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13. ABSTRACT (Maximum 200 words) We performed a molecular dynamics study of water at room temperature to examine the dynamics of hydrogen bond formation. It was carried out through an application of the reactive flux formalism. Computed long time relaxation functions are not consistent with a first-order process. Statistical (non dynamical) theories of hydrogen bond breaking, such as transition state theory with a single dividing surface, are found to be unsatisfactory. Further, our dynamical results indicate that at least two elementary processes contribute to hydrogen bond breaking.			
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by

A. Luzar and D. Chandler

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