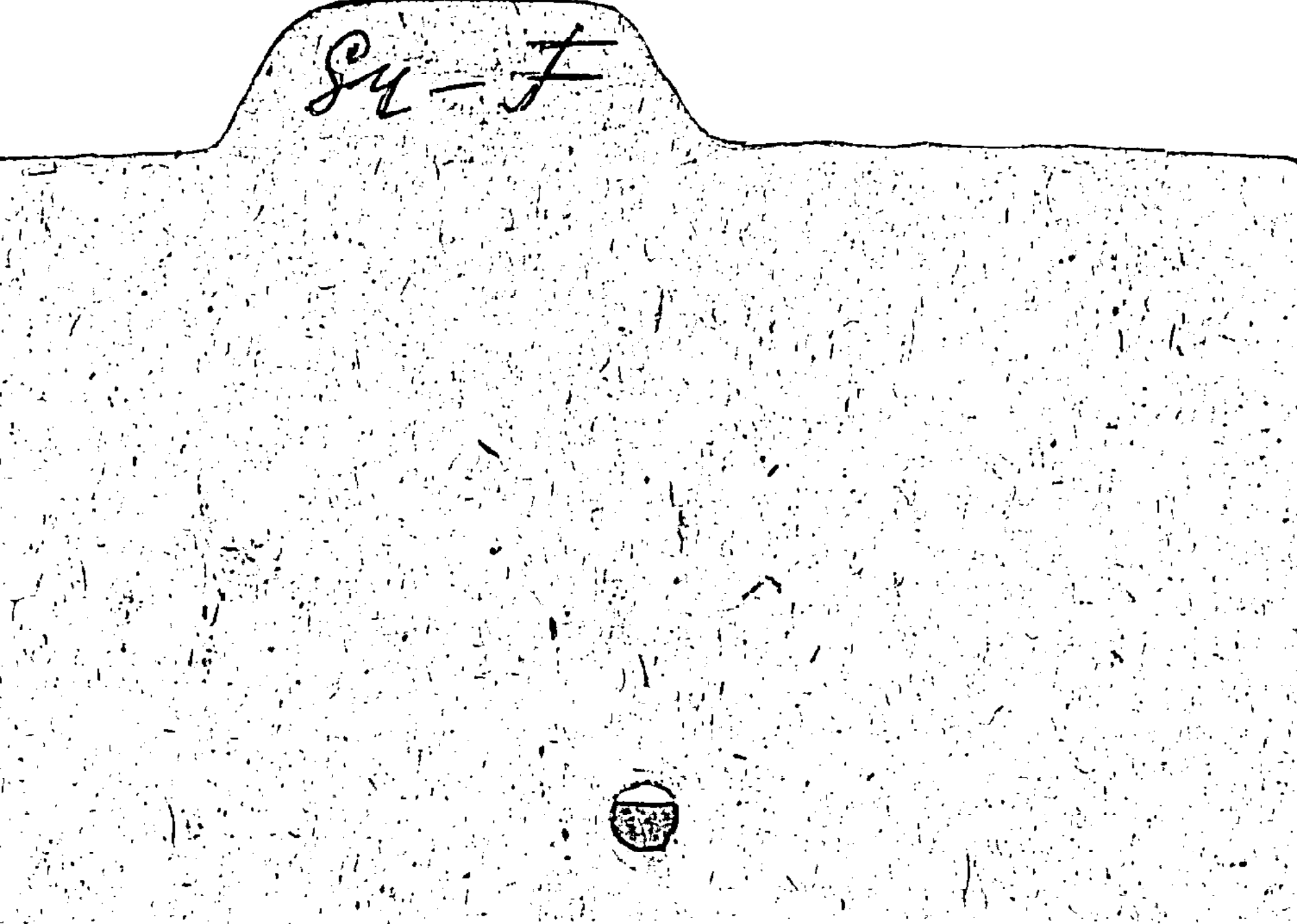

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110: 45179w **Comparison of the calcium + hydrogen fluoride (deuterium fluoride) and strontium + hydrogen fluoride (deuterium fluoride) reaction dynamics.** Zhang, Rong; Rakestraw, David J.; McKendrick, Kenneth G.; Zare, Richard N. (Dep. Chem., Stanford Univ., Stanford, CA 94305-5080 USA). *J. Chem. Phys.* 1988, 89(10), 6283-94 (Eng). A comparative study of the reaction family, Ca and Sr with rovibrationally selected HF or DF, has been carried out under single-collision conditions. A thermal beam of the alk. earth atoms, Ca or Sr, is fired into a low-pressure gas of HF or DF in which the reagent mols. have been prepd. in a selected vibration-rotation state by the use of a tunable IR light source (optical parametric oscillator). The resulting alk. earth monofluoride reaction products are detected by using laser induced fluorescence. The HF mol. is aligned with its rotational angular momentum pointing preferentially either along or perpendicular to the metal atom beam. For both Ca + HF(v = 1) and Sr + HF (v = 1) the cross section and the product state distribution are found to be independent of the approach geometry, which is consistent with reaction through a bent transition state. The state-to-state reaction dynamics for Ca + HF(DF) and Sr + HF(DF) show marked differences. The Ca + HF(DF) → CaF + H(D) reaction has attributes of a statistical internal energy distribution, whereas Sr. + HF(DF) are consistent with a model in which the Ca atom inserts into the HF bond to form a long-lived H-Ca-F intermediate; the findings for Sr + HF(DF) are interpreted as competition between direct reaction and reaction which samples the deep H-Sr-F potential well.

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