

Abstract Submitted
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Variable (T_g , T_s) Measurements of Alkane Dissociative Sticking Coefficients LETICIA VALADEZ, KRISTY DEWITT, HEATHER ABBOTT, KURT KOLASINSKI, IAN HARRISON, Dept. of Chemistry, University of Virginia — Dissociative sticking coefficients $S(T_g, T_s)$ for CH_4 and C_2H_6 on Pt(111) have been measured as a function of gas temperature (T_g) and surface temperature (T_s) using an effusive molecular beam. Microcanonical unimolecular rate theory (MURT) was employed to extract transition state characteristics [e.g., $E_0(\text{CH}_4) = 52.5 \pm 3.5$ kJ/mol⁻¹ and $E_0(\text{C}_2\text{H}_6) = 26.5 \pm 3$ kJ/mol⁻¹]. MURT allows our $S(T_g, T_s)$ values to be directly compared to other supersonic molecular beam and thermal equilibrium sticking measurements. The $S(T_g, T_s)$ depend strongly on T_s , however, only for CH_4 is a strong T_g dependence observed. The fairly weak T_g dependence for C_2H_6 suggests that vibrational mode specific behavior and/or molecular rotations play stronger roles in the dissociative chemisorption of C_2H_6 than they do for CH_4 . Interestingly, thermal $S(T_g = T_s)$ predictions based on MURT modeling of our $\text{CH}_4/\text{Pt}(111)$ data are three orders of magnitude *higher* than recent thermal equilibrium measurements on supported Pt nanocrystallite catalysts [J. M. Wei, E. Iglesia, J. Phys. Chem. B **108**, 4094 (2004)].

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