DEPERTURBATION STUDIES OF AlO : INTERACTIONS IN THE $A^2\Pi \sim X^2\Sigma^+$ STATES

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The rotational structure of $D^2\Sigma^+$ - $A^2\Pi$ band system of AlO molecule, at moderate high resolution, was photographed by Singh et. al[a]. They carried out the rotational analyses of seven bands of this system, involving vibrational levels v′= 0 - 5 and v′′= 0 - 4 for both the sub-transitions $D^2\Sigma^+$ - $A^2\Pi_{1/2}$ and $D^2\Sigma^+$ - $A^2\Pi_{3/2}$ and reported several rotational perturbations in the $A^2\Pi_i$ state. In this work, we present a deperturbation analysis which yields deperturbed molecular constants of the $X^2\Sigma^+$, $A^2\Pi_i$, and $D^2\Sigma^+$ states. The revised molecular parameters for the $X^2\Sigma^+$ and $D^2\Sigma^+$ states are first obtained from a simultaneous fit performed using previous high resolution data of the $D^2\Sigma^+$ - $X^2\Sigma^+$ system [b] involving v′=0 - 6 and v′′= 0 - 4 vibrational levels and $B^2\Sigma^+$ - $X^2\Sigma^+$, system [c] involving v′= 0 - 11 and v′′= 0 - 7 vibrational levels. PGOPHER program is used to simulate and fit the observed spectra[d] . The branch frequencies involving the $D^2\Sigma^+$ - $A^2\Pi_i$ transitions from our earlier studies have been incorporated into a single Hamiltonian to obtain improved molecular constants together with the L- doubling and spin splitting coefficients for these states. Further, invoking perturbing state ($X^2\Sigma^+$) molecular parameters in this fit, deperturbation of the vibrational levels within the $A^2\Pi_i$ state of AlO up to v′′ = 4 is obtained. A global least squares fit to all the data allows determination of $A^2\Pi_i$ state molecular constants with much improved precision. The results of this study will be presented.

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[a] M. Singh and M. D. Saksena, Can. J. Phys. 63, 1162 (1985).

[b] M. Singh and M. D. Saksena, Proc. Indian Acad. Sci. 77, 139 (1973).

[c] M. D. Saksena, M. N. Deo, K. Sunanda, S. H. Behere and C. T. Londhe, 247, 47(2008).

[d] PGOPHER, a Program for Simulating Rotational Structure, C. M.Western, University of Bristol.