2
CMLE method		
w.a.CMLE	w.e.CMLE	
8.6	0.8	
Δ		
-0.58		

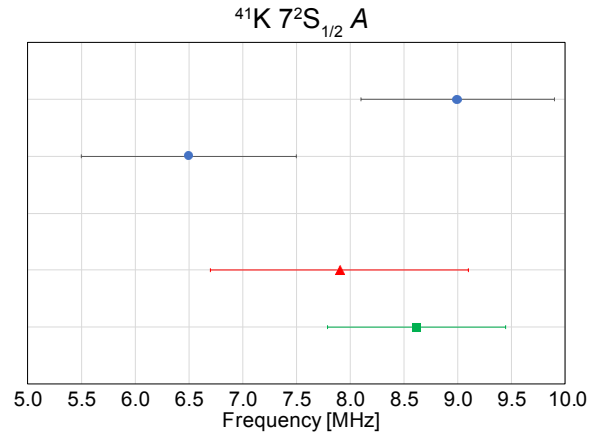


FIG. 6. $^{41}\text{K } 7^2S_{1/2}$ state: A constant.

TABLE VII. $^{85}\text{Rb } 4^2D_{5/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
3.465	0.816	1.861
w.a.	w.e.	w.e.e.
-4.983	0.0037	0.007
CMLE method		
w.a.CMLE	w.e.CMLE	
-4.979	0.0040	
Δ		
-0.571		

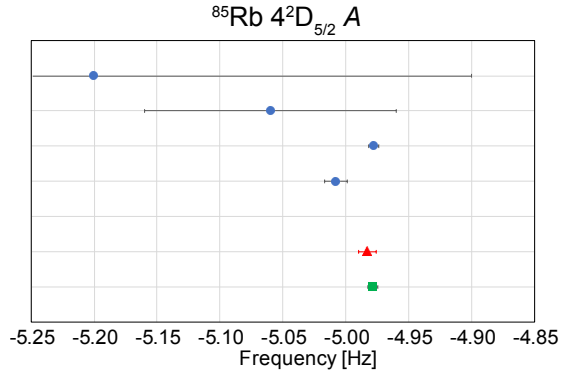


FIG. 7. $^{85}\text{Rb } 4^2D_{5/2}$ state: A constant.

TABLE VIII. $^{85}\text{Rb } 5^2P_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
61.21742	0.707107	7.824156
w.a.	w.e.	w.e.e.
120.605	0.0041	0.029
CMLE method		
w.a.CMLE	w.e.CMLE	
120.644	0.0048	
Δ		
-0.182		

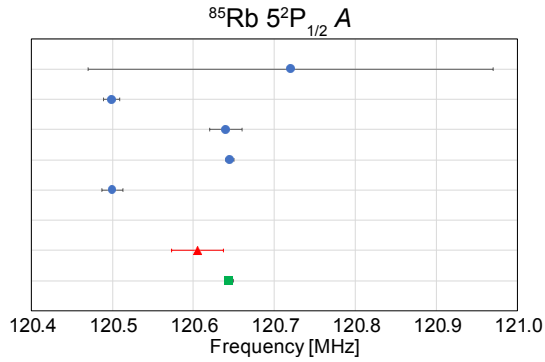


FIG. 8. $^{85}\text{Rb } 5^2P_{1/2}$ state: A constant.

TABLE IX. $^{85}\text{Rb } 5^2P_{3/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
23.756	0.632	4.874
w.a.	w.e.	w.e.e.
26.000	0.0046	0.022
CMLE method		
w.a.CMLE	w.e.CMLE	
26.009	0.005	
Δ		
0.409		

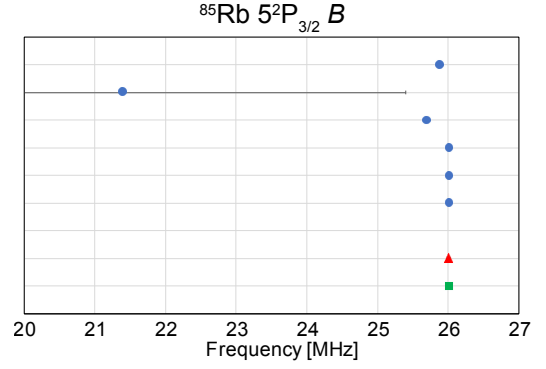


FIG. 9. $^{85}\text{Rb } 5^2P_{3/2}$ state: B constant.

