SCF TREATMENT OF HIGHER EXCITED STATES OF ATOMS. TRANSITION PROBABILITIES BETWEEN EXCITED STATES OF PIII

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A non-relativistic SCF method for higher excited states of atoms has been developed with orthogonality conditions for states of the same symmetry. The modification of the steepest descent method, based on the pair mixing idea of Rossi, was adpated for several states of PIII. With the help of this method the energies of some *s* and *p* states were determined.

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1. Introduction

The method described in [1] was used to calculate the energies and wave functions for some excited states of PIII. With the help of these wave functions the oscillator strenghts and lifetimes for some states were calculated.

2. Results and discussion

In Table I the calculated and observed [2] excited state energies are compared. There are the energies of excitation relative to the ground state. The agreement of the presented results with experiment is comparable with one in paper [1].

Table II and Table III contain the oscillator strenghts (in dipole moment and dipole velocity approximation) and appropriate lifetimes. The calculated values of oscillator strenghts are compared, where possible with the semiempirical method reported by Migdałek [3].

Except for one case, there are no experimental data with which to compare. The agreement in that single case is good. There is also good agreement with the semiempirical results of [3].

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TABLE I

Values of energy of excitation for PIII in a.u.

Energy level	Our result	Ch. Moore
3*p*	0.0	0.0
4*p*	0.646	0.645
5*p*	0.841	0.875
6*p*	0.931	—
4*s*	0.540	0.540
5*s*	0.797	0.804
6*s*	0.909	0.918
7*s*	0.968	—

TABLE II

Oscillator strenghts for PIII

Transition	$g_{nl} f_{nln'l'}$	
	Our result $\frac{\text{dipole moment}}{\text{dipole velocity}}$	Other result (see Ref.)
3*p*—4*s*	$\frac{0.595}{0.602}$	0.612 [3]
3*p*—5*s*	$\frac{0.0949}{0.0984}$	0.979 [3]
3*p*—6*s*	$\frac{0.0349}{0.0377}$	0.0358 [3]
4*p*—5*s*	$\frac{1.281}{1.182}$	1.260 [3]
4*p*—6*s*	$\frac{0.177}{0.160}$	0.175 [3]
5*p*—6*s*	$\frac{1.931}{1.830}$	
4*s*—4*p*	$\frac{2.558}{2.126}$	2.496 [3] 2.370 [4] 2.340 [5]
4*s*—5*p*	$\frac{0.0055}{0.0144}$	
5*s*—5*p*	$\frac{3.270}{3.042}$	

TABLE III

Lifetimes for PIII

Level	$\tau_{nl} \times 10^{-9}$ sec	
	Our result $\frac{\text{dipole moment}}{\text{dipole velocity}}$	Other result (see Ref.)
$4p$	$\frac{2.146}{2.550}$	3.1±0.1 [6] 2.8±0.2 [7] 3.2±0.2 [8]
$5p$	$\frac{9.341}{8.846}$	
$4s$	$\frac{0.359}{0.355}$	
$5s$	$\frac{0.695}{0.695}$	
$6s$	$\frac{1.240}{1.226}$	

The calculated lifetime for the $4s$ state lies between two experimental results.

In other cases, neither theoretical nor experimental values exist with which one can compare. In all these cases the present work gives a first estimation of the appropriate oscillator strenghts and lifetimes.

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