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LANDÉ FACTORS MEASUREMENTS IN THE B ³Σ_u⁻ STATE OF ⁸⁰Se₂

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Résumé. — Nous avons mesuré les facteurs de Landé de plusieurs niveaux de l'état B ³Σ_u⁻ de ⁸⁰Se₂ excités par laser. Les résultats sont en assez bon accord avec les valeurs théoriques et les déterminations de structure fine récemment publiées.

Abstract. — We have measured Landé factors in several laser excited levels of the B ³Σ_u⁻ state of ⁸⁰Se₂. The results are in reasonably good agreement with recently published theoretical values and fine structure determinations.

In a previous paper [1] we have used the technique of the resonances in a modulated light beam [2] to measure the Landé factor of the B 1_u, v' = 0, J' = 105 level of ⁸⁰Se₂ excited by the 4 727 Å line from an Ar⁺ laser. We have now extended these measurements to several other laser excited levels of ⁸⁰Se₂. The experimental set up is described in [1]. The Landé factors are given in table I together with the identification of the excited levels.

TABLE I

Laser line	v', J'	10 ³ .g _J
5 145 Å	B 1 _u , 0, 94 F ₃	+ (8.0 ± 0.8)
4 965 Å	B 0 _u ⁺ , 0, 131 F ₁	- (8.5 ± 0.8)
4 880 Å	B 1 _u , 1, 39 F ₃	+ (7.4 ± 0.7)
4 765 Å	B 1 _u , 0, 16 F ₂	- (6.9 ± 0.7)
4 727 Å	B 1 _u , 0, 105 F ₃	+ (8.2 ± 0.5)

The signs of the Landé factors have been obtained by the use of dispersion shaped Hanle effect curves [3]. The B state of Se₂ is known to be near a Hund's case ³Σ state [4]. However, as already remarked in [1] the experimental Landé factors cannot be explained by the expression

$$g_{\Omega,J} = - \frac{2 \Omega^2}{J(J+1)}$$

valid for a pure case of a ³Σ state. A striking example of this is that, in this case, g_J(B 0_u⁺) should be zero. In fact Buchler and Meschi [5] (hereafter referred as B. M.) have shown that the rotation of the molecule mixes the Ω = 0 and Ω = 1 states of the same parity

(called respectively F₁ and F₃), the Ω = 1 state of opposite parity (F₂) remaining unaffected. This process is in fact a transition from Hund's coupling case a) to case b) which causes large variations of the Landé factor values. However B. M. have treated the F₁ ↔ F₃ interaction only to 2nd order in perturbation theory. It is worthwhile here to quote the results of the exact diagonalization of the 2 × 2 Hamiltonian. If we define

$$\text{tg } \theta = \frac{2 B [J(J+1)]^{1/2}}{\lambda - B}$$

where B ≈ 7 × 10⁻² cm⁻¹ is the rotational constant of the molecular state and λ ≈ 37.5 cm⁻¹ the recently published value [6] of the Ω-splitting constant in the B state.

Then the appropriate wavefunctions become

$$\begin{cases} |F_3\rangle = \cos \theta/2 \, |\Omega = 1^+\rangle - \sin \theta/2 \, |\Omega = 0^+\rangle \\ |F_2\rangle = |\Omega = 1^-\rangle \\ |F_1\rangle = \sin \theta/2 \, |\Omega = 1^+\rangle + \cos \theta/2 \, |\Omega = 0^+\rangle. \end{cases}$$

Using these *perturbed* wavefunctions the Landé factors may easily be calculated to be :

$$\begin{cases} g_1 = -2 \left\{ \frac{\sin^2 \theta/2}{J(J+1)} + \frac{2 \sin \theta/2 \cos \theta/2}{[J(J+1)]^{1/2}} \right\} \\ g_2 = -2 [J(J+1)]^{-1} \\ g_3 = -2 \left\{ \frac{\cos^2 \theta/2}{J(J+1)} - \frac{2 \sin \theta/2 \cos \theta/2}{[J(J+1)]^{1/2}} \right\}. \end{cases}$$

If g > 0 the molecular magnetic moment is parallel to J.
If g < 0 the molecular magnetic moment is anti-parallel to J.

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The B. M. treatment corresponds to the approximation $\theta \simeq \tan \theta$, and is valid only for small values of θ , that is for small J values. In fact for the B state of Se_2 $\theta = \pi/4$ for $J \simeq 260$. Therefore for J values of about 100 as observed, there are small deviations between the B. M. and the exact calculation (10 % for the g_1 and g_3 values). Note incidentally that the exact theory allows one to find the case b) g_J values in the limit of very high J ($\theta \rightarrow \pi/2$). The B. M. and exact g_J values are plotted against J on figure 1 together with the positions of the experimental points. The agreement between experiment and theory is within 10 to 20 %. This should be considered as a first important step in the understanding of the g factors. Let us just point out some probable causes of deviation from the present theory.

i) The $\text{B } ^3\Sigma_u^-$ state of Se_2 is not in fact a pure triplet $S = 1$ state ; it contains a small admixture of $S = 0$ Σ and Π states. This is the well known origin of the important fine structure splitting $2\lambda \simeq 75 \text{ cm}^{-1}$. This singlet-triplet mixing certainly causes changes in the g values.

ii) The $\text{B } ^3\Sigma_u^-$ state is also known to be locally perturbed even in the $v = 0$ and 1 vibrational levels by other electronic states [7]. This in turn may cause local variations of the g values close to the crossing points.

To investigate these questions further we need systematic measurements of g values as functions of v , and J in the B state of Se_2 . Such a study is now under way in our laboratory using a pulsed dye laser excitation.

FIG. 1. — Theoretical and experimental Landé factors : — exact diagonalization, ●●● Buchler and Meschi, ♦ experimental points.

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