Kinetic Studies of 1,3-bis(4-chlorophenyl)triazene

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While the main focus of this project was to study the kinetics of the thermal cis-to-trans isomerization of 1,3-bis(4-chlorophenyl)triazene, some preliminary work had to be done. First, the compound was prepared using the amine method, by combining chloroaniline and sodium hexanitrocobaltate(III) in a one-pot synthesis. Second, the pK_a of the substrate was determined using UV-visible absorption spectroscopy. The pK_a (in a 30:70 THF:H₂0 solution) was found to be 13.2. Third, also using UV-visible absorption spectroscopy, the kinetics of the hydrolytic decomposition of the compound was studied. The decomposition was found to follow a first order reaction and to accelerate as the pH decreases.



1,3-bis(4-chlorophenyl)triazene

The thermal cis-to-trans isomerization of the substrate was studied using time-resolved laser-flash photolysis with laser excitation at 355 nm. The results obtained from this study agree with the mechanism proposed from previous triazene studies. That is, two processes were observed. The first process is attributed to the interconversion of rotamers around the N-N single bond while the substrate is in the cis form. The second process is attributed to the cis-to-trans isomerization, which takes place *via* an 1,3-prototropic rearrangement and is catalyzed by general acids and bases.