THE $\tilde{B}\ ^1A_1$ ELECTRONIC STATE OF SiH_2

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The $\tilde{B}\ ^1A_1$ electronic state of SiH_2 is the second excited singlet state of the molecule and, like the analogous $\tilde{c}$ state of CH_2, it is quasilinear with symmetry $^1\Sigma_g^+$ at linearity. Using *ab initio* methods, we calculate the potential energy of the state, and the in-plane y and z dipole moments, at 89 nuclear geometries. In a fitting we determine the optimum values of the parameters in an analytical function for the potential energy, and use the MORBID program to calculate the term values of the state. We adjust some of the potential energy parameters in a fitting to the term values for SiH_2 and SiD_2 obtained by experiment[a]. Using the refined potential, and our *ab initio* dipole moment surfaces, we simulate the rotation-vibration spectrum of the state. Although lying above the $Si(^1D)$+$H_2(^1\Sigma_g^+)$ dissociation limit there is calculated to be a barrier of more than 3 eV to adiabatic dissociation; the dissociation process will be discussed.

[a] Y. Muramoto, H. Ishikawa, and N. Mikami, *J. Chem. Phys.* in press.