TABLE X. $^{85}\text{Rb } 6^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
7.579	1	2.753
w.a.	w.e.	w.e.e.
239.069	0.0095	0.026
CMLE method		
w.a.CMLE	w.e.CMLE	
239.058	0.0100	
Δ		
0.423		

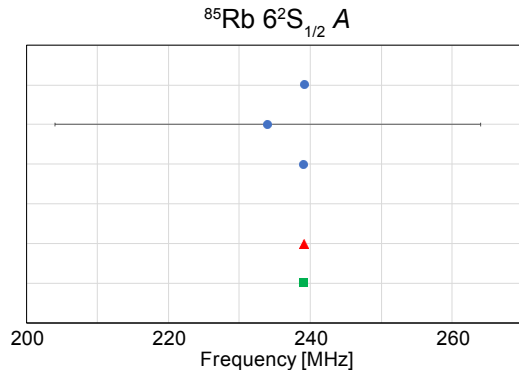


FIG. 10. $^{85}\text{Rb } 6^2S_{1/2}$ state: A constant.

TABLE XI. $^{85}\text{Rb } 7^2D_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
2.949	1	1.717
w.a.	w.e.	w.e.e.
1.35	0.009	0.016
CMLE method		
w.a.CMLE	w.e.CMLE	
1.342	0.010	
Δ		
0.50		

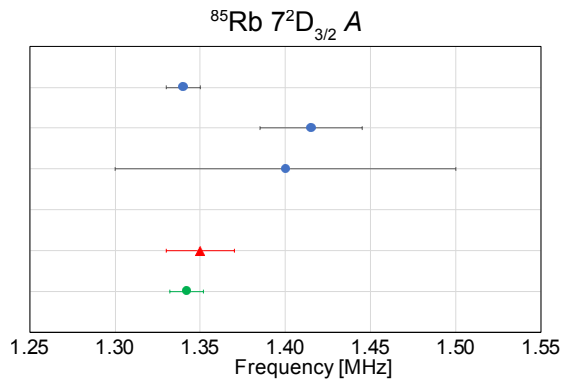


FIG. 11. $^{85}\text{Rb } 7^2D_{3/2}$ state: A constant.

TABLE XII. $^{85}\text{Rb } 8^2D_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
9.274	1.414	3.045
w.a.	w.e.	w.e.e.
0.864	0.0062	0.019
CMLE method		
w.a.CMLE	w.e.CMLE	
0.877	0.008	
Δ		
-0.684		

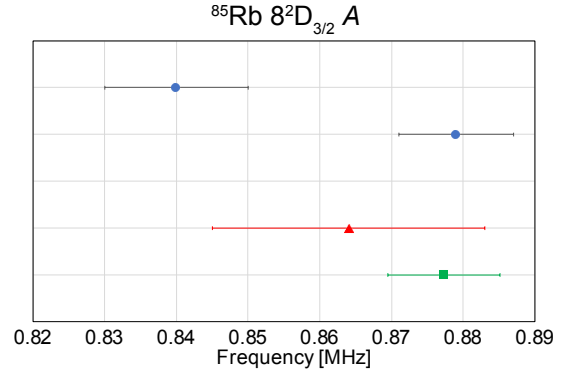


FIG. 12. $^{85}\text{Rb } 8^2D_{3/2}$ state: A constant.

TABLE XIII. $^{87}\text{Rb } 4^2D_{5/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
8.535	0.816	2.921
w.a.	w.e.	w.e.e.
-16.786	0.0036	0.010
CMLE method		
w.a.CMLE	w.e.CMLE	
-16.779	0.006	
Δ		
-0.700		

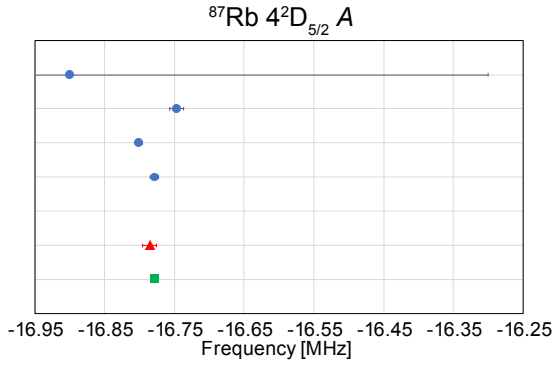


FIG. 13. $^{87}\text{Rb } 4^2D_{5/2}$ state: A constant.

