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*Ab initio* study of band strength distribution for the  $D^2 \Sigma^+ - A^2 \Pi$  transition of AlO and the effect of  $R$  dependence of the electronic transition moment on the distribution

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PII: S2210-271X(14)00522-2

DOI: <http://dx.doi.org/10.1016/j.comptc.2014.11.019>

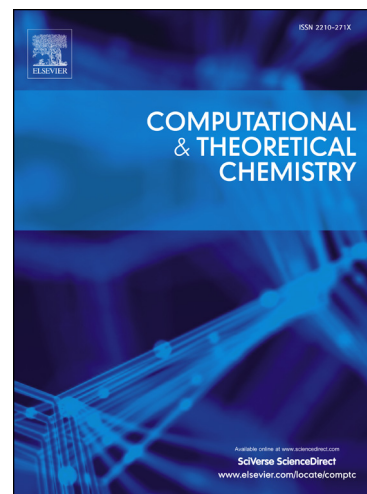
Reference: COMPTC 1683

To appear in: *Computational & Theoretical Chemistry*

Received Date: 28 September 2014

Revised Date: 24 November 2014

Accepted Date: 27 November 2014



Please cite this article as: N. Honjou, *Ab initio* study of band strength distribution for the  $D^2 \Sigma^+ - A^2 \Pi$  transition of AlO and the effect of  $R$  dependence of the electronic transition moment on the distribution, *Computational & Theoretical Chemistry* (2014), doi: <http://dx.doi.org/10.1016/j.comptc.2014.11.019>

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***Ab initio* study of band strength distribution for the  $D^2\Sigma^+-A^2\Pi$  transition of AIO and the effect of  $R$  dependence of the electronic transition moment on the distribution**

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**Abstract:** The band strength distribution for the  $D^2\Sigma^+ \nu'-A^2\Pi \nu''$  electronic transition of AIO, and the effect of  $R$  dependence of the electronic transition moment on the distribution, are studied based on the *ab initio* band strengths and the Franck-Condon factors (FCFs) for bands with vibrational quantum numbers  $\nu'=0-18$  and  $\nu''=0-18$ . The band strength distribution exhibits a Condon parabola of the bands involving  $\nu'=0-9$  and 11 of all the inner-well levels of the  $D^2\Sigma^+$  double potential well. Five unobserved bands calculated among the ten largest band strength bands are found to involve the  $\nu'$  levels near the  $D^2\Sigma^+$  potential barrier top. The effect of the  $R$  dependence is examined for the FCF maximum bands in the  $\nu''$ -progressions for  $\nu'=0-9$  and 11-18 (excluding  $\nu'=10$  of the  $D^2\Sigma^+$  outer-well level) by using the ratio of the band strength to the FCF, both relative to the 0-0 band. Large (Small) ratios of value 1.276-1.559 (0.619-0.841) are found for ratio>1 (ratio<1) bands with  $\nu'=8, 9$  and 11-18. An analysis using a model of transition matrix element shows that the difference between (1) the electronic transition moment in the region represented by the  $R$ -centroid for each large ratio band and (2) that for the 0-0 band makes the greatest contribution to the ratio. The  $R$ -centroids do not properly represent the important  $R$  regions ( $R<3.0 a_0$ ) for the small ratio bands with  $\nu'=11-18$ ; a possible explanation is discussed. The results imply that the avoided crossings influence the band strength distribution. The Einstein  $A$  coefficients have been evaluated for the D-A bands with  $\nu'=0-9$  and 11 and  $\nu''=0-18$  from the calculated band strengths and transition energies.

**Keywords:** AIO; *Ab initio*; Band strength; Electronic transition moment;  $R$ -centroid; Einstein  $A$  coefficient;

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