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Evidence of Carbenes in the Explosion Chemistry of Nitroaromatic Anion Radicals

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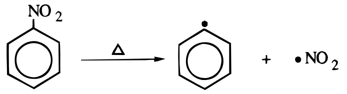
The solid potassium salts of the nitrobenzene anion radical [$K^+C_6H_5NO_2{}^{\bullet-}{}_{(solid)}$] and all three nitrotoluene anion radicals were generated via the potassium reduction of the nitroaromatic in liquid ammonia followed by removal of the ammonia. These solid salts were found to be very shock- and impact-sensitive explosives, which emit a number of gasses, including CO, CO_2, CH_4, and H_2, upon detonation. No other low molecular weight products are formed, and mass spectral analysis of the solid "ash" shows that all organic components of it are polymeric in nature. The initiation step in the detonations appears to be the cleavage of the C−NO_2 bond (e.g., $K^+C_6H_5NO_2{}^{\bullet-}{}_{(solid)} \rightarrow C_6H_5{}^{\bullet} + KNO_{2(solid)}$). The polymerization results in the release of the hydrogen gas, and trapping experiments indicate that the methane is formed from an intermediate carbene that reacts with the molecular hydrogen. Indeed, carrying out the explosions under an atmosphere of CH_4 results in the formation of ethane, presumably via carbene insertion into the H_3C−H bond. On the basis of this and deuterium labeling experiments, a mechanism is proposed that accounts for the formation of $NO_2{}^-$ (detected via IR in the ash) H_2, CH_4, and polymeric material.

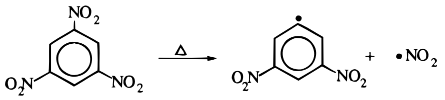
Introduction

As noted by Brill's and Tsang's groups, the homolytic cleavage of the C−NO_2 bond (reaction 1) is the most important primary step in both the thermal decomposition of nitrobenzene and in the impact initiated explosion of trinitrobenzene.[1,2] Due to the high energy of activation ($k = 1.5 \times 10^{15}e^{-297.9\text{kJ/mol}/RT}$)[3] the dissociation of nitrobenzene (first reported in this journal)[4a] is rapid only at very elevated temperatures (>1000 K). Further, the aromatic ring structure maintains much of its integrity after bond cleavage at temperatures up to 750 K.[2] This inhibits the formation of carbon-containing gasses and yields a variety of liquid products resulting from phenyl radical reactions.[4] Benzene, phenol, benzonitrile, biphenyl, dibenzofuran, terphenyls, and several more minor species make up the liquid products during pyrolysis from 673 to 900 K.[4] The factors discussed above and the formation of gaseous products with positive heats of formation (NO_2, NO, N_2O) and the small amounts of CO_2 and CO render nitrobenzene ($C_6H_5NO_2$) shelf stable and impervious to detonation via thermal or physical shock.



(1)

Trinitrobenzene (TNB) is a relatively thermally stable explosive, as the analogous homonuclear bond cleavage (reaction 2) represents the explosion initiation step, which has an energy of activation (266.3 kJ/mol)[1] nearly identical to that for reaction 1. However, the inhibition of carbon-containing gasses is compromised, and when TNB is heated to temperatures as low as 790 K, large amounts of both CO_2 and CO are produced.[1] It is believed that both IR-inactive N_2 and H_2 are also formed,[1] and the high heat of explosion[5] results from the formation of products with negative heats of formation (CO, CO_2, and HNCO) and the lack of formation of products with positive heats of formation (NO, HCN, and N_2O).[1] Despite the complexity of the reaction steps following the homolysis of trinitrobenzene, the energy of activation (E_a) is very close to the bond dissociation energy, which suggests that reaction 2 is the rate-determining step.[1]



(2)

Gas phase $C_6H_5NO_2$ accepts an electron exothermically (EA = 95.3 kJ/mol),[6] and potassium anion radical salts typically have crystal lattice energies of >700 kJ/mol.[7] This, in conjunction with the ionization potential of potassium, places the $K^+C_6H_5NO_2{}^{\bullet-}$ solid anion radical salt energetically downhill from $C_6H_5NO_2$, Scheme 1.[8,9]

(enthalpies in kJ/mol)

$$\begin{array}{rl}
C_6H_5NO_{2(gas)} + e^-{}_{(gas)} \rightarrow C_6H_5NO_2{}^{\bullet-}{}_{(gas)} & \Delta H° = -95.3 \\
K_{(gas)} \rightarrow K^+{}_{(gas)} + e^-{}_{(gas)} & \Delta H° = +418 \\
K_{(solid)} \rightarrow K_{(gas)} & \Delta H° = +89.5 \\
K^+{}_{(gas)} + C_6H_5NO_2{}^{\bullet-}{}_{(gas)} \rightarrow K^+C_6H_5NO_2{}^{\bullet-}{}_{(solid)} & \Delta H° \sim -700 \\
C_6H_5NO_{2(liquid)} \rightarrow C_6H_5NO_{2(gas)} & \Delta H° = +51 \\
\hline
C_6H_5NO_{2(liquid)} + K_{(solid)} \rightarrow K^+C_6H_5NO_2{}^{\bullet-}{}_{(solid)} & \Delta H° \sim -237
\end{array}$$