TABLE XIV. $^{87}\text{Rb } 4^2D_{5/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
48.309	1	6.950
w.a.	w.e.	w.e.e.
3.825	0.024	0.165
CMLE method		
w.a.CMLE	w.e.CMLE	
4.13	0.04	
Δ		
-1.94		

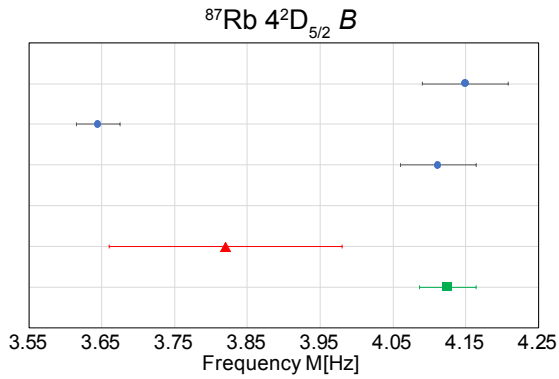


FIG. 14. $^{87}\text{Rb } 4^2D_{5/2}$ state: B constant.

TABLE XV. $^{87}\text{Rb } 5^2P_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
3293.197	0.577	57.386
w.a.	w.e.	w.e.e.
406.48	0.006	0.33
CMLE method		
w.a.CMLE	w.e.CMLE	
408.33	0.014	
Δ		
-5.61		

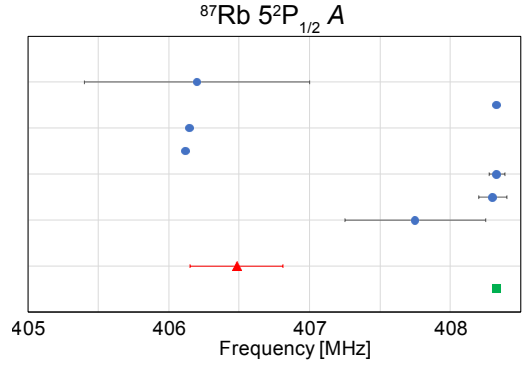


FIG. 15. $^{87}\text{Rb } 5^2P_{1/2}$ state: A constant.

TABLE XVI. $^{87}\text{Rb } 5^2P_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
4.276	0.632	2.068
w.a.	w.e.	w.e.e.
84.720	0.001	0.002
CMLE method		
w.a.CMLE	w.e.CMLE	
84.7193	0.0011	
Δ		
0.5		

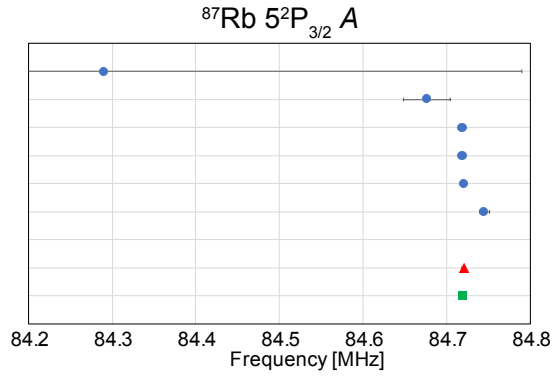


FIG. 16. $^{87}\text{Rb } 5^2P_{3/2}$ state: A constant.

