

Abstract Submitted
for the DAMOP15 Meeting of
The American Physical Society

Electronic Transition Dipole Moment and Radiative Lifetime Calculations of Sodium Dimer Ion-Pair States AYDIN SANLI, BEDIHA BESER, JOHN EDWARDSON, Temple University, SYLVIE MAGNIER, Universite Lille, ERGIN AHMED, MARJATTA LYYRA, Temple University — Alkali dimer M_2 and alkali hydride MH molecular electronic states with ion-pair character are known to exhibit multiple minima and shoulders in their potential energy curves. This exotic behavior of the of the $1\Sigma_g^+$ symmetry states is caused by an avoided crossing of the zero-order covalent and ionic ($M^+ + M^-$) potential energy curves. We present a computational study of lifetimes and transition dipole moment matrix elements for the sodium dimer ion-pair states of $1\Sigma_g^+$ symmetry. We report here the ab initio calculated electric transition dipole moments between the $n 1\Sigma_g^+$ and the $A1\Sigma_u^+$ states, that vary strongly as a function of internuclear distance. In addition, we have calculated the radiative lifetimes, τ , of these ion-pair states of and compared them with the experimental results from literature when available.

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Date submitted: 02 Feb 2015

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