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Wavefunctions and pseudopotential for sodium atoms*

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In a recent paper[1] we reported the wave functions and pseudopotential for the 2*s*, 2*p*, 3*s* and 3*p* states of Li. In the present paper we extend the same method to the 3*s*, 3*p*, and 3*d* states of Na. The outer electron is assumed to move in the pseudopotential

$$V(r)=(-\epsilon^2/r)\{10e^{-r/\alpha}[1+(r/2\alpha)]+1\}, \qquad (1)$$

and the Schroedinger equation is solved numerically for this potential with α adjusted[2] to give the correct energy for the 3*s* state. Retaining this value of α, the Schroedinger equation was again solved numerically for the excited states. The energies so found were labelled ϵ_{num}, and are compared with spectroscopic values ϵ_{sp} in Table I. Analytical functions were accurately fitted to the numerical solutions, and the radial functions are given below:

$$R_{3s}(r)=0.702244(r-0.961)[\exp(-0.71r)-14(0.34-r)\exp(-3.6r)],$$

$$R_{3p}(r)=0.148743r[25.4\exp(-3.8r)-\exp(-0.44r)],$$

$$R_{3d}(r)=0.00907928r^2\exp(-0.334r).$$

Plots of these functions are available from the authors. These functions are nearly exact solutions of the radial Schroedinger equation with the potential given in Eq. (1). They should be useful in atomic scattering calculations involving Na.

TABLE I. Comparison of energy levels of Na (ϵ_{sp}=spectroscopic, ϵ_{num}=by numerical solution of the Schroedinger equation with the pseudopotential, ϵ_{an}=variation energy of analytical fit)—atomic units.

State	ϵ_{sp}	ϵ_{num}	ϵ_{an}
3*s*	−0.1889	−0.1889	−0.1867
3*p*	−0.1116	−0.1141	−0.1115
3*d*	−0.0559	−0.0556	−0.0556

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[1] D. Rapp and C. Chang, J. Chem. Phys. 57, 4283 (1972).

[2] α was found to be 0.278196.

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EPR study of the photochemical reaction of hypofluorites with compounds of tetravalent sulfur. II. Thionyl fluoride and sulfur dioxide*

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The high reactivity of alkoxy radicals makes them particularly valuable reagents for the generation of paramagnetic entities for EPR studies. Hydrogen abstraction is the principal mode of reaction of these radicals in many instances,[1] but there are now a few established cases of adduct formation with certain acceptor molecules.[2,3] Such intermediates are important in the reaction of, for example, SF_4 with certain peroxides.[4] During the course of our investigation of this reaction we discovered that in many instances hypofluorites were more useful sources of alkoxy radicals than were the corresponding peroxides. Aside from the practical advantages of lower freezing points and higher extinction coefficients than peroxides, hypofluorites are also photochemical sources of both alkoxy radicals and fluorine atoms, so that hypofluorite photolysis often results in both RO and F attack on the host molecule, with a corresponding increase in the information provided by the EPR spectrum.

As a logical extension of our experiments[4] with SF_4, we chose to explore the reactions of RO and F radicals with OSF_2 and SO_2. This has enabled us to establish