# THEORETICAL STUDIES ON THE ELECTRONIC SPECTRA OF AlCl

SUNIL K. MISHRA[a], SUSHIL SRIVASTAV and VIPIN B. SINGH, *Department of Physics, Udai Pratap Autonomous College, Varanasi-221002, India.*

The spectra of AlCl molecule are of astrophysical interest since AlCl has been detected in the envelope of the carbon star IRC + 10216 by microwave spectroscopy[b]. Ab initio and Density Functional Theory calculations on the spectra and structure of AlCl molecule and their cation are carried out. The Einstein A spontaneous emission coefficients for the ro-vibrational transitions in the $A^1\Pi$-$X\,^1\Sigma^+$ electronic band systems of AlCl molecule for v = 0 - 4 and J = 0-100 in each electronic state have been computed using LEVEL program. The values of radiative lifetimes of $A^1\Pi$ state for $v' \leq 9$ levels are determined. We have obtained the high transition probabilities for the diagonal bands in this electronic system. The results obtained in the present work are found in agreement with the experimental value.

[a] present address: Department of Physics, Agrasen Kannya PG College, Varanasi

[b] I.Cernicharo, M.Guelin, Astron. Astrophy., 183, (1987) L10