Abstract Submitted
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Chemical pathways in ultracold reactions of SrF molecules[1] EDMUND MEYER, Kansas State University, JOHN BOHN, JILA — We present a theoretical investigation of the chemical reaction SrF + SrF $\rightarrow$ products, focusing on reactions at ultralow temperatures. We find that bond swapping, SrF + SrF $\rightarrow$ Sr_2 + F_2, is energetically forbidden at these temperatures. Rather, the only energetically allowed reaction is SrF + SrF $\rightarrow$ SrF_2 + Sr, and even then only singlet states of the SrF_2 trimer can form. A calculation along a reduced reaction path demonstrates that this abstraction reaction is barrierless, and proceeds by one SrF molecule "handing off" a fluorine atom to the other molecule.

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