INTERPRETATION OF NITROGEN MOLECULE SPECTRA

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The analytical quantum-mechanical decision for nitrogen molecula spectra and forbidden Vegard-Kaplan band ($A^3\Sigma_u^+ - X^1\Sigma_g^+$) have been obtained. The ground $X^1\Sigma_g^+$ state of nitrogen molecule have been calculated by MINDO/3 method under the intermolecular distance R=1,09 $\mathring{A}$ and then MO LKAO coefficients were used for the CI and SOC calculations to determine the radiative lifetime. The lifetime of metastable $A^3\Sigma_u^+$ state was calculated to be τ=5,58 s. The obtained lifetime $A^3\Sigma_u^+$ state is in a good agreement with Piper experimental values 2,37 s [1] and recent ab initio computation values 3,87 s [2]. Thus, even account single excitation in minimal CI basis have been obtained sufficiently good results. The analitical decision as alternative theoretical method spectroscopic investigation will be presented.