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Study of Excited State Relaxation Pathways of 2,4,6-Trinitrobenzene-1,3,5-triamine Using Transient Absorption Spectroscopy

by Frank De Lucia and Nhan Dang

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14. ABSTRACT
Excited states are thought to play a role during the very early stages of energetic initiation. In this work, we used ultrafast pump-probe spectroscopy to resolve the excited states and subsequent relaxation pathways of the explosive 2,4,6-trinitrobenzene-1,3,5-triamine (TATB). A 400-nm, 35-fs laser pulse was used to pump the TATB into an excited state. We used transient absorption to analyze the excited state's absorption features and lifetimes. We collected transient absorption spectra at various delay times relative to the pump pulse over a range of 0.5 to 30 ps to resolve the excited states. Using global lifetime analysis, we found two prominent excited states with lifetimes of 0.72 and 4.4 ps. Based on results from our experiments and the literature, there are two possible relaxation pathways: the relaxation to a triplet state and relaxation to a "hot" ground state/relaxed structure.

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1. Introduction

The molecular response of an energetic molecule to external stimuli is dependent on how the energy couples into the material and how fast this process occurs. Following the energy flow processes from initial stimulus through explosive initiation is complicated in such an extreme environment that includes rapidly changing chemical and electronic structure dynamics and large increases in temperature and pressure. Furthermore, the processes occur on a timescale of tens of picoseconds (ps). To monitor the energy flow under these conditions, experiments must be designed to resolve this short timescale as well as be able to deconvolve the various effects of the extreme environment. Ultrafast pump-probe experiments allow us to use a singular external stimulus, the pump, to perturb the molecule from equilibrium and then probe the energetic molecule to resolve the electronic and chemical changes in the molecule. It has been shown that short-lived, excited state species play a role at this early stage.[1–3] We would like to obtain a better understanding of the role excited state species play in the very beginnings of the initiation process.

In previous studies, decomposition products from shocked samples of 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) and 2,4,6-trinitrobenzene-1,3,5-triamine (TATB) have been studied.[4,5] Researchers found that the products from the shock decomposition are identical to decomposition due to ultraviolet photolysis. The first step in photolytic decomposition involves an electronic excitation, which suggests that shock decomposition could also involve electronic excitations.[4,5]

We set up a femtosecond (fs) transient absorption experiment to observe the evolution of excited state species that arise after interrogating an energetic material with an on-resonance pump beam. The probe beam allows us to collect data on the same timescale as that used when the initiation takes place. The goal of this work was to use the US Army Combat Capabilities Development Command (DEVCOM) Army Research Laboratory (ARL) transient absorption experimental setup to collect high-quality transient absorption spectra of an energetic material. We chose TATB as our target molecule because there have been some limited studies that would allow us to compare our data. In a previous study, Chu et al.[6] used fs transient absorption and time-dependent density function theory (DFT) to analyze TATB. However, the experimental transient absorption spectra were less than ideal. Initially, we wanted to generate high-quality, high signal-to-noise transient absorption spectra of TATB for analysis and then expand to other energetic materials in the future. We performed global fitting analysis to determine the lifetimes of the observed excited state species.

2. Experimental Setup

The fs pump-probe transient absorption experimental layout is shown in Fig. 1. Initially, an fs laser system (Coherent Astrella Integrated titanium-sapphire [Ti:S] Amplifier) produces a pulse train of 6-mJ, 800-nm, and 35-fs pulses at a 1-kHz repetition rate. The pulse train is divided by a 10:90 beamsplitter (Semrock, FS01-BsTis-1090P) into a probe and pump beam path. The pump pulse passes through a delay line (Thorlabs, IMS600PP), an attenuator made up of a zero-order half-wave plate (Newlight Photonics, WPM03-H-NIR), and a thin-film polarizer (Newlight Photonics, TFP2103-800); a beta barium borate crystal for Type I second harmonic generation (Newlight Photonics, THG800-A10-35fs) and another zero-order half-wave plate (Newport, 10RP02-41) control the polarization of the pump beam.