Here we report that despite the negative heats of generation of their anion radical salts from the metal and neutral molecules in their standard states, $K^+C_6H_5NO_2{}^{\bullet-}{}_{(solid)}$ and $K^+CH_3C_6H_5NO_2{}^{\bullet-}{}_{(solid)}$ are very

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shock- and impact-sensitive explosives. We were motivated to investigate the detonation chemistry and the explosive nature of these anion radicals and compare them to those of the neutral nitroaromatics and the common explosive TNB in terms of a particular question: does the nature of the decomposition of solid nitroaromatic anion radical salts resemble that of the nitroaromatic explosives or is it basically the same as that for neutral nitroaromatics but with a lower E_a due to a weakening of the $C-NO_2$ bond?

Experimental Section

Samples of the anion radical of nitrobenzene (1.5−2.5 mmol) were generated via reduction of nitrobenzene in an evacuated apparatus on a potassium metal mirror in 30−40 mL of liquid ammonia at −78 °C as previously described.[10] The solvent was removed under reduced pressure, leaving dark red crystals. The solid $K^+C_6H_5NO_2^{\bullet-}$ was then left exposed to vacuum (10^{-3} Torr) to ensure the complete removal of the ammonia. The resulting crystals are extremely shock sensitive. To prevent premature detonation, the apparatus had to be supported so as to protect it from the vibration of the vacuum pump, and the all glass apparatuses were always kept behind explosion shields. The quantity of anion radical salt was always small, and detonation normally did not rupture the 100 mL glass bulb containing it. The detonations were initiated by simple agitation of the glass bulb.

To ensure that NH_3 did not remain in the solid salt, samples of it were quenched with H_2O and the resulting H_2O solution divided into two equal portions. One portion was boiled for 15 min to eliminate any dissolved ammonia, and both were titrated with a standard solution of HCl. Both titrations proved to be identical, indicating the absence of ammonia. In one experiment a detonation occurred just as the water entered the bulb. Apparently, the initial contact of the water with the salt caused a detonation.

The bulb containing the detonation products was connected to the high vacuum system through U-tube no. 1, which was cooled to −78 °C. After the line was pumped down to about 10^{-6} Torr, the stopcock separating the bulb and the high vacuum system (stopcock J) was opened and the gasses allowed into the line, Figure 1. The pressure in the vacuum system was monitored with a Fluid Precision Inc. capacitron pressure gauge to ±0.01 Torr. The final pressures ranged from 50 to 100 Torr. From the known volume of the vacuum system (831.6 mL), the number of moles of noncondensable gases that passed through the U-tube was obtained. The relative amounts of the gaseous products vary slightly from experiment to experiment. However, in a typical experiment involving 2.5 mmol of $K^+C_6H_5NO_2^{\bullet-}{}_{(\mathrm{solid})}$, 0 to as much as 0.20 mmol of NO_2 was evolved along with 2.6 mmol of noncondensable (−78 °C) gasses. Of these noncondensable gasses, 1.6 mmol proved to be hydrogen.

When these noncondensable gases were exposed to a 300 °C Cu−CuO furnace, the pressure dropped due to the oxidation of the H_2 to form water, which was trapped in U-tube no. 2. In separate experiments mixtures of methane and hydrogen were injected into the system to verify that the hot CuO would selectively oxidize the H_2 leaving the CH_4. This vacuum system was fitted with a 10 cm gas IR cell, allowing us to take an IR sample at any time.

The characteristic blue (brown gas) NO_2 was the only material found in U-tube no. 1. After the reaction gasses were pumped from the line, the NO_2 was condensed through stopcock C into a standardized NaOH solution, which was subsequently titrated with standardized HCl. GC−mass spectral analysis failed to show the existence of any other substance in U-tube no. 1. Thus, the liquid products (benzene, etc.) formed during the pyrolysis of nitrobenzene do not form during the detonation of its anion radical.

