Derivation of C_6-coefficients from B3LYP calculations of the long-range parts of the $Si(^3P_J) + O_2(^3\Sigma^-_g)$ potential energy surface.

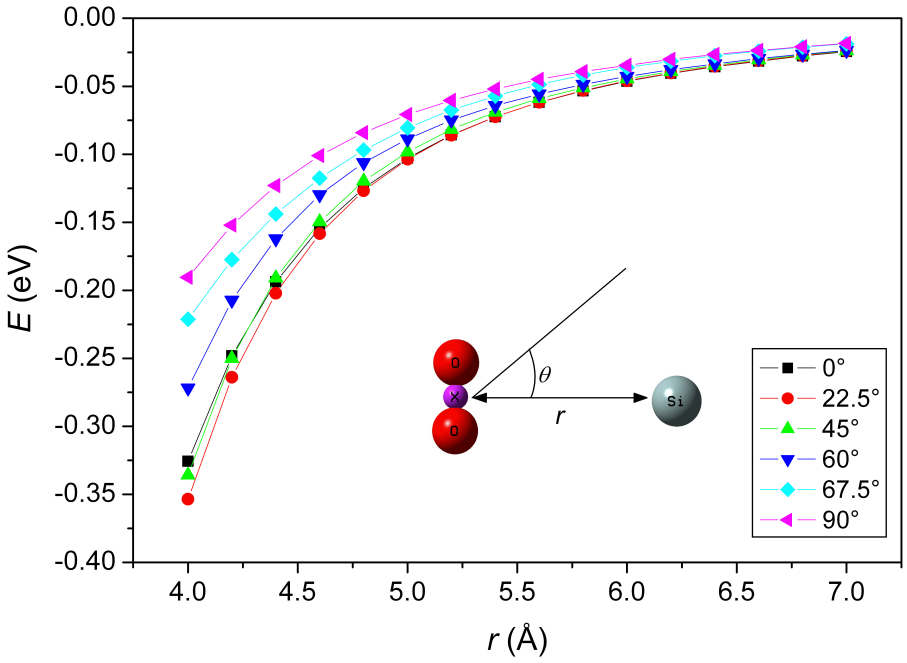

Figure S1: Long-range part of the singlet PES at the B3LYP/6-311+G(2d,p) level of theory. The optimization was carried out on a grid of 16 values of the Si-X distance r ranging from 4 to 7 Å, and 13 values of the Jacobi angle θ ranging from 0 to 90°.

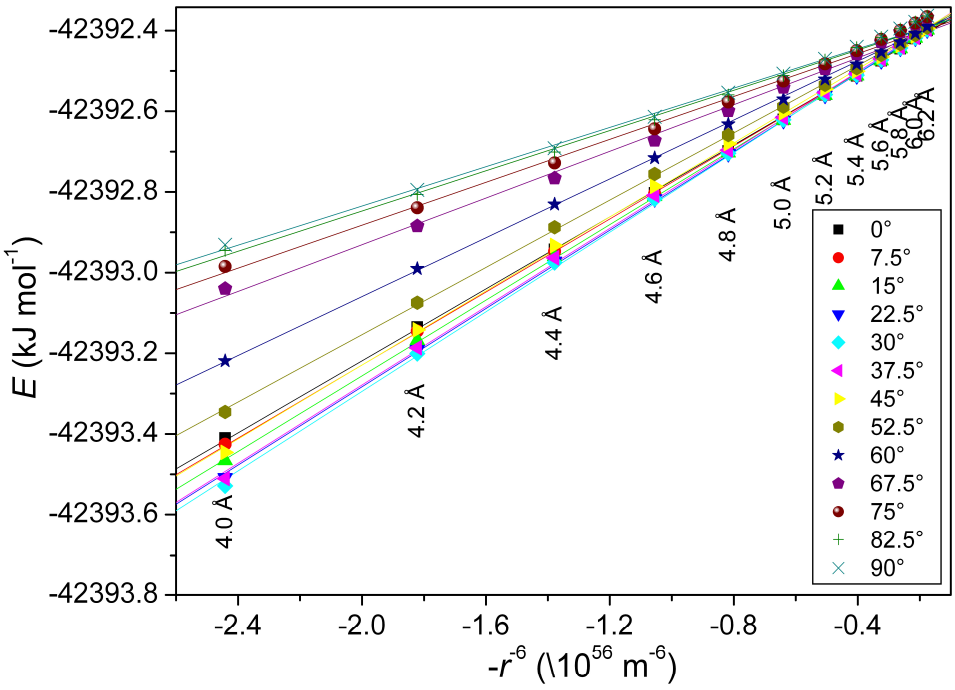

Figure S2: A $C_6 \times r^{-6}$ potential was fitted to the PES and C_6 values were obtained for the range of Jacobi angles (0 – 90°). For $\theta > 67.5°$ departure from r^{-6} behaviour was observed for $r > 6$ Å and therefore only values of r between 4 and 6 Å were considered in the fit.

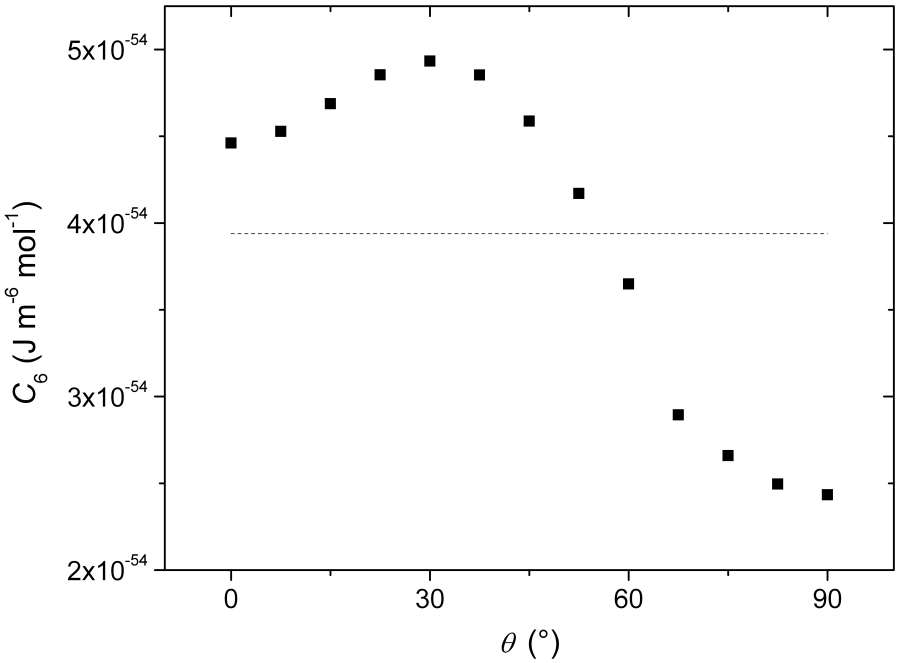

Figure S3: C_6 coefficients as a function of the Jacobi angle. The angle-averaged C_6 is 3.9×10^{-54} J m^{-6} molecule^{-1}, which agrees reasonably well with the value calculated with the London formula (6.0×10^{-54} J m^{-6} molecule^{-1}). The maximum variation of ~ 40% with respect to the averaged C_6 indicates that there is not a very strong dependence on the Jacobi angle.