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Hyperfine Structures ab-initio Calculations of the $2p^4(^3P)3d^{2S+1}L_J$ States in theFluorine Atom

Fatima Zahra Boualili[1*], Messaoud Nemouchi[1], Michel Godefroid[2], and Per Jönsson[3]

[1]Laboratoire d'Électronique Quantique, Faculté de Physique, USTHB, BP32, El-Alia, Algiers, Algeria

[2]Spectroscopy, Quantum Chemistry and Atmospheric Remote Sensing (SQUARES),CP160/09, Université libre de Bruxelles, 1050 Brussels, Belgium

[3]Department of Materials Science and Applied Mathematics, Malmö University, SE-20506 Malmö, Sweden

[*]Corresponding author

ABSTRACT

In previous work devoted to ab initio calculations of hyperfine structure constants in nitrogen and fluorine atoms, we observed sizeable relativistic effects, a priori unexpected for such light systems, that can even largely dominate over electron correlation. We observed that the atomic wave functions calculated in the Breit-Pauli approximation describe adequately the relevant atomic levels and hyperfine structures, even in cases for which a small relativistic LS-term mixing becomes crucial. In the present work we identify new levels belonging to the spectroscopic terms $2p^4(^3P)3d^{2,4}(P; D; F)$ of the fluorine atom, for which correlation effects on the hyperfine structures are small, but relativistic LS-term admixtures are decisive to correctly reproduce the experimental values. The Breit-Pauli analysis of the hyperfine matrix elements nails cases with large cancellation, either between LS pairs for individual hyperfine operators, or between the orbital and the spin-dipole contributions. Multiconfiguration Dirac-Hartree-Fock calculations are performed to support the Breit-Pauli analysis.

Introduction

In previous work [1,2] devoted to ab-initio calculations ofhyperfine constants of certain states of nitrogen and fluorine atoms, the authors concluded that there were anomalously large effects of relativity on the hyperfine interaction. In the present work, we have taken the opportunity of new experimental measurements [3] of hyperfine constants in the fluorine atom to study the influence of relativistic effects. The states concerned by this study areall the states of the $2p^4(^3P)3d$ configuration.

Theoretical Study

We used three methods to evaluate relativistic effects. The nonrelativistic multiconfigurational Hartree-Fock (MCHF) approach combined with the Breit-Pauli (BP) approximation to introduce relativistic effects. The second approach, purely relativistic, is the Dirac Hartree-Fock multiconfigurational method (MCDHF) combined with a relativistic configuration interaction (RCI) calculation. The third approach is the Pauli approximation (RCI-P) which is the non- relativistic limit of the Dirac theory.

Results and Discussion

In this table we reports only the case of the hyperfine structure constants (in MHz) of $2p^4(^3P)3d\ ^4D$

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for the Actif space [9f] calculated with (SD)-MR-MCHF by using the simultaneous optimization strategy, (SD)-MR-BP and (SD)-MR-RCI-P methods. These values are compared with fully relativistic results calculated with the (SD)-MCDHF-RCI method, and with observation. We notice the large differences between the nonrelativistic and Breit-Pauli results are most likely due to the strong relativistic interaction between the terms, and the good agreement between the Breit-Pauli and the other relativistic results.

J	1/2	3/2	5/2	7/2
MCHF	3472	1453	813	190
BP	4646	2262	1461	852
RCI-P	4640	2258	1458	850
MCDHF-RCI	4608	2257	1463	855
Exp[3]	4541±50	2290±50	1481±20	793 ± 20

Conclusion

In this work, we present the results of elaborate ab initio variational calculations of hyperfine constants for 17 levels in fluorine, all arising from the 6 terms $2p^4(^3P)3d\ ^4D$, ^2D, ^4F, ^2F, ^4P and ^2P. The global theory-observation agreement is very good.

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