MARCH 1, 1933 PHYSICAL REVIEW VOLUME 43

LETTERS TO THE EDITOR

Prompt publication of brief reports of important discoveries in physics may be secured by addressing them to this department. Closing dates for this department are, for the first issue of the month, the twentieth of the preceding month; for the second issue, the fifth of the month. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents.

The *C* State of Li_2

Some time ago[1] the writer called attention to the fact that a simple Heitler-London calculation makes the known $^1\Pi S^N$ state[2] of Li_2 repulsive, in qualitative disagreement with experiment. A later calculation showed that the modified method proposed by Slater,[3] which takes account of the influence of the corresponding polar state, gives just the same results as the ordinary Heitler-London treatment.

Thus it appears that the mutual polarization of the two atoms, neglected in the simple Heitler-London calculation, is of decisive importance, and that the inclusion of the polar wave functions does not account for any appreciable part of this influence. The direct description of the polarization given by Rosen[4] for the ground state of H_2 is instructive; but this procedure is not available in other problems, since it does not take account of the effects of inner electrons. The correct modification in the general case has been indicated by Eisenschitz and London.[5] One must use as wave function a linear combination of the original Heitler-London wave function with similar functions for other molecular states. The program of successive approximations given by Eisenschitz and London is not well suited to actual calculation, as is illustrated by their very poor results for the ground state of H_2. Slater[6] has pointed out that the best way to get accurate results in practice is to treat the problem as if it were degenerate and obtain the energy from a secular equation.

A good example of a successful application of this procedure is provided by the work of Ireland[7] on the BeH molecule. In the case of the ground state of BeH the inclusion of the influence of a single higher state sufficed to change complete disagreement with experiment into good qualitative agreement. Thus though the simple Heitler-London method itself fails in this case, a modification which does not unduly increase the labor involved gives good results.

In the present note the writer wishes to call attention to the fact that such a result cannot be obtained in the case of the *C* state of Li_2. In Table I are listed some of the atomic configurations which can give rise to $^1\Pi S^N$ states of Li_2. It is seen that there are a number of higher states whose influences should be of the same sort and which are about the same distance from the *C* state, and that there are an infinite number less than twice as far away as the nearest. Thus to give a correct account of the influence of polarization one would have both to calculate the influences of a considerable number of states and to show that the influence of states lying still higher is negligible.

Table I.

Configuration	Energy (in Rh)	Distance above $2\,^2S+2\,^2P$
$2\,^2S+2\,^2P$	−0.657	0.000
$2\,^2P+2\,^2P$	−0.521	0.136
$2\,^2S+3\,^2P$	−0.511	0.146
$2\,^2S+3\,^2D$	−0.508	0.149
$2\,^2S+4\,^2P$	−0.461	0.196
$2\,^2S+4\,^2D$	−0.459	0.198
$2\,^2S+4\,^2F$	−0.459	0.198
$\lim_{n\to\infty} [2\,^2S+n\,^2(P, D, F, \cdots)]$	−0.396	0.261

The influence of the $^1\Pi S^N$ state arising from the $2\,^2P+2\,^2P$ configuration is probably somewhat smaller than those of the states next above it, but its influence can be calculated much more readily. The calculation shows that the *C* state, at the distance at which the experimental curve has its minimum, is pushed down by roughly one-tenth the amount required to make it agree with experiment. This is a reasonable share of the effect for this state to have, if one supposes that a considerable number of higher states also play an appreciable part.

There is no reason to suppose that this is a very exceptional case. We are led to the conclusion that the Heitler-London method, which has great value as a general approach to valence problems, is likely even in very simple cases to fail to give us any feasible way to explain quantitatively the position of a state. The reliability of general rules based on first order Heitler-London studies seems to be in part a mysterious coincidence.

An alternative way of attack is to use two-center functions, as Hylleraas[8] did for H_2. This has been attempted for the *C* state of Li_2. The motion of the π electron, being nearly hydrogenic, presents no difficulty; but for the σ

---

[1] W. H. Furry, Phys. Rev. **39**, 1015L (1932).

[2] Named by Mulliken, Rev. Mod. Phys. **4**, 1 (1932), the *C* state.

[3] J. C. Slater, Phys. Rev. **35**, 509 (1930).

[4] N. Rosen, Phys. Rev. **38**, 2099 (1931).

[5] R. Eisenschitz and F. London, Zeits. f. Physik **60**, 491 (1930).

[6] J. C. Slater, Phys. Rev. **38**, 1109 (1931).

[7] C. E. Ireland, Phys. Rev. **43**, 329 (1933).

[8] E. A. Hylleraas, Zeits. f. Physik **71**, 739 (1931).

electron the effect of the K-shells cannot be neglected even in first approximation, and an attempt to use a variation method here leads to integrals whose numerical tabulation is not feasible.