TABLE XVII. $^{87}\text{Rb } 5^2P_{3/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
2.130	0.632	1.456
w.a.	w.e.	w.e.e.
12.497	0.002	0.003
CMLE method		
w.a.CMLE	w.e.CMLE	
12.496	0.002	
Δ		
0.333		

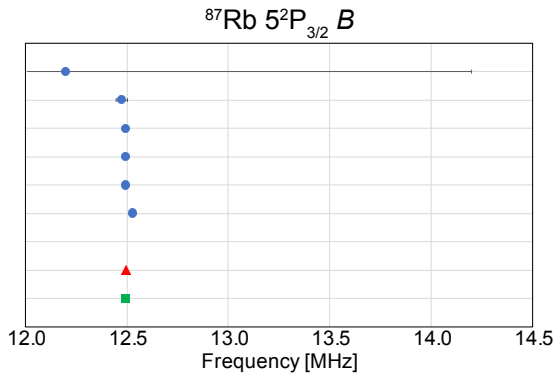


FIG. 17. $^{87}\text{Rb } 5^2P_{3/2}$ state: B constant.

TABLE XVIII. $^{87}\text{Rb } 6^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
7.740	1	2.782
w.a.	w.e.	w.e.e.
807.352	0.015	0.041
CMLE method		
w.a.CMLE	w.e.CMLE	
807.342	0.015	
Δ		
0.25		

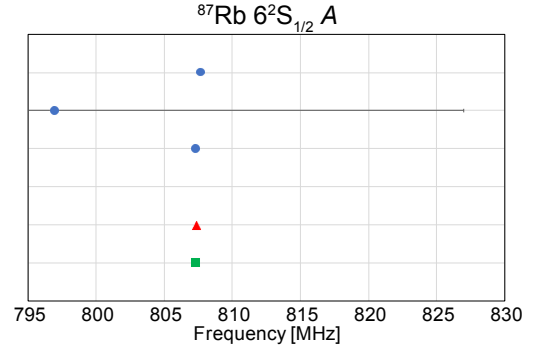


FIG. 18. $^{87}\text{Rb } 6^2S_{1/2}$ state: A constant.

TABLE XIX. $^{133}\text{Cs } 6^2P_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
13.86264	0.53452	3.72326
w.a.	w.e.	w.e.e.
291.9263	0.0007	0.0025
CMLE method		
w.a.CMLE	w.e.CMLE	
291.92969	0.00077	
Δ		
-1.354		

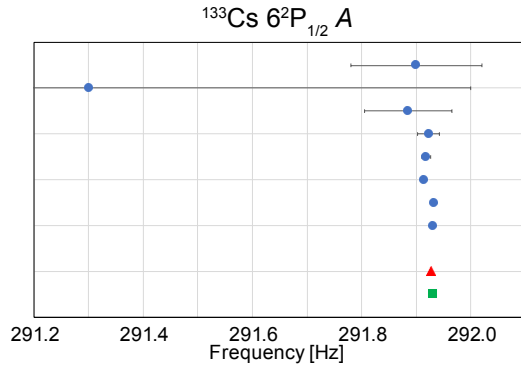


FIG. 19. $^{133}\text{Cs } 6^2P_{1/2}$ state: A constant.

TABLE XX. $^{133}\text{Cs } 6^2P_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
25.593	0.816	5.059
w.a.	w.e.	w.e.e.
50.2878	0.0002	0.0011
CMLE method		
w.a.CMLE	w.e.CMLE	
50.2883	0.00022	
Δ		
-0.4545		

TABLE XXI. $^{133}\text{Cs } 6^2P_{3/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
11.715	0.816	3.423
w.a.	w.e.	w.e.e.
-0.496	0.002	0.006
CMLE method		
w.a.CMLE	w.e.CMLE	
-0.492	0.002	
Δ		
-0.667		

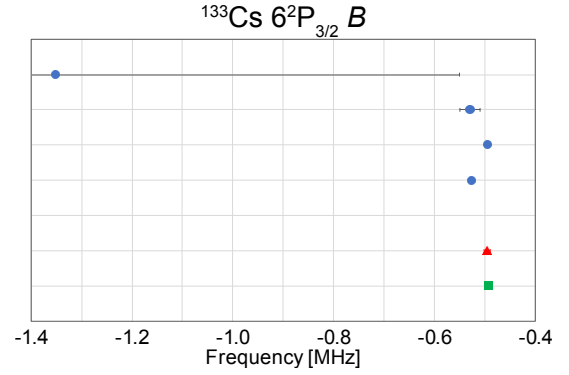


FIG. 21. $^{133}\text{Cs } 6^2P_{3/2}$ state: B constant.

