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Research paper

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ACCEPTED MANUSCRIPT

Ultrafast Electron Diffraction Study of Single-Crystal (EDO-TTF)₂SbF₆: Counterion Effect and Dimensionality Reduction

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Highlights

The ultrafast structural dynamics of single crystal (EDO-TTF) $_2$ SbF $_6$ upon photoexcitation at 800 nm were studied using ultrafast electron diffraction with femtosecond time resolution.

Singular value decomposition of the $(EDO-TTF)_2XF_6$ diffraction data shows that there are only two principal modes for X = Sb, and three principal modes for X = P.

In contrast to the case of the smaller isostructural analogue, no photoinduced insulator-to-metallic phase transition was observed when X = Sb. Instead, transition to a non-thermal excited state was observed to occur after +100 ps.

Abstract

Ultrafast electron diffraction is a sensitive tool to directly study molecular dynamics in structural detail. Here, we report the influence of counterion size on the photoinduced insulator-to-metal phase transition in two derivatives of the organic salt (EDO-TTF) $_2$ XF $_6$. For X = P, three dominant motions are present and the molecules undergo the transition, whereas in the case of X = Sb, only two dominant motions are found and the molecules do not evolve into the metallic state. This reduction in dimensionality is supported by a novel data analysis method involving singular value decomposition of time-resolved electron diffraction data in reciprocal space.

Keywords

Ultrafast electron diffraction, femtosecond structural dynamics, photoinduced phase transition, singular value decomposition, dimensionality reduction.

Introduction

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