

Experimental and Theoretical Investigations on the Visible Spectrum of AlD^+

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The emission spectrum of the AlD^+ ion has been studied by Fourier transform spectroscopy technique, as a further step of our investigation of the AlD neutral molecule.² The $0-0$ and $1-1$ bands of the $\text{AX}\rho l$ system have been recorded in the $27,000-29,000\text{ cm}^{-1}$ region with an instrumental resolution of 0.03 cm^{-1} . In total, almost 500 rotational frequencies were measured with an absolute accuracy of about 0.005 cm^{-1} . It improved the experimental accuracy of the determined frequencies by the factor 10 compared to the previous work.³ The rotational analysis has shown irregularities in the Λ -doubling splitting of the $\text{A}\rho l$ $v=0,1$. Consequently, the $\text{A}\rho l$ state has been represented by the rotational term values, while the regular $\text{X}\rho l$ state by the molecular constants. The causes of the irregularities were identified in the interaction between the $\text{A}\rho l$ state the lying higher the $\text{B}\rho l$ state.

Ab initio calculations on the ion were performed using a parallel version of the MOLPRO⁴ (version 2010.1) suite of quantum chemistry codes. The static electron correlation was calculated using SA-CASSCF method.⁵ The active space consisted of all the occupied valence orbitals of the aluminum atom plus the $1s$ orbital from the deuterium atom. The $1s$ orbital of the Al^+ atom is kept frozen while the $2s2p$ orbitals are closed (kept doubly occupied in all configurations). In addition, SA-CASSCF can be used to calculate the excited electronic states corresponding to the $\text{Al}^+(\text{}^3\text{P}) + \text{D}(\text{}^2\text{S})$ asymptote so a total of five states are included ($2\times \text{}^2\Sigma^+, \text{}^2\Pi, \text{}^4\Sigma^+, \text{}^4\Pi$). The accuracy of the potentials can be improved by including dynamic electron correlation, that was handled here by using MRCI method.⁶

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