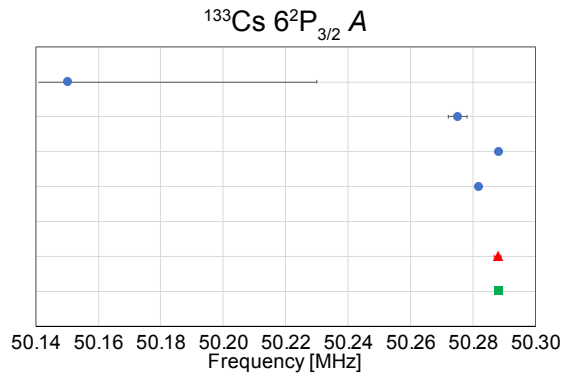


FIG. 20. $^{133}\text{Cs } 6^2P_{3/2}$ state: A constant.

TABLE XXII. $^{133}\text{Cs } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
2.619	0.8165	1.618
w.a.	w.e.	w.e.e.
545.856	0.008	0.014
CMLE method		
w.a.CMLE	w.e.CMLE	
545.868	0.0010	
Δ		
-0.857		

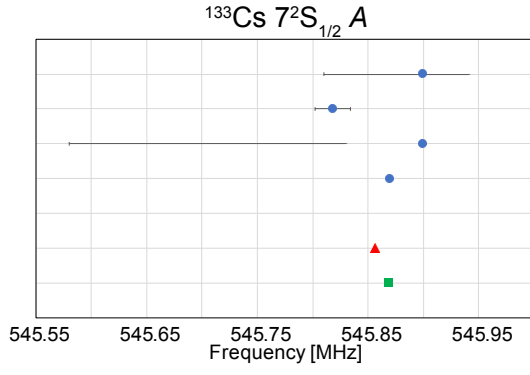


FIG. 22. $^{133}\text{Cs } 7^2S_{1/2}$ state: A constant.

TABLE XXIII. $^{204g}\text{Fr } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
27.268	1.414	5.222
w.a.	w.e.	w.e.e.
13146.6	0.7	3.6
CMLE method		
w.a.CMLE	w.e.CMLE	
13146.7	0.7	
Δ		
-0.0		

TABLE XXIV. $^{206g}\text{Fr } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
7.396	1.414	2.720
w.a.	w.e.	w.e.e.
13056.5	0.87	2.4
CMLE method		
w.a.CMLE	w.e.CMLE	
13057.6	1.0	
Δ		
-0.5		

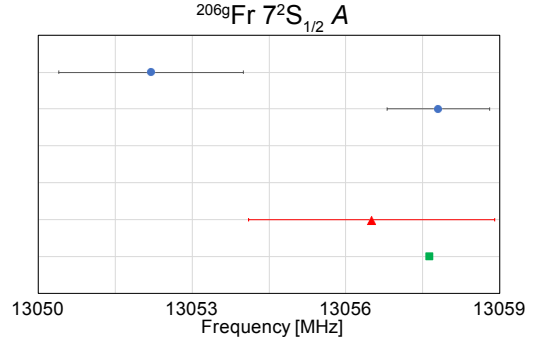


FIG. 24. $^{206g}\text{Fr } 7^2S_{1/2}$ state: A constant.

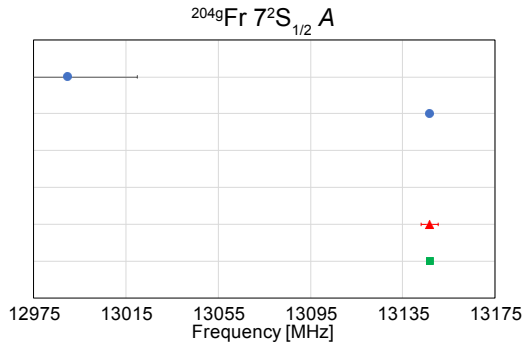


FIG. 23. $^{204g}\text{Fr } 7^2S_{1/2}$ state: A constant.

