AN AB INITIO MODEL HAMILTONIAN FOR THE $e' \otimes e'$ and $e' \otimes e''$ SINGLET STATES OF Si_3

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The recent[a] mass-selected REMPI spectrum of the silicon trimer in the 2.25-2.6 eV region has been partially assigned in terms of a triplet-triplet transition. However, several remaining features appear to be due to transitions from the ground singlet to one of two upper singlet states, both of these belonging to the same electron configuration. To aid in the assignment of these features, a model Hamiltonian has been developed for the $e' \otimes e'$ and $e' \otimes e''$ singlet states of Si_3 (7 states in total), including quadratic vibronic (Jahn-Teller and psuedo-Jahn-Teller) interactions and a quartic expansion of the diabatic potential. This Hamiltonian has been fit to *ab initio* single-point energies calculated using the full EOMDEA-CCSDT method and the Widmark-Roos ANO basis set.

[a] N. J. Reilly, D. L. Kokkin, J. F. Stanton and M. C. McCarthy, submitted.