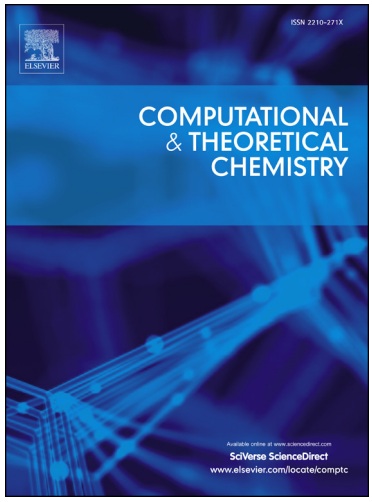

Ab initio study of band strength distribution for the $D^2\Sigma^+$-$A^2\Pi$ transition of AlO and the effect of *R* dependence of the electronic transition moment on the distribution

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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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Abstract: The band strength distribution for the $D^2\Sigma^+$ v'-$A^2\Pi$ v'' electronic transition of AlO, 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 v'=0-18 and v''=0-18. The band strength distribution exhibits a Condon parabola of the bands involving v'=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 v' levels near the $D^2\Sigma^+$ potential barrier top. The effect of the *R* dependence is examined for the FCF maximum bands in the v''-progressions for v'=0-9 and 11-18 (excluding v'=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 v'=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 v'=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 v'=0-9 and 11 and v''=0-18 from the calculated band strengths and transition energies.

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