

Features of the Zeeman splitting and g-factors of $2p5f$ configuration levels of carbon atom

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Abstract: The gyromagnetic ratios of levels (the g-factors) – are one of the most important characteristics of atoms. There are no corresponding experimental data in the literature for $npn'l$ configurations of carbon atom. That is why the theoretical study of the fine and the Zeeman structures for the determination of the g-factors is ongoing. All the calculations are effected in one configuration approximation, with the energy operator matrix, in which the maximum possible number of interactions is taken into account, including the magnetic, spin-orbit (own and other) and spin-spin interactions. The fine structures were studied in three approximations (LS , LK , JK) for the establishment of the character of the coupling in $2p5f$ C I configuration. During the study of Zeeman splitting (except the g-factors) features of it were determined: the fields of crossings and anticrossings of magnetic components. In all steps of calculations the numerical digitalization of corresponding energy operator matrices were effected, e.g. the results presented in the paper were obtain in the intermediate coupling approximation.

Keywords: Fine Structure, Zeeman Splitting, Crossings and Anticrossings of Magnetic Components, G-Factors, Energy Operator Matrix

1. Introduction

For all $2pnl$ C I configurations, including $l = 3$, there are no experimental data except the fine structure energy levels. For this reason, it is possible to precise semiempirical calculations of the fine structure parameters, with numerical diagonalization of the energy operator matrix in the absence of a magnetic field, and taking into account the interaction of the atom with the magnetic field. It seems of interest to determine the Lande factors from the calculated Zeeman pattern. This is possible if, in the absence of magnetic field, upon diagonalization of the matrix of the energy operator separated with respect to quantum number J (J is the total electron angular momentum of the atom), the obtained energy levels are almost coincide with corresponding experimental quantities (zero energy residuals). For the considered $2p5f$ configuration of C I this was reached, which will be confirmed

below by corresponding figures and tables.

2. Fine Structure

The fine structure of higher excited $2p4f$ and $2p5f$ C I configurations were studied in detail in our work [1]. The experimental energies are taken from [2], where they are measured with accuracy of 0.001 cm^{-1} . The classification of levels in [2] is given in the JK -coupling. There are also experimental energies in [3]. Their accuracy is 0.01 cm^{-1} , and the classification of levels is given in the LK -coupling. The authors [2] and [3] differ in assessing the closeness of the systems considered to JK or LK types of coupling. Our calculation of fine structure parameters in [1] were executed with energies taken from [2] in the JK -coupling approximation. Further the numerical values of fine structure parameters (see [1]) were introduced in the energy operator matrices, written in the LK and LS types of coupling approximation with further

level is total, it is quasi-total for 3D_2 . One can consider that these levels are nearest to jK -coupling, as the calculation of fine structure parameters is effected in the jK -coupling approximation. If all the configuration levels were nearest to jK -coupling, then there must be coincidence of g_{LS} , g_{LK} , g_{JK} as for the 1G_4 level in the Table 1. From the Table 1 it is seen that this is not the case. That is why the g-factors of the rest of the levels, coinciding in two bases, are compared with their vector counterparts. One obtains the following: the 3F_3 and 1D_2 levels are nearest to LS -coupling; 1F_3 , 3G_3 , 3F_4 , 3G_4 levels are near to jK -coupling; 3D_3 level is near to LK -coupling; 3F_2 level is approximately in the middle of the LK and jK -couplings.

Thus the majority of the levels of 2p5f configuration lie close to the jK -coupling. The classification in [2] is confirmed by the doublet structure of the energy spectrum in the Fig.1.

3. Zeeman Splitting and it's Particularities

The magnetic field totally erases the degeneracy of levels due to the quantum number M [7]. The energy operator matrix is labeled with M for the following values: $M = \pm 5$ (first rank); $M = \pm 4$ (fourth rank); $M = \pm 3$ (eighth rank); $M = \pm 2$ (eleventh rank); $M = \pm 1$ and $M = 0$ (twelfth rank). In the numerical experiment, all the cited matrices were diagonalized when the magnetic field varied from zero to 62 kOe.

The energy operator matrix for the $n p n' f$ configurations in the absence of the field was published in the works [8-12]. The coefficients of radial integrals (fine structure parameters) are calculated in two representations: $LSJM$ (LS -coupling approximation) and in the independent moments approximation in order to exclude possible errors. In the matrix the following interactions were taken into account: electrostatic, spin-orbit (own and other), spin-spin, orbit-orbit, which are represented by 18 radial integrals. The numerical values of fine structure parameters can be seen in [1].

