COMPUTATIONAL STUDIES OF NONADIABATIC ALIGNMENT OF ASYMMETRIC TOP MOLECULES

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We numerically simulated rotational wavepacket dynamics in asymmetric top molecules. The molecules are aligned impulsively using a short, intense linearly-polarized laser pulse. The alignment of molecules is important for capturing dynamics in the molecular frame and for molecular imaging. The alignment process is challenging to simulate because of the large number of initial rotational states involved. The alignment is simulated under the rigid-rotor assumption and field-free conditions. The evolution of the degree of alignment and angular distributions of 4-fluorobenzotrifluoride (FC6H4CF3) are calculated and the numerical results show good agreement with the experimental results.