

THEORETICAL OSCILLATOR STRENGTH FOR THE NI  $2p^23s(^4P)-2p^3(^4S)$  TRANSITION\*

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A measurement of the oscillator strength for the  $2p^23s(^4P)-2p^3(^4S)$  transition of atomic nitrogen has recently been reported by Fairchild and Clark.<sup>1</sup> Since the rather small result of  $1.2 \times 10^{-4}$  differs by three orders of magnitude with a previous estimate made by one of us,<sup>2</sup> a more thorough theoretical investigation has been performed. In the course of computing the Planck mean absorption coefficient for atomic nitrogen, as reported in reference 2, the value of 0.12 was obtained for the total  $f$  number of the above multiplet transition. Accordingly, the  $f$  numbers for the three components corresponding to the states of  $2p^23s(^4P)$  having  $J = \frac{1}{2}, \frac{3}{2},$  and  $\frac{5}{2}$  would be 0.02, 0.04, and 0.06, respectively. This result was obtained by means of the Bates-Damgaard Coulomb approximation<sup>3</sup> as supplemented by the work of Burgess and Seaton.<sup>4</sup>

Although considerable uncertainty<sup>5</sup> in this  $f$ -number estimate is to be expected for a transition of this type (involving equivalent electrons in one state), our experience in comparing values so computed for OI  $2p^4-2p^33s$  transitions with values obtained from analytical Hartree-Fock wave functions indicates that the uncertainty is of the order of a factor of two or less, not several orders of magnitude. We have now calculated an  $f$  number for this nitrogen transition from analytical Hartree-Fock wave functions. The result of 0.10 for the total  $f$  number obtained by this means confirms the Coulomb approximation result within the expected uncertainty, and should provide a more reliable value. This is particularly true for this transition, as cancellation of positive and negative contributions to the radial integral is not severe. The ratio of positive to negative areas is about 7 to 1.

The wave functions used for the  $1s^22s^22p^3(^4S)$  and  $1s^22s^22p^23s(^4P)$  states of neutral nitrogen were obtained by our using computer programs designed by C. C. J. Roothaan and his co-workers.<sup>6</sup> The

programs are based on the expansion method for self-consistent-field solutions to the wave equation. Our wave functions represent exact solutions to the restricted Hartree-Fock equations to at least three figures, possibly more.

It is interesting to note that, although  $2p-3d$  transition  $f$  numbers are usually larger than those for the  $2p-3s$  transitions (as noted by Fairchild and Clark), this is not the case (at least for Coulomb approximation values) for any of the  $2p^3-2p^23s$  and  $2p^32p^23d$  transitions of NI, all of which were computed in performing the work of reference 2. The  $2p-3s$  values obtained were all equal to or greater than the  $2p-3d$  values.

To avoid ambiguities in the choice of average or total  $f$  numbers, it is desirable to note that the radial dipole integral factor,<sup>3</sup>  $\sigma^2$ , obtained by the Coulomb approximation was 0.16, and the value we have obtained by means of analytical SCF functions is 0.12. These values yield the  $f$  numbers quoted above.

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<sup>1</sup>C. E. Fairchild and K. C. Clark, Phys. Rev. Letters **9**, 100 (1962).

<sup>2</sup>B. H. Armstrong *et al.*, J. Quant. Spectry. Radiative Transfer **1**, 143 (1961).

<sup>3</sup>D. R. Bates and A. Damgaard, Phil. Trans. Roy. Soc. London **A242**, 101 (1949).

<sup>4</sup>A. Burgess and M. J. Seaton, Monthly Notices Roy. Astron. Soc. **120**, 121 (1960).

<sup>5</sup>Part of the uncertainty in the Coulomb approximation relates to the choice of one-electron energy parameter. The choice of the experimental ionization potential to the  $^3P$  parent yields the result quoted. The choice of the Hartree-Fock one-electron orbital energy lowers the value to  $f=0.09$ , which brings the Coulomb approximation result into closer agreement with the Hartree-Fock result.

<sup>6</sup>C. C. J. Roothaan and P. Bagus (to be published).