Reprinted from:

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 58, NUMBER 6 15 MARCH 1973

Wavefunctions and pseudopotential for sodium atoms*

Donald Rapp and Chi-Ming Chang

The University of Texas at Dallas, Dallas, Texas 75230

(Received 20 November 1972)

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

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

and the Schroedinger equation is solved numerically for this potential with α adjusted[2] to give the correct energy for the $3s$ 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}
$3s$	−0.1889	−0.1889	−0.1867
$3p$	−0.1116	−0.1141	−0.1115
$3d$	−0.0559	−0.0556	−0.0556

* Partial support under Grant AT-464 from the Robert A. Welch Foundation is gratefully acknowledged.

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

[2] α was found to be 0.278196.