Multiconfiguration Dirac-Hartree-Fock calculations of EDM for Ra, Hg, Yb

2014 J. Phys.: Conf. Ser. 488 122001

(http://iopscience.iop.org/1742-6596/488/12/122001)

Multiconfiguration Dirac-Hartree-Fock calculations of EDM for Ra, Hg, Yb

Gediminas Gaigalas,[†1] **Jacek Bieroń,**[*] **Laima Radžiūtė**[†]

[†] Vilnius University, Institute of Theoretical Physics and Astronomy, A. Goštauto 12, Vilnius, Lithuania
[*] Uniwersytet Jagielloński, Instytut Fizyki imienia Mariana Smoluchowskiego, Kraków, Poland

Synopsis Using multiconfiguration Dirac-Hartree-Fock (MCDHF) method, we calculated the atomic electric dipole moment (EDM) for Ra, Hg, Yb, arising from nuclear Schiff moment, (P,T)-odd electron-nucleon interactions, and interaction of electron EDM with nuclear electromagnetic field.

Atomic EDM for Ra, Hg, Yb were calculated using recently developed program in the framework of GRASP2K [1]. EDM may be induced by tensor-pseudotensor, scalar-pseudoscalar e-N (P,T)-odd interactions, nuclear Schiff moment, and the electron EDM. All three elements are diamagnetic with closed outer s shell (Ra $6p^6 7s^2$, Hg $5d^{10} 6s^2$, Yb $4f^{14} 6s^2$). As an example we present the Schiff moment of ^{199}Hg. This interaction is the dominant nuclear contribution to the EDM of diamagnetic atoms. Table 1 presents results calculated with theoretical as well as experimental values of transition energies [2], and compared with d_{at}^{SM} values calculated with other methods: DHF and RPA.

Table 1. The values d_{at}^{SM} for ^{199}Hg in units $\{10^{-17}[S/(|e|\,\mathrm{fm}^3)]\,|e|\,\mathrm{cm}\}$.

Virtual space	Theoretical energy	Experimental energy
6	-2.86	-2.46
7	-1.64	-1.94
8	-1.63	-2.23
9	-0.37	-2.33
DHF [3]	-1.2	
RPA [3]	-3.0	

The matrix elements of all interactions were calculated between ground state of ^{199}Hg, and excited states np with opposite parity. The multiconfiguration expansions for ^{199}Hg atom were generated by single and restricted double substitutions from valence and core orbitals to four sets of virtual orbitals, limited by the principal quantum number (up to n=9). Table 2 presents percentage contributions of the lowest excited levels in four different multiconfiguration approximations (for each level the first line with theoretical energy, and the second line with experimental energy [2]). As can be seen, the largest contribution to d_{at}^{SM} arises from the lowest singlet ^1P and triplet ^3P states.

[1]E-mail: gediminas.gaigalas@tfai.vu.lt

Table 2. Percentage contribution of excited levels to d_{at}^{SM} for ^{199}Hg.

Levels	Virtual space 6	7	8	9
6p ^3P	12.7%	14.3%	16.3%	13.1%
	11.2%	14.7%	17.1%	16.4%
6p ^1P	87.3%	85.2%	82.1%	88.3%
	88.8%	84.6%	80.0%	84.9%
7p ^3P		0.9%	-0.6%	-1.4%
		1.5%	-1.1%	-1.4%
7p ^1P		-0.5%	0.3%	0.0%
		-0.8%	0.5%	0.0%
8p ^3P			2.6%	
			4.6%	
8p ^1P			-0.6%	0.0%
			-1.1%	0.0%
9p ^3P				0.0%
				0.0%

In all mechanisms which induce atomic EDM the dominant contribution arises from the lowest levels of the opposite parity. Higher levels (7p ^3P, 7p ^1P, and still higher levels of ^{199}Hg) have significantly weaker influence on atomic EDM. We will present the details of the calculations of EDM of Ra, Hg, Yb, together with a comparison with the data obtained by Dzuba et al [3].

References

[1] Jönsson P, Gaigalas G, Bieroń J, Froese Fischer C and Grant I P 2013 *Comput. Phys. Commun.* in press

[2] Ralchenko Yu, Kramida A E, Reader J and NIST ASD Team 2012 NIST Atomic Spectra Database (ver. 5.0), [Online]. Available: http://physics.nist.gov/asd [2013, February 11]. National Institute of Standards and Technology, Gaithersburg, MD

[3] Dzuba V A, Flambaum V V and Porsev S G 2009 *Phys. Rev. A* 80, 032120