

Relaxation of Photoexcited Na₃F

J.M. L’Hermite, V. Blanchet, A. Le Padellec, P. Labastie

Lab. Collisions Agrégats Réactivité (CNRS UMR 5589, IRSAMC, Toulouse, France)

Some small Na_nF_{n-p} clusters present a significant difference between the ionisation potential of different isomers. This strong correlation between the structure and the ionisation potential allows an ideal excitation scheme to study selectively the dynamics of one isomer through time-resolved experiment. Indeed for geometric rearrangement like isomerisation, the ionisation probability may become time-dependent if the probe pulse energy is low enough to photoionise only one isomer. Na₃F is a two-excess electrons cluster whose two lowest energy isomers are a quasi-planar of C_{2v} isomer (deformed rhombic structure) and a 3D triagonal pyramidal one of C_{3v} symmetry, which lies slightly higher (~65 meV of difference).[1]

Moreover, this system fulfills the requirements stated above for an ideal system, since the vertical ionisation potential of the C_{3v} pyramidal structure is 0.5eV lower than the C_{2v} one.[2]

We have studied the relaxation dynamics of excited Na₃F in a femtosecond pump-probe experiment using two NOPA laser pulses. The pump pulse brings the C_{2v} isomer into an excited state and the evolution of the system is probed *via* a photoionisation transition close to the ionisation threshold of the C_{3v} geometry. This time-resolved experiment shows a decay and oscillations providing an insight on nuclear dynamics.

[1] V. Bonacic-Koutecky, J. Pittner and J Koutecky, Chem. Phys., **210**, 313, (1996).

[2] V. Bonacic-Koutecky and J. Pittner, Chem. Phys., **225**, 173, (1997).