The difficulties in the diatomic fixed-nuclei problem come from the necessity of taking into account both the effect of inner electrons and that of polarization. The use of atomic wave functions, characteristic of the simple Heitler-London method and its modifications, gives a ready account of the effects of inner electrons, at the expense of introducing complications when the effect of polarization is important. The procedure then required is clearly defined by the work of Eisenschitz and London and in this note we have seen an example of what an unpleasant situation will sometimes result. In the two-center method the original assumption disposes of the effect of polarization, and we are left with the problem of dealing with the effects of the inner electrons, which, except in H_2, are always important. This problem would seem to deserve more attention than it has received so far, since its solution might provide a method of treating valence problems which could give satisfactory results where the atomic-function method cannot.

WENDELL H. FURRY

University of California,
December 28, 1932.

Lack of Observed Hyperfine Structure in the Al III Line, 5722.6A

Tolansky[1] has reported attempts to obtain the hyperfine structure of lines of Al III with a Fabry-Perot etalon, using a high potential discharge in a liquid air cooled hollow cathode lamp. Because of broadening of the fringes by reason of Stark effect, negative results were obtained.

Recently we have attempted to obtain the hyperfine structure of the Al III line at 5722.6A, given by the transition $4s^2S_{\frac{1}{2}}-4p^2P_{\frac{1}{2}}$. Use was made of a Fabry-Perot etalon and a Shüler lamp with a spark gap in series. In order to excite the lines with sufficient intensity to photograph them, it was necessary to run the cathode at a temperature near the melting point of aluminum. Etalon separations of 1, 3, 5, 8, and 12 mm were used. Visual observation of the various photographed interference patterns failed to reveal any evidence of structure. Microphotometer records show that the fringes are very symmetrical and are quite broad, having a half-width of 0.10A; in fact the Doppler broadening of the fringes is such that high resolutions cannot be obtained. A careful study of the small irregularities on the records led to the conclusion that they are due entirely to plate grain. The symmetrical shape of the curves indicate either that there is no structure to the line at all, or that the structure consists of two very close unresolved components of approximately equal intensity or several still closer components. The vapor-pressure of aluminum is so low that it is impossible to excite Al III lines without at the same time introducing other effects which make the determination of the hyperfine structure very difficult.

ROBLEY C. WILLIAMS
GEORGE B. SABINE

Department of Physics,
Cornell University,
February 1, 1933.

---

[1] S. Tolansky, Zeits. f. Physik **74**, 336–43 (1932).

Emission of γ-rays by Nuclei Excited by Neutrons, and Nuclear Energy Levels

TABLE I. *Amount of energy (in 10^6 electron-volts) which disappears in the reaction and is presumably converted into γ-rays.*

	N^{14}	$+\ n^1 \rightarrow$	$N^{15} \rightarrow$	$B^{11} + He^4$	
1.	1.4	(*HA*)	1.4 (*FB*)	1.3 (*FC*)	
2a.	2.3	(*HA*)	2.0 (*FB*)	2.0 (*FB*)	2.3 (*FC*)
	2.8	(*FA*)	2.5 (*FC*)		
3.	3.8	(*FA*)	3.8 (*FA*)	3.9 (*FB*)	
4.	5.0	(*FC*)	5.8 (*FC*)		

Neutrons seem to be remarkably efficient in the excitation of atomic nuclei with which they unite. When nitrogen, by the impact of a neutron is converted into boron and helium, mass is lost (energy equivalent to 1.4 million electron-volts), if Aston's mass values are entirely correct. In the disintegrations with capture of the neutron which have thus far been investigated, kinetic energy has either been conserved, or a part of it has disappeared and presumably has been transformed into γ-rays.

While examining half a dozen photographs of the disintegration of nitrogen obtained by Gans, Newson and the writer, two remarkably good (*A*) photographs were found which represent capture of the neutron. These are marked (*HA*) in Table I, where they are compared with results from three of the best photographs obtained by Feather (*FA*), together with four (*FB*) from slightly imperfect, and five less perfect (*FC*) photographs.

If the rest masses alone of N^{14} and n^1 are considered the rest mass of the newly formed N^{15} is 15.0147 ± 0.004, which undoubtedly represents an excited state of this nucleus. In addition there has been 0.002 or more mass units of kinetic energy to dispose of in the cases which have thus far been investigated. The excess energy is presumably emitted as a γ-ray.

A possible explanation of the constancy of the lowest value, 1.4×10^6 electron-volt as found in the table, is that this value is due to this amount of error in Aston's mass values. Obviously the error may be in any or all of the four masses involved.

On the basis of the last paragraph the amount of energy which is converted into γ-rays in the disintegration process would be as shown in Table II which also strongly suggests differences between definite energy levels.