To calculate the Zeeman splitting in the fundamental energy operator matrix from [8-12], elements of energy operator matrix of interaction of the atom with the magnetic field are added. The results are published in [5] for all the cited upper values of M . The Zeeman structure was calculated with the energy operator matrix in the LS -coupling approximation. In this approximation it is more compact as compared to the many matrices in the non-coupling moments representation.

Table 2. The fields of the crossing of Zeeman components with $\Delta M = \pm 1, \pm 2$ in the range $H = 0 - 62$ kOe.

№	The crossing sublevels		H, Oe	№	The crossing sublevels		H, Oe
	Upper	Lower			Upper	Lower	
1	$^3G_5 (M = -2)$	$^1G_4 (M = -4)$	266.44	37	$^3D_2 (M = -1)$	$^3D_1 (M = 1)$	3777.942
2	$^3G_5 (M = -1)$	$^1G_4 (M = -3)$	282.55	38	$^3G_4 (M = -3)$	$^3G_3 (M = -2)$	3945.23
3	$^3G_5 (M = 0)$	$^1G_4 (M = -2)$	316.627	39	$^3F_4 (M = -2)$	$^1F_3 (M = -1)$	4155.77
4	$^3G_5 (M = 1)$	$^1G_4 (M = -1)$	345.642	40	$^1D_2 (M = -1)$	$^3D_3 (M = 0)$	5379.17
5	$^3G_5 (M = 3)$	$^1G_4 (M = 1)$	398.44	41	$^3G_4 (M = -2)$	$^3G_3 (M = -1)$	6269.47
6	$^3G_5 (M = 4)$	$^1G_4 (M = 2)$	448.72	42	$^3F_4 (M = -1)$	$^1F_3 (M = 0)$	7393.77
7	$^3F_2 (M = 1)$	$^3F_3 (M = 3)$	736.97	43	$^3G_4 (M = -1)$	$^3G_3 (M = 0)$	13387.2
8	$^3F_2 (M = 0)$	$^3F_3 (M = 2)$	919.215	44	$^3F_4 (M = 0)$	$^1F_3 (M = 1)$	16146.62
9	$^1D_2 (M = 1)$	$^3D_3 (M = 3)$	998.58	45	$^3F_4 (M = -4)$	$^3F_2 (M = -2)$	17944.28
10	$^3F_2 (M = 2)$	$^3F_3 (M = 3)$	1089.45	46	$^1F_3 (M = -3)$	$^3F_2 (M = -1)$	18392.091
11	$^1D_2 (M = 0)$	$^3D_3 (M = 2)$	1153.298	47	$^1F_3 (M = -2)$	$^3F_2 (M = 0)$	18820.231
12	$^3F_2 (M = -1)$	$^3F_3 (M = 1)$	1157.779	48	$^1F_3 (M = -1)$	$^3F_2 (M = 1)$	19242.028
13	$^1D_2 (M = -1)$	$^3D_3 (M = 1)$	1334.829	49	$^1F_3 (M = 0)$	$^3F_2 (M = 2)$	19653.551
14	$^1D_2 (M = 2)$	$^3D_3 (M = 3)$	1403.93	50	$^1F_3 (M = 1)$	$^3F_3 (M = 3)$	20059.62
15	$^3F_2 (M = -2)$	$^3F_3 (M = 0)$	1453.241	51	$^3F_4 (M = -3)$	$^3F_2 (M = -1)$	25533.8
16	$^1D_2 (M = -2)$	$^3D_3 (M = 0)$	1542.691	52	$^1F_3 (M = -3)$	$^3F_2 (M = -2)$	26601.64
17	$^3F_4 (M = -3)$	$^1F_3 (M = -1)$	1544.09	53	$^3F_4 (M = -2)$	$^3F_2 (M = 0)$	27069.411
18	$^3G_5 (M = 3)$	$^3G_4 (M = 2)$	1559.65	54	$^1F_3 (M = -2)$	$^3F_2 (M = -1)$	27713.96
19	$^3G_5 (M = 2)$	$^1G_4 (M = 1)$	1560.21	55	$^3F_4 (M = -4)$	$^3F_3 (M = -2)$	28029.52
20	$^3G_5 (M = 4)$	$^1G_4 (M = 3)$	1650.93	56	$^3F_4 (M = -1)$	$^3F_2 (M = 1)$	28621.461
21	$^3F_4 (M = -2)$	$^1F_3 (M = 0)$	1765.643	57	$^1F_3 (M = -1)$	$^3F_2 (M = 0)$	28772.43
22	$^3G_4 (M = -4)$	$^3G_3 (M = -2)$	1896.89	58	$^1F_3 (M = -3)$	$^3F_3 (M = -1)$	29224.634
23	$^3F_4 (M = -1)$	$^1F_3 (M = 1)$	2026.208	59	$^1F_3 (M = 0)$	$^3F_2 (M = 1)$	29738.99
24	$^3F_4 (M = -4)$	$^1F_3 (M = -3)$	2045.19	60	$^1F_3 (M = -2)$	$^3F_3 (M = 0)$	30165.902
25	$^3G_4 (M = -3)$	$^3G_3 (M = -1)$	2166.68	61	$^3F_4 (M = 0)$	$^3F_2 (M = 2)$	30169.305
26	$^1D_2 (M = 1)$	$^3D_3 (M = 2)$	2203.53	62	$^1F_3 (M = 1)$	$^3F_2 (M = 2)$	30600.9
27	$^3F_4 (M = 0)$	$^1F_3 (M = 2)$	2328.976	63	$^1F_3 (M = -1)$	$^3F_3 (M = 1)$	30842.604
28	$^3G_4 (M = -2)$	$^3G_3 (M = 0)$	2486.016	64	$^1F_3 (M = 0)$	$^3F_3 (M = 2)$	31176.379
29	$^3F_4 (M = 1)$	$^1F_3 (M = 3)$	2676.22	65	$^1F_3 (M = 2)$	$^3F_3 (M = 3)$	31360.94
30	$^3F_4 (M = -3)$	$^1F_3 (M = -2)$	2765.09	66	$^3F_4 (M = 1)$	$^3F_3 (M = 3)$	31705.65
31	$^3G_4 (M = -4)$	$^3G_3 (M = -3)$	2855.91	67	$^3F_4 (M = -3)$	$^3F_2 (M = -2)$	46529.71
32	$^3G_4 (M = -1)$	$^3G_3 (M = 1)$	2860.29	68	$^3F_4 (M = -4)$	$^3F_3 (M = -3)$	51690.18
33	$^3D_2 (M = -2)$	$^3D_1 (M = -1)$	3013.9	69	$^3F_4 (M = -2)$	$^3F_2 (M = -1)$	53669.27
34	$^3G_4 (M = 0)$	$^3G_3 (M = 2)$	3290.421	70	$^3F_4 (M = -3)$	$^3F_3 (M = -1)$	55535.76
35	$^1D_2 (M = 0)$	$^3D_3 (M = 1)$	3378.59	71	$^3F_4 (M = -1)$	$^3F_2 (M = 0)$	61835.15
36	$^3G_4 (M = 1)$	$^3G_3 (M = 3)$	3774.32				