TABLE XXV. $^{208g}\text{Fr } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
7.452	1	2.730
w.a.	w.e.	w.e.e.
6653.1	0.36	1.0
CMLE method		
w.a.CMLE	w.e.CMLE	
6653.6	0.4	
Δ		
-0.5		

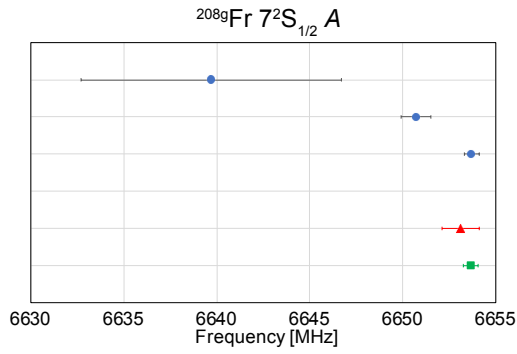


FIG. 25. $^{208g}\text{Fr } 7^2S_{1/2}$ state: A constant.

TABLE XXVII. $^{221g}\text{Fr } 7^2S_{1/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
4.464	0.632	2.113
w.a.	w.e.	w.e.e.
6207.2	0.505	1.1
CMLE method		
w.a.CMLE		w.e.CMLE
6209.2		0.7
Δ		
-1.9		

TABLE XXVI. $^{212g}\text{Fr } 7^2P_{3/2}$ state: A constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
2.215	1	1.488
w.a.	w.e.	w.e.e.
97.21	0.0705	0.10
CMLE method		
w.a.CMLE		w.e.CMLE
97.20		0.07
Δ		
-0.0		

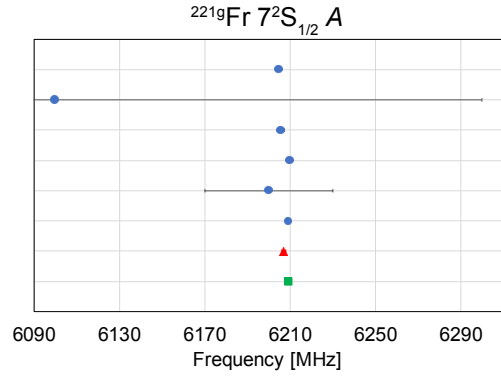


FIG. 27. $^{221g}\text{Fr } 7^2S_{1/2}$ state: A constant.

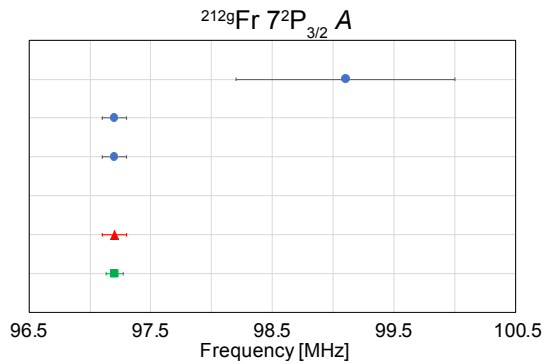


FIG. 26. $^{212g}\text{Fr } 7^2P_{3/2}$ state: A constant.

TABLE XXVIII. $^{221g}\text{Fr } 8^2P_{3/2}$ state: B constant

χ^2 method		
χ_{red}^2	σ_{rcs}	$(\chi_{\text{red}}^2)^{1/2}$
2.485294	1.414214	1.576482
w.a.	w.e.	w.e.e.
-86.9	0.19	0.3
CMLE method		
w.a.CMLE		w.e.CMLE
-86.9685		0.1976
Δ		
0.228		

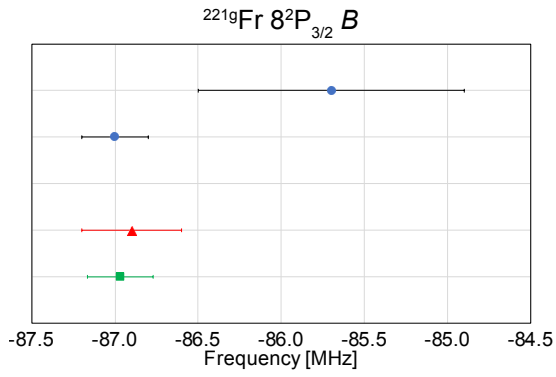


FIG. 28. $^{221g}\text{Fr } 8^2P_{3/2}$ state: B constant.

III. ACKNOWLEDGMENTS

The authors are indebted to the referee for providing the Excel algorithm of the CMLE approach.

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