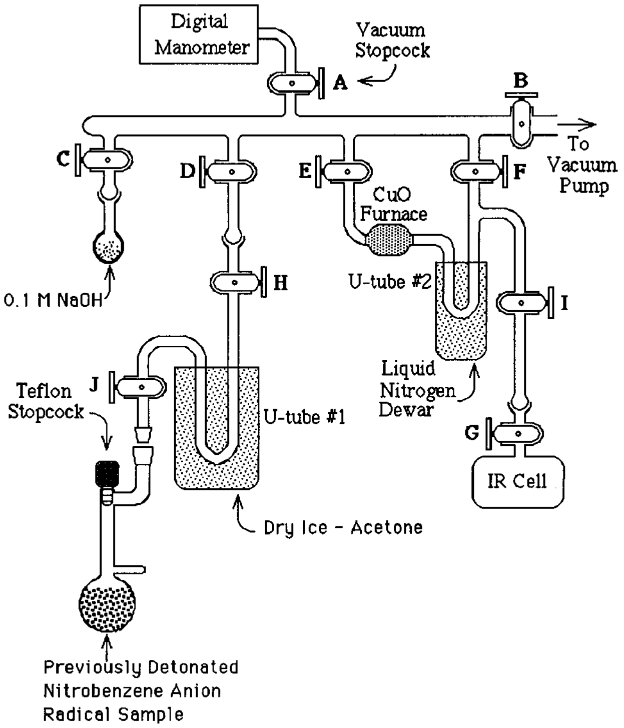

Figure 1. Vacuum apparatus used for the analysis of the gasses produced from the detonation of the solid potassium salt of the nitrobenzene anion radical. The system was pumped down to 10^{-6} Torr prior to opening the Teflon stopcock to allow the gasses into the vacuum line.

Spectroscopic analyses were carried out using a Nicolet FT-IR using a gas cell fitted with sodium chloride windows. Matrix-assisted laser desorption time of flight mass spectra were obtained in the Mass Spectrometry Laboratory, School of Chemical Sciences, University of Illinois.

Results and Discussion

The reduction of nitrobenzene in liquid ammonia with a stoichiometric amount of potassium metal results in the formation of the corresponding solvated anion radical, which exhibits the characteristic 54 line pattern upon EPR analysis.[10] Removal of the solvent under reduced pressure leaves the dark red salt, $K^+C_6H_5NO_2^{\bullet-}{}_{(\mathrm{solid})}$. After exposure to high vacuum for about 1 h, the solid anion radical salt is free of residual ammonia. This was evidenced by the fact that the addition of H_2O to this solid yields a water solution that is free of ammonia. This is in contrast to the anion radical alkaline earth metal salts that do retain ammonia in the complex, e.g., $Ba^{2+}(NH_3)_2(\text{naphthalene}^{\bullet-})_2$.[11]

The most remarkable feature of $K^+C_6H_5NO_2^{\bullet-}{}_{(\mathrm{solid})}$ is its extreme thermal and shock sensitivity. In over 90% of the samples generated,[12] a gentle agitation of the evacuated reaction vessel containing the salt resulted in a violent detonation that was concomitant with a yellow flash of light and the production of a dark cloud inside of the reaction vessel. To avoid the shattering of the

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[8] For the ionization potential of potassium see: Lotz, W. *J. Opt. Soc. Am.* **1967**, *57*, 873.

[9] For the $\Delta H_{(\mathrm{sublimn})}$ of potassium see: Hicks, W. T. *J. Phys. Chem.* **1963**, *38*, 1873.

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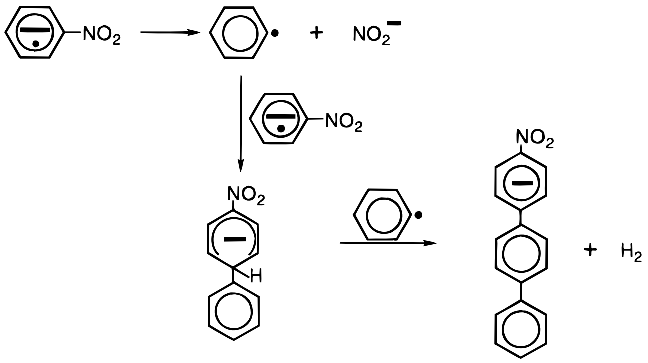
[12] Shock and impact sensitivity are influenced by crystal size, crystal defects, and crystal orientation; see ref 1.

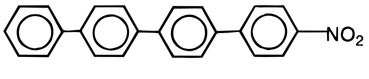
Scheme 2



reaction vessel, care was taken to use small amounts of salt (<200 mg) and large glass reaction vessels (100 mL), which can accommodate the volume of evolved gas. It should be noted that, even under these conditions, the apparatus was occasionally shattered.

The noncondensable (in dry ice−acetone) gasses, which amount to about 1.0 mol per mole of solid salt, were allowed into a high vacuum system, Figure 1. The vacuum system was equipped with a CuO oven and an IR cell. Heating of the CuO furnace resulted in an immediate drop in the total pressure to 38% of its original value ($CuO + H_2 \rightarrow Cu + H_2O$), indicating that 62% of the gas was hydrogen. The concomitant deposition of water ice in the frozen U-tube was also observed.

It seems probable that the release of hydrogen results from a polymerization that is analogous to that of the naphthalene anion radical.[13] In agreement with this mechanism, a granular black solid polymeric material remained after the detonation. This material was quenched under vacuum with I_2 in diethyl ether. Laser desorption mass spectral analysis of the quenched material reveals major positive ion peