Transition probabilities of forbidden lines in Bi I

Paweł Syty, Józef E. Sienkiewicz
Faculty of Applied Physics and Mathematics, Technical University of Gdańsk
ul. Narutowicza 11/12, 80-952 Gdańsk, Poland

Jerzy Kwela Institute of Experimental Physics, University of Gdańsk ul. Wita Stwosza 57, 80-952 Gdańsk, Poland

Introduction

Decay rates calculated for strong transitions are in reasonable agreement with experiment, but in the case of weak transitions the predictions often strongly disagree with the experimental data. It results from the fact that weak transition rates are especially sensitive to even small modifications to the wave functions and a careful choice of the theoretical method to be used is required.

Our work

In our calculations the code GRASP92 has been used. It implements the Multiconfiguration Dirac-Fock Method (MCDF). Using this program we have calculated transition amplitudes for the magnetic dipole (M1) forbidden transitions within the ground $6s^26p^3$ configuration of neutral bismuth. Moreover, to check the accuracy of the method, we calculated the energies for all five levels of the configuration $6s^26p^3$.

Energies of the low-lying states of bismuth (in cm⁻¹)

		Experiment ^a	MBPT ^b	CI°	This work
Odd	⁴ S ^o _{3/2}	0	0	0	0
	$^{2}D_{3/2}^{\circ}$	11 419.0	11 672	11 521	11 550
	² D° _{5/2}	15 437.7	15 593	15 969	15 867
	${}^{2}P^{o}_{1/2}$	21 661.0	21 806	22 222	22 321
	${}^{2}P^{o}_{3/2}$	33 164.8	33 337	33 185	33 180
Even	⁴ P _{1/2}	32 588.2	-	32 823	32 800
	⁴ P _{3/2}	44 865.1	-	44 418	44 873
	$^{2}P_{1/2}$	45 915.6	-	45 814	46 013
	⁴ P _{5/2}	48 498.9	-	48 940	48 676
	² P _{3/2}	49 456.6	-	49 599	49 612

^a Moore (1958)

Calculations

- CSF including single and double excitations from the reference configurations (6s²6p³, 6p⁵).
- Inclusion of the core polarisation effect (excitations from the inner 5p and 5d shells).
- Generation of atomic wave functions including Breit interactions.
- Calculation of transition properties using GRASP92.

References

V. A. Dzuba et al, Phys. Lett. 141A (1989) 147

M. J. D. Macpherson et al, J. Physique II 2, (1992) 749

M. G. Kozlov et al, J. Phys. B 29 (1996) 689

C. E. Moore, Atomic Energy Levels 3, NBS Circular No 467 (1954)

S. J. Rose et al, J. Phys. B 11 (1978) 3499

F. A. Parpia et al, Comput. Phys. Commun. 94 (1996) 249

M1 transition amplitudes for the states of configuration 6s² 6p³

Transition	⁴ S ^o _{3/2} - ² D ^o _{3/2}	⁴ S ^o _{3/2} - ² D ^o _{5/2}	⁴ S ^o _{3/2} - ² P ^o _{1/2}	Х
Wavelength	876 nm	648 nm	462 nm	
Experiment ^a	-	-	-	8.75
MBPT ^b	1.747	0.615	0.625	8.07
MBPT ^c	1.696	0.563	0.590	9.06
CI ^d	1.618	0.510	0.573	10.07
This work	1.603	0.523	0.598	9.39

^a Macpherson *et al.* (1992), X is the squared ratio of the first and second amplitudes

^b Dzuba et al (1989)

^c Kozlov *et al* (1996), 354 relativistic configurations

 $^{^{\}rm b}$ Dzuba $\it et\,al\,$ (1989), second order in the residual e-e interaction

^c Dzuba *et al* (1989), semi-empirical higher order corrections

^d Kozlov et al (1996), 354 relativistic configurations