Hyperfine Structure of the $3p^4 4s\ ^4p$ State of the Chlorine Atom

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Introduction

This work followed upon preceding work[1, 2, 3] devoted to calculations *ab-initio* of hyperfine constants of certain atomic states of nitrogen and fluorine. The interest caused by these elements was due to experimental work of spectroscopy to very high resolution completed by the same laboratory and measuring hyperfine spectra several elementsof which nitrogen, fluorine, oxygen and chlorine[4, 5, 6, 7]. The multi-configuration nonrelativistic Hartree-Fock methodcombined with the approximation of Breit-Pauli[8] to take account of the relativistic effects was used successfully in calculation of the hyperfine constants. This same method was also employed successfully in the hyperfine structural analysis of the fundamental state of chlorine[9]. We use it in this work to calculate the hyperfine structures of the excited state $3p^4\,4s\ ^4P$ of the atom of chlorine.

Theoretical Study

We used the ATSP code to calculate the energy of hyperfinelevels of our state. The wave functions associated with the state are calculated using the nonrelativistic method ' Multiconfigurationnelle Hartree-Fock' (MCHF), whereas the influence of the relativistic effects on the hyperfine structures of the state areanalyzed through the approximation of Breit-Pauli (BP). We carried out several types of calculations MCHF with the purpose of highlighting the nature of the effects of correlation that describe correctly the hyperfine interaction in this atomic state of chlorine.

Results and Discussion

The results of calculations corresponding to the approachesdescribed above are given in the table1 and are compared with the experiment[4]. The comparison of the single-configuration Hartree-Fock computation (HF) with that of the multi-configuration Hartree-Fock (MCHF) shows the importance of the electronic correlation in the determination of the hyperfineconstants. The comparison of the SR-C-MCHF and SR-C-BP approaches show that relative variations related to the relativistic effects on the magnetic constants do not exceed 2% whereas they are respectively about 12% and 5% on $A1/2,3/2(^4P)$.

The effect of the electronic correlation is very remarkable onthe constant $A1/2\ (^4P)$ whereas it is not negligible on the two others constants $A3/2,5/2\ (^4P)$. Broadly our values for these three last constants are in concord with the experiment. The most remarkable result is that of the MR2-BP calculation which is in very good agreement with theexperiment.

With regard to constant B, our results show that the interaction of the electronic electric field with the nuclearquadruple moment is insensitive with the effects of correlation and relativity.

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Hyperfine constants	**A1/2**	**A3/2**	**A5/2**	B1/2	B3/2	B5/2
HF	-26.6	52.6	72.1	0.0	47.4	-59.2
SR- **MCHF**	31.4	74.5	284.7	0.0	50.2	-62.7
SR-C-	51.5	84.5	289.3	0.0	50.2	-62.8
MCHF **MR2-**	57.9	85.9	293.9	0.0	49.9	-62.4
MCHF **MR4-**	61.0	87.1	293.9	0.0	49.9	-62.4
MCHF	65.2	89,5	301.0	0.0	50,2	-64,4
MR2-BP **Exper-**	67.0 ±09	101.1 ±0.2	299.6 ±0.2	0.0	47.3 ±0.3	-62.5 ±0.5

Conclusion

In the context of nonrelativistic MCHF approach, the study of the properties in general of the atom of chlorine is complex because of the sizes, very large, of configuration spaces. This with for effect to make difficult the treatment ofthe correlation electronic. However, preliminary results, relating to the hyperfine constants, which we obtained are satisfactory. We think that we can improve our results withinthe framework of a calculation MR2-BP for the stat ^{4}P. The variation which still remains between these results and the experiment possibly requires to consider a calculation of the type multi-configuration Dirac-Fock (MCDF).

References

[1]T. Carette, M. Nemouchi, P. Jönsson, and M. Godefroid, Eur. Phys. J. D 60, 231–242 (2010)

[2]P. Jönsson, M. Nemouchi, T. Carette, and M. Godefroid, J. Phys. B: At.Mol. Opt. Phys. 43 (2010) 115006 (6pp).

[3]Thomas Carette, Messaoud Nemouchi, Jiguang Li, and Michel Godefroid,Physical Review A 88, 042501 (2013).

[4]D.A. Tate and J.P. Walton, Phys. Rev. A 59,1170 (1999).

[5]R.M. Jennerich, A.N. Keiser, and D.A. Tate, Eur. Phys. J. D 40, 81–89(2006)

[6]R. M. Jennerich and D. A. Tate Physical Review A, Volume 62, 042506.

[7]D. A. Tate and D. N. Aturaliye, Physical Review A 56, (29 January 1997),(10pp).

[8]C. Froese Fischer, T. Brage, P. Jönsson, Computational Atomic Structure.An MCHF Approach,

[9]T Carette and M R Godefroid, J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 105001 (9pp) Institute of Physics Publishing, Bristol/Philadelphia, 1997.

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