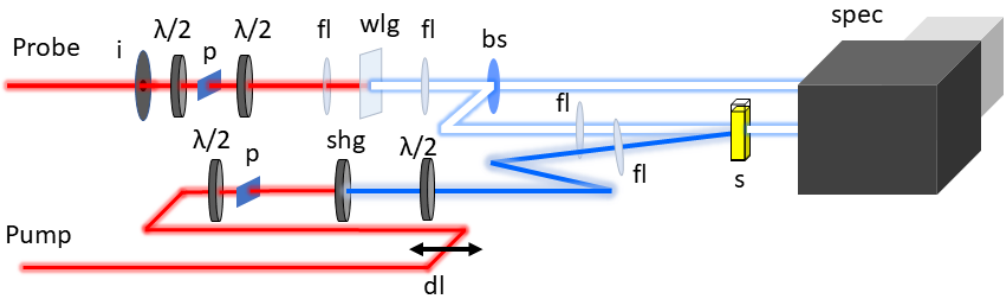

Fig. 1 Femtosecond transient absorption experimental setup: i, iris; λ/2, half-wave plate; p, polarizer; fl, focusing lens; wlg, white light generation; bs, beamsplitter; s, sample cuvette; spec, spectrometer; dl, delay line; shg, second harmonic generator

Next, a 50-cm focal length lens focuses the pump beam onto the sample. The pump beam is 12 μJ. The probe pulse passes through an iris and an attenuator made up of a zero-order half-wave plate (Newlight Photonics, WPD03-H800-F400-SP) and a thin-film polarizer. Another zero-order half-wave plate controls the polarization, and a 10-cm focal length lens focuses the probe pulse onto a calcium fluoride plate (Newport, 10CF20) to generate white light. The plate then rasters back and forth on a 2-mm linear path to prevent damage. The iris and the attenuator create a stable white-light probe pulse, and a 10-cm focal length lens collimates the white light and passes through a broadband plate beamsplitter (Thorlabs, BSW26R) to form a reference pulse and a probe pulse. The reference pulse goes into the spectrometer while a 10-cm focal length lens focuses the probe pulse into the sample. The probe pulse and the pump pulse overlap spatially and temporally in a quartz cuvette (5-mm path length; Starna Scientific).

In the next step, to avoid formation of a bubble in the solution due to laser-sample interaction, a micro-stirrer perturbs the solution in the sample holder. After the

sample, the white light goes into the spectrometer, a grating (50 × 50 mm, 300 nm, 2.5° blaze, 300 grooves/mm; Newport, Ruled Diffraction Grating) disperses the probe pulse and the reference pulse, and focuses them onto a camera (Q Imaging Retiga R6 CCD).

Finally, the experiment is then performed as follows: in the optical path of the pump pulse, a shutter (Thorlabs, SH05) opens for 1 ms. The pump pulse excites the sample and then the probe pulse arrives relative to the pump pulse determined by the delay line position. The camera then records the probe pulse spectrum with the pump pulse and the reference pulse spectrum. The shutter then closes for 1 ms, and the camera records the probe pulse spectrum without the pump pulse and the reference spectrum. During the measurements, the probe pulse spectrum is normalized with respect to the reference at the same time to account for any laser fluctuations during measurements. The percentage of transient transmission T for the probe pulse is first obtained using the equation:

$$T = \left[\frac{T_{pump\ on}}{Reference} - \frac{T_{pump\ off}}{Reference}\right] / \frac{T_{pump\ off}}{Reference} \quad (1)$$

where $T_{pump\ on}$ and $T_{pump\ off}$ are the transmitted probe pulse spectrum with the pump pulse on and off, respectively. The transient absorption A for a particular delay time is then calculated using the equation:

$$A = -\log(T + 1) \quad (2)$$

This process is repeated many times to obtain an averaged spectrum with a good signal-to-noise ratio. Experiments are repeated multiple times on different days under identical conditions to test repeatability and further improve the signal-to-noise ratio. In this case, we collected a total of 2600 transient absorption spectra at each time delay over the course of four days.

The TATB is not soluble in most solvents and only slightly soluble in dimethyl sulfoxide (DMSO). We placed several milligrams of TATB in a 40-mL vial. The DMSO was added to the vial to dissolve some of the TATB. This created a clear solution with a yellow color; undissolved TATB settled to the bottom of the vial. The TATB in DMSO was decanted into another vial such that no undissolved TATB was transferred. The concentration of the TATB in DMSO we used for transient absorption is estimated to be approximately 100 ppm or 4×10^{-4} molarity (M).[7–9] We collected ground state absorption spectra of TATB samples using a CCD array ultraviolet visible (UV-Vis) spectrometer (Si Photonics 400 Series) after diluting the 4×10^{-4} M solution to 5×10^{-5} M.

We used two fitting methods to determine lifetimes of the transient absorption data. First, we used single exponential fits to determine the lifetime of a particular wavelength range within the transient absorption spectrum:

$$f(x) = Aexp\left(\frac{-x}{t}\right) + y_0 \quad (3)$$

where *f(x)* is the difference absorption as a function of wavelength, x is the wavelength, t is the lifetime, and y_0 is the vertical offset. It would become tedious to determine the single exponential fit at each wavelength over the entire wavelength range. In additional, the single exponential fit may not be sufficient to describe a multicomponent system often found in photophysical processes, that is, there could be wavelength overlap between two different excited states that have different lifetimes that would not be described accurately by a single exponential fit. To describe the system more thoroughly, we used global lifetime analysis (IGOR Pro) to determine decay dynamics of the entire spectral range simultaneously. At each wavelength, λ_i the data are fit to a sum of exponentials:

$$f(x, \lambda_i) = \sum_{i=1}^{n} A_i(\lambda_i) exp\left(\frac{-x}{t_i}\right) + y_{0i} \quad (4)$$

where n is the number of wavelengths collected over a wavelength range. To perform the global lifetime analysis, the lifetime at each wavelength is held constant because the lifetime that describes the absorption of each excited state is independent of wavelength. The amplitudes determined from the global analysis of each excited state component vary as a function of wavelength. Plotting these amplitudes creates a decay-associated difference spectrum (DADS) and represents the spectrum of an excited state component.[10–13] Finally, at early times after excitation (<0.5 ps), coherent artifacts that interfere with the transient absorption spectrum are present.[10] In this report, we do not address excited state species at this timescale, so methods for diminishing coherent artifacts are not discussed.

3. Results and Discussion

3.1 Steady State Absorption

The TATB in DMSO solution was diluted to 5×10^{-5} M to collect ground state UV-VIS absorption spectra (no pump) with a maximum absorption of approximately 1.0. In the ground state absorption spectrum of TATB shown in Fig. 2, we observe a TATB absorption band from 300 to 450 nm that peaks at 355 nm. Chu et al.[14] used quantum chemical calculations to predict the electronic excitations of several nitro-containing explosives. They also observed that the π-

antibonding orbital of the nitro group is an unoccupied orbital with a relatively low energy level. It is expected that excitation of TATB will follow a similar pathway. Using the second harmonic from the fs laser, TATB can be excited because the 400-nm pump beam is absorbed efficiently on the red edge of the absorption band. Thus, during excitation, an electron is promoted to the nitrogen dioxide (NO_2) π^* orbital, and we attribute the observed absorption band at 355 nm to $n \rightarrow \pi^*$ transitions. Furthermore, using a combination of experiment and DFT, Chu et al.[6] showed that NO_2 groups are significant for photophysical excitation properties in nitro-containing energetics. The DFT calculations show that upon excitation, the electron density is transferred to the NO_2 groups.

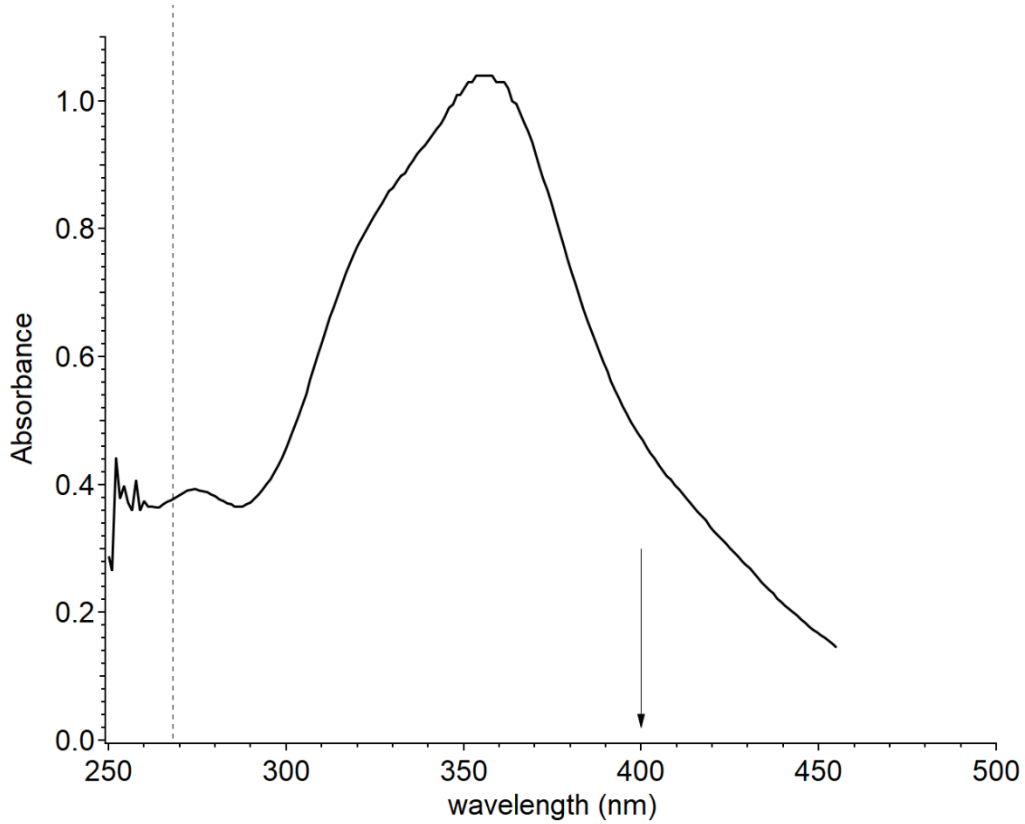

Fig. 2 Ground state UV-Vis absorption spectrum of 5×10^{-5}M TATB. Arrow indicates pump wavelength during transient absorption spectroscopy.

3.2 Transient Absorption

To observe the evolution of the TATB excited states due to an excitation laser pulse, we collected fs transient absorption spectra at various time delays. The transient absorption spectra were calculated from the difference between the absorption spectrum with the 400-nm pump on and the ground state absorption spectrum with no 400-nm pump. Therefore, only absorption changes from species formed due to excitation from the 400-nm pump will be observed. The time evolution of the

excited state species can then be followed at various time delays. In Fig. 3, we show each transient absorption spectrum of TATB from 390 to 700 nm at delay times ranging from 0.5 to 30 ps. There are two prominent absorption bands found in the TATB transient spectra: one is centered at 420 nm and the other is centered at 630 nm. The lifetime of the 630-nm feature is shorter than the lifetime of the 420-nm feature. We used a single exponential model to fit the average intensities from 405 to 435 nm and 620 to 640 nm at each delay time to estimate the lifetime of the 420- and 630-nm bands, respectively. The average intensity from 620 to 640 nm at each time delay as well as the single exponential fit is shown in Fig. 4a. The lifetime was calculated to be 0.64 ± 0.02 ps. The average intensity from 405 to 435 nm at each time delay as well as the single exponential fit is shown in Fig. 4b. The lifetime was calculated to be 4.77 ± 0.06 ps. Next, we used global fit analysis to thoroughly analyze the excited state lifetimes and determine the DADS of each excited state. We used a double exponential fit at each wavelength to perform global lifetime analysis because the single exponential fit analysis in each region yielded different lifetimes:

$$f(x) = A_1 exp\left(\frac{-x}{t_1}\right) + A_2 exp\left(\frac{-x}{t_2}\right) + y. \quad (5)$$

The two lifetimes calculated using global lifetime analysis were t_1 = 0.721 ± 0.003 ps and t_2 = 4.43 ± 0.01 ps. We plotted the amplitudes of each component (A_1 and A_2) at each wavelength from 390 to 700 nm to form the two DADS in Fig. 5. These DADS show the absorption features of the two prominent excited state components of TATB found over this wavelength and time range. The DADS with an approximately 0.7 ps lifetime has two absorption features at 477 and 650 nm, whereas the longer-lived DADS only has one absorption feature at 420 nm.

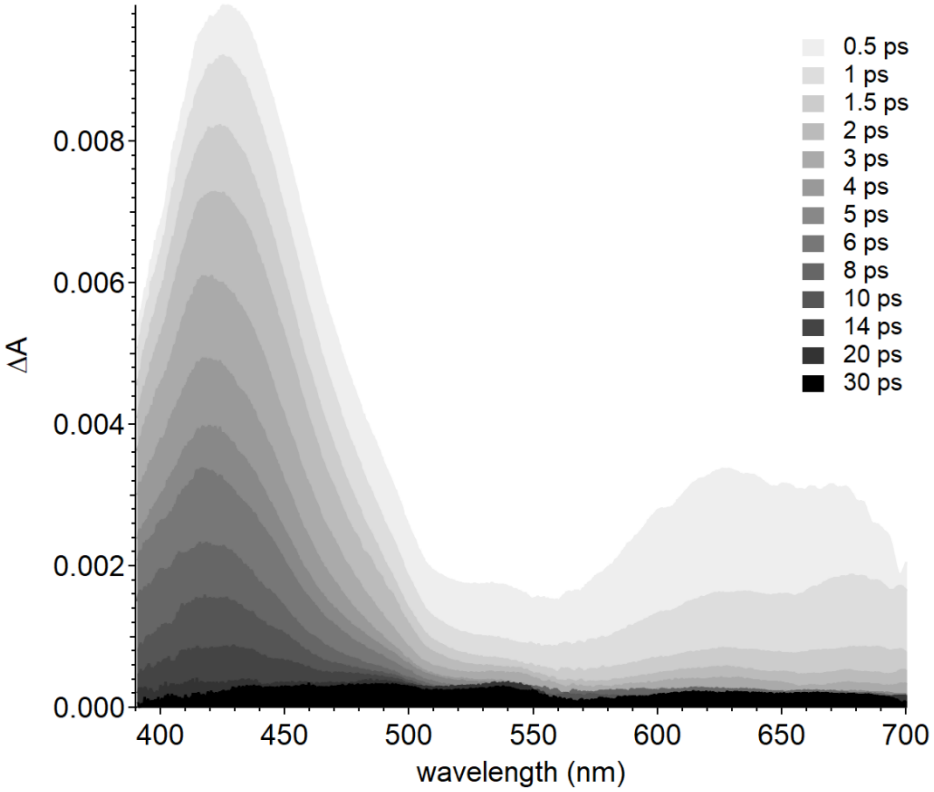

Fig. 3 Transient absorption spectra of TATB at various time delays

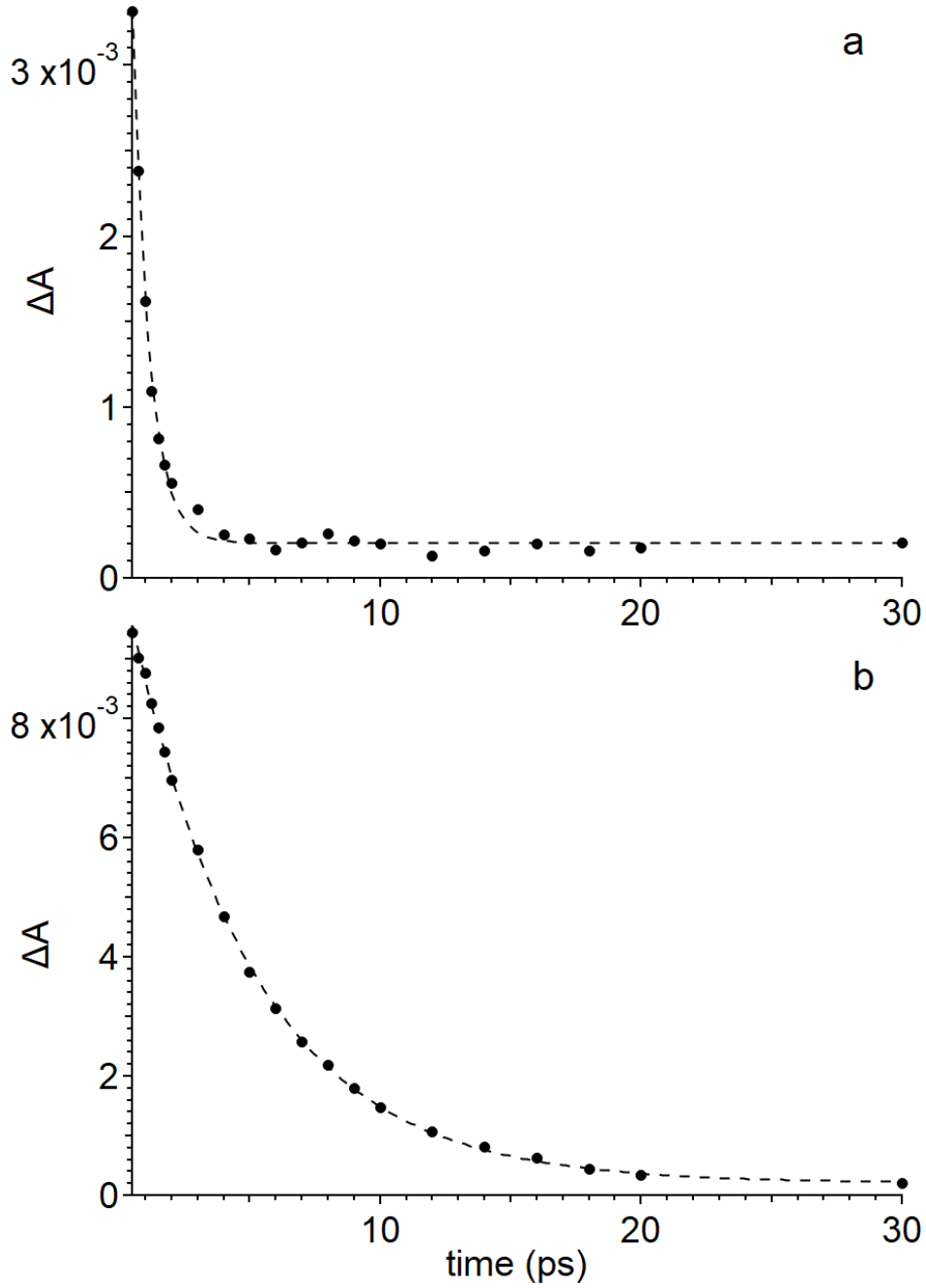

Fig. 4 The difference absorption values at a) 630 nm and b) 420 nm for each time delay collected using transient absorption fitted to a single exponential decay

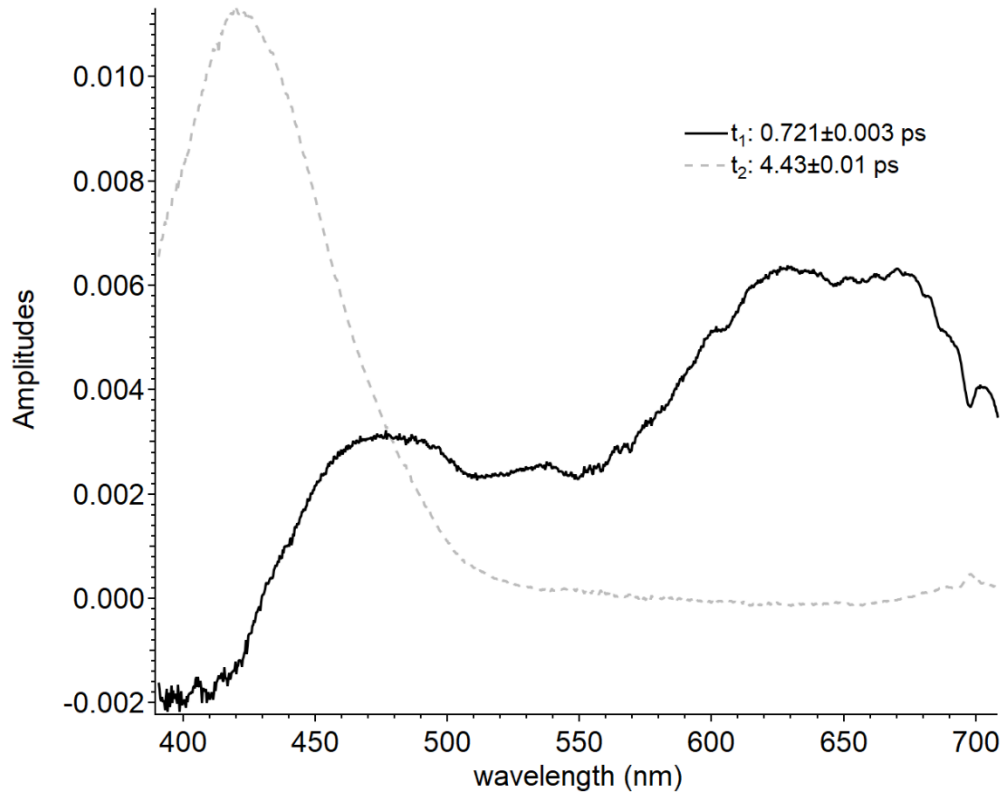

Fig. 5 DADS calculated from the transient absorption spectra

3.3 Potential Photoinduced Relaxation Pathways

In previous work, DFT calculations of TATB have shown that upon initial excitation, charge transfer occurs rapidly to the NO_2 groups.[6] Upon relaxation, the charge density is redistributed and localized onto one NO_2 group. This excited state and subsequent electron redistribution are assigned to a $S_1^* \rightarrow S_1$ vibrational relaxation transition.[6] From this S_1 state, two possible relaxation pathways present themselves according to previous studies.[6,14,15] First, according to Chu et al.,[6] the S_1 state leads to intersystem crossing to a triplet state in a time frame of 6 ps. This is comparable to the 4.4-ps lifetime we determined for the longer-lived component in Fig. 5. The nonbonding orbitals of the nitro group can increase the likelihood of triplet excited state formation. The DFT calculations indicate that such a transition occurs along a S_1-T_1 conical intersection.[6] Thus, the longer-lived component can be attributed to the transient absorption of the S_1 state and its subsequent intersystem crossing to a triplet state. In this relaxation pathway, the shorter-lived component from Fig. 5 can be attributed to the transient absorption of the S_1^* state and its subsequent vibrational relaxation due to charge density redistribution. For the shorter-lived component, we calculated a 0.72-ps lifetime. This is comparable to the 0.64-ps lifetime determined by Chu et al.[6] The authors propose several

reasons that a relaxation to a triplet state from the S_1 state is a reasonable assumption. However, there is no experimental evidence of triplet formation in this work or our own experiments, that is, no long-lived component on an ns timescale one would expect from a triplet state. Another nitro-containing explosive, hexanitrostilbene, did show evidence of an ns component in its measured transient absorption spectra.[16] The lack of any long-lived component in TATB transient absorption spectra seems to diminish the likelihood that triplet formation is a dominant relaxation pathway.

The second possible relaxation pathway is a transition from the S_1 state to a hot ground state via a conical intersection.[15] Previous studies have shown that energetic materials and nitrated amines use conical intersections for fast relaxation from excited states to the ground state.[15,17] According to Tang and Fang,[15] the lifetime of the S_1 state in 3-nitrotyrosine is estimated to be approximately 0.4 ps before it reaches the conical intersection and relaxes to the hot ground state. Chu et al.[14] have shown a relaxed structure using time-dependent DFT for several energetics: RDX, 1,3,5,7-tetranitro-1,3,5,7-tetrazocane, 2,6-diamino-3,5-dinitropyrazine-1-oxide, etc. that is formed after relaxation from an excited state. This relaxed state is similar to the hot ground state observed in 3-nitrotyrosine in that they are both higher energy ground states. The lifetime of the 0.72-ps component from TATB in Fig. 5 is comparable to the estimated 0.4-ps lifetime of the S_1 state in 3-nitrotyrosine. We attributed the transient absorption of the S_1 state to the short-lived component, keeping in mind we are comparing two different molecules: TATB versus 3-nitrotyrosine. We attributed the 4.4-ps component from the TATB global analysis in Fig. 5 to the absorption of the hot ground state. Tang and Fang[15] used a biexponential decay model to calculate the lifetimes (1 and 9 ps) of the hot ground state. A single lifetime (4.4 ps) describes the hot ground state in TATB, but the lifetime occurs in the same time frame as the two lifetimes found in 3-nitrotyrosine. In this excitation and relaxation pathway, we do not observe the short-lived S_1* state that describes the first distribution of electron density upon excitation at each nitro group.[6] However, this S_1* state could be a very fast lived, excited state (<0.4 ps) we do not observe in our current experimental setup due to interference from coherent artifacts arising from pump probe pulse overlap.

4. Conclusion

We collected transient absorption spectra of the energetic TATB over a 30-ps range using our system built at ARL. Using this system, we collected high-quality, low-noise transient spectra at various time delays. We then used a global analysis fit with a biexponential model to analyze the data set and determine the kinetics and the DADS associated with each decay lifetime. The two DADS represented excited

states found during excitation of TATB—a 0.72-ps component and a longer-lived 4.4-ps component. Assigning each of these components to a particular excited state was not straightforward because there were two potential excitation and subsequent relaxation pathways found in literature. In particular, what is the lifetime of the S_1 excited state, and does it relax to a triplet state or a hot ground state? There is evidence for both pathways, but the more likely pathway is that a hot ground state is formed because there is a lack of experimental evidence of a longer-lived (ns) triplet state in ours and others experiments.[6]

In future work, investigation of nitro-containing model systems such as 4-nitroaniline, 3-nitroaniline, and 2-nitroaniline will be performed to observe the photophysics of the excitation and relaxation pathways due to the positions of the amine groups relative to the nitro groups compared to TATB. Modeling and theoretical studies should also be performed on the transient absorption data collected from TATB and any other nitroanilines collected in the future. In addition, multicomponent regression (MCR) analysis could be used to analyze the data set. There are some advantages to using MCR as opposed to global analysis.[10] Finally, it would be advantageous to be able to observe shorter lived excited state species (<400 fs) by eliminating interference due to pump probe pulse overlap. According to Bhattacharya et al.,[17] the initial step in excited state decomposition of an energetic could be ultrafast (<200 fs) and lead to rapid energy transfer from the upper excited states to the ground state. With less interference, we could potentially observe any extremely short-lived excited states, similar to that observed in 3-tyrosine,[15] which could lend more experimental evidence to the hypothesis that the S_1 state relaxation pathway leads to a hot ground state.

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List of Symbols, Abbreviations, and Acronyms

ARL	Army Research Laboratory
DADS	decay-associated difference spectrum
DEVCOM	US Army Combat Capabilities Development Command
DFT	density functional theory
DMSO	dimethyl sulfoxide
M	molarity
MCR	multicomponent regression
RDX	1,3,5-trinitroperhydro-1,3,5-triazine
TATB	2,4,6-trinitrobenzene-1,3,5-triamine
Ti:S	titanium-sapphire
UV-Vis	ultraviolet visible

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