Table 3. Minimal energy intervals and corresponding values of the magnetic fields in the anticrossing “necks” magnetic components with $\Delta M = 0$

The anticrossing sublevels		H, Oe	$\Delta E, \text{cm}^{-1}$
Upper	Lower		
$^1F_3 (M=0)$	$^3F_2 (M=0)$	66605 ± 5	0.11821
$^1F_3 (M=1)$	$^3F_2 (M=1)$	70050 ± 50	0.19252
$^1F_3 (M=-1)$	$^3F_2 (M=-1)$	61035 ± 15	0.06489
$^1F_3 (M=2)$	$^3F_2 (M=2)$	70905 ± 5	0.29085
$^1F_3 (M=-2)$	$^3F_2 (M=-2)$	54550 ± 10	0.0286

In the studied range of the magnetic field (0 - 62 kOe) 71 crossings of Zeeman components with $\Delta M = \pm 1, \pm 2$ and 5 anti-crossing with $\Delta M = 0$ were detected. The crossing of sublevels and their corresponding values of the magnetic field are presented in the Table 2.

From the Table 2 it is seen that, the crossings of magnetic

components of levels of $2p5f$ configuration start with comparatively smaller magnetic fields (a hundred Oest). As the crossings are many, the general view of Zeeman splitting is not shown. Let's pay attention to the anticrossings. They are represented on the Fig. 2. The most narrow anticrossings with $M = -1$ and $M = -2$ in increasing order are shown on the Fig. 3.

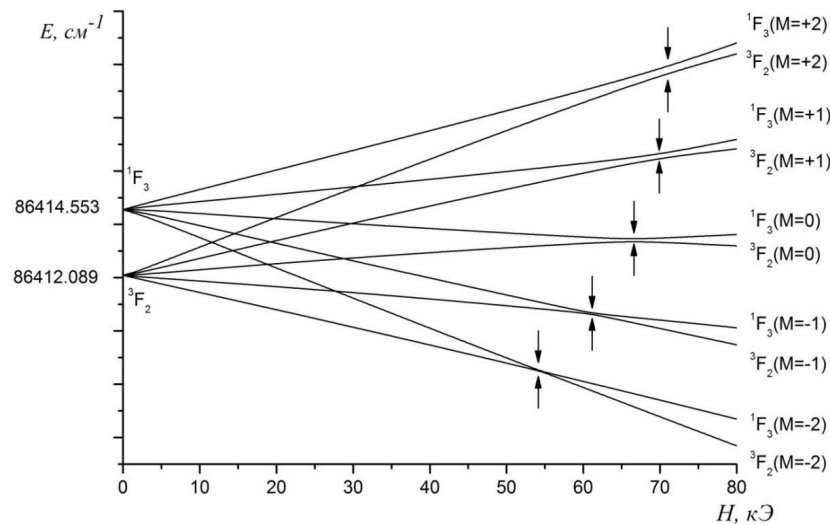
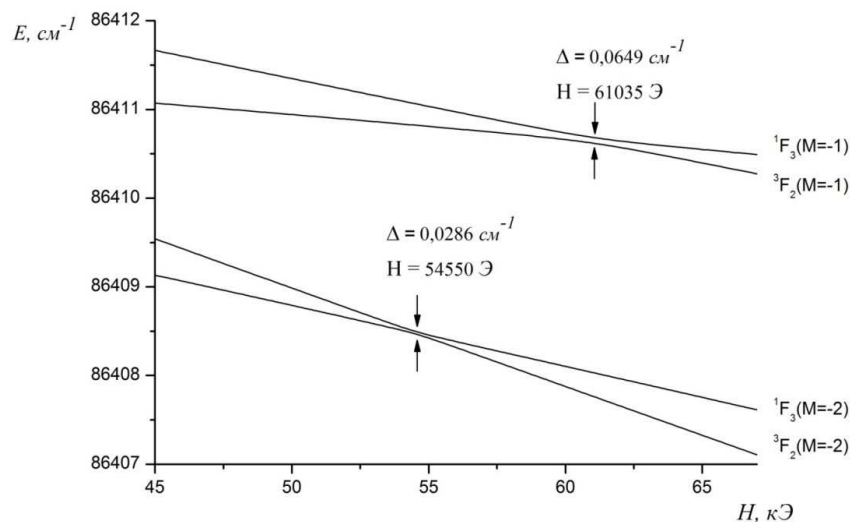
**Figure 2.** Anticrossings of magnetic components with $\Delta M=0$ of the 1F_3 and 3F_2 levels of the $2p5f$ configuration of C I.**Figure 3.** Fragment of the Zeeman pattern in the range of anticrossing of magnetic components with $M = 0$.

Table 3 shows the minimum energy intervals in the anticrossing “necks” and the corresponding values of the magnetic fields. This error defines the area of the magnetic field, where the curves $E(H)$ are parallel.

As is known, anticrossings are experienced by sublevels

from different terms. Figure 2, 3, and Table 3 show that in the LS -coupling approximation, 1F_3 and 3F_2 – the terms are different. In the JK -coupling,

$$\frac{1}{2} \begin{bmatrix} 7 \\ 2 \end{bmatrix}_3 \text{ and } \frac{1}{2} \begin{bmatrix} 5 \\ 2 \end{bmatrix}_2$$

the terms are different also, as they have different intermediate moments K . The anticrossing from different terms is observed also in series of Helium atom configurations (see for example, [6]).

4. The Gyromagnetic Ratios

The gyromagnetic ratios can be calculated from Zeeman splitting only in a linear range, in which the spacing between the positive and negative values of M with respect to $M = 0$ is the same. Our calculation of g-factors are executed with the field $H = 40$ Oe. The demonstration of the linearity is presented in the Table 4. To this effect in the given point of the magnetic field the diagonalization of the energy operator matrix is done for the values $M = 0$, $M = +1$, $M = -1$. As a result the energies of Zeeman components are obtained when

Table 4. The energies of Zeeman components with $M = 0, \pm 1$ and the gyromagnetic ratios of levels of the 2p5f C I configuration when $H = 40$ Oe

Levels	$M = 0$	$M = +1$	$M = -1$	g-factors
3F_3	86412.004	86412.007	86412.002	1.11931 (1.11936)
3F_2	86412.089	86412.090	86412.088	0.76972 (0.76967)
1F_3	86414.553	86414.555	86414.552	0.88777 (0.88776)
3F_4	86414.723	86414.725	86414.721	1.13187 (1.13187)
3G_3	86469.520	86469.522	86469.518	0.89714 (0.89713)
3G_4	86469.760	86469.762	86469.758	1.14671 (1.14672)
3D_3	86482.680	86482.682	86482.678	1.26279 (1.26280)
1D_2	86482.808	86482.810	86482.806	0.96902 (0.96900)
1G_4	86487.976	86487.978	86487.974	1.02222 (1.02211)
3G_5	86488.009	86488.011	86488.007	1.20035 (1.20046) ^{LS}
3D_1	86498.540	86498.541	86498.539	0.49886 (0.49884) ^{LS}
3D_2	86498.745	86498.747	86498.743	1.09426 (1.09427)

From Table 4 it is seen that, the g-factors, calculated when $H = 40$ Oe, with accuracy 0.001 totally coincide with g_{LS} from the Table 1 (the intermediate coupling with respect to the diagonalization of the energy operator matrix in the LS-coupling approximation). The distinctions are seen in the fourth or in the fifth decimal place. That is why in the brackets of the last column of Table 4, the g-factors are presented (in the absence of the field in the LS basis) with an accuracy of 0.00001. The same is extended also to 3G_5 , 3D_1 levels. Their g-factors coincide with analogous LS-couplings (g^{LS}) only with a 0.001 accuracy. The insignificant deviation from the LS-coupling is remarkable when the accuracy is great.

Thus, for the 2p5f configuration of carbon atom the magnetic field in the linear range does not bring important changes in the calculation of values of g-factors in comparison with similar values in absence of the field with accuracy of 0.001. In other words for the carbon atom the energy of interaction with the magnetic field is small as compared to the rest of the interactions, in particular with the electrostatic interaction and the spin-own orbit interaction ($\xi_p = 42$ cm⁻¹ [1]). With the increase of nuclear charge (for example, the 3p5f Si I configuration [5]) the role of the magnetic field increases a bit. Namely, the divergence of g-factors of 3G_5 , 3D_1 levels, with respect to Zeeman splitting and the corresponding vector analogues to (g^{LS} in Table 1) are observed in the third decimal place. It is due to the fact that, for the atom of silicon $\xi_p \approx 190$ cm⁻¹ [1], that means 4 times greater as compared to carbon.

$H = 40$ Oe and coefficients of expansion of the wave functions with respect to LS-coupling basis (coefficients of intermediate coupling). It is seen that, the distances $\Delta E (M = +1) - (M = 0)$ cm⁻¹ and $\Delta E (M = -1) - (M = 0)$ cm⁻¹ are perfectly the same for all levels of the configuration.

The coefficients of intermediate coupling were used in the calculation of the g-factors when $H = 40$ Oe (see the method of calculation in [6]). The gyromagnetic ratios with accuracy 0.00001 are presented in the last column of Table 4. For comparison, in brackets, the g-factors with the same accuracy are indicated, calculated in the absence of the magnetic field (see Table 2 paragraph 2 in this work). In contrast to the Table 1, where the results of 10 levels of configuration are presented, in Table 4 we have all the 12 levels, including 3G_5 and 3D_1 with the unit value of the quantum number J .

Further let's consider, what will happen to Germanium atom.

The constant of spin-orbit splitting (spin-own orbit) $\xi_p = 1178$ cm⁻¹ (4p4f Ge I) and $\xi_p = 1176.9$ cm⁻¹ (4p5f Ge I) [1]. That means for germanium the magnetic interaction is sensibly 28 times greater as compared to carbon and 6 times greater as compared to silicon. The significant increase of the role of magnetic interactions for germanium was the cause of strong deviation from LS-coupling [1].

5. Conclusions

The Zeeman splitting and its features are determined for 12 levels 2p5f configuration of carbon atom. For this purpose the numerical diagonalization of energy operator matrices for all values of quantum number M in the range of the magnetic field from zero to 62 kOe was effected. In the established linear range when $H = 40$ Oe the energy of Zeeman sublevels and the coefficients of expansion of wave functions with respect to the LS-coupling basis were calculated, and later used for the calculation of the g-factors. A comparative analysis of the g-factors in the sense of splitting with similar values in the absence of the field (the fine structure) was done. The character of the coupling in the 2p5f configuration was established. It was shown that, the majority of levels of configuration are really near the jK -coupling in accordance with the experimental work [2].

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