IRS2012-311-3
International Radiation Symposium 2012
Dahlem Cube, Berlin, Germany, 06 – 10 August 2012

Theoretical study of the lowest - lying states of LuI located below 40 000 cm-1

J. Assaf (1,2), S. Magnier (1), F. Taher (3), and F. Haj Hassan (4)

(1) Laboratoire de PhLAM,Universite Lille 1 Sciences et Technologies,France.(joumana.assaf@yahoo.com), (2) Universite Libanaise, Ecole doctorale des Sciences et Technologies, Liban., (3) Universite Libanaise,Faculte de Genie (III), Liban., (4) Universite Libanaise,Faculte des Sciences (I), Liban.

A theoretical investigation of the lowest-lying electronic states of Lutetium monoiodide LuI molecule is presented. Calculations have been performed through CASSCF and MRCI (single and double excitations) methods, in a range of internuclear distance R from 1.80 (Å) to 3.50 (Å), taking without and with the Spin-orbit coupling. The Lutetium atom is described by a relativistic pseudopotential ECP28 [1] while for the Iodine atom, the pseudopotential ECP 46 is used [2]. Calculations have been performed via the computational chemistry program MOLPRO [3]. Potential energy curves of the lowest-lying 22 $^{2S+1}\Lambda^{(\pm)}$ electronic states located below 40.000 cm^{-1} and that of the corresponding 43 $^{2s+1}\Omega^{(+/-)}$molecular states have been determined. Spectroscopic constants (Re (Å), ωe, Te, Be in cm^{-1}) have been calculated and part of the results are compared with available experimental and theoretical values [4, 5]. A satisfying agreement has been obtained. Calculations have been used to predict the spin - orbit constant (A) in different triplet states of $\Lambda \neq 0$ and the composition (in percentage) of state wavefunctions in term of $^{2s+1}\Omega^{(+/-)}$. A discussion is done to identify the Hund' case in LuI.

References:

[1] X. Cao, M. Dolg, J. Chem. Phys., 115, 7348 (2001).

[2] H. Stoll, B. Metz, M. Dolg, J. Comput. Chem., 23, 767 (2002).

[3] J.Werner, P.J. Knowles, with contributions from R.D. Amos, A. Berning,

D.L. Cooper, P.J. Knowles and H.-J. Werner,"Chem. Phys. Lett.", 115, 5053.

[4] J. Kramer, J. Chem. Phys., 69 (6), 15 September (1978).

[5] V. Solomonik , A. Smirnov, J.Struct.Chem., 46, (6), 973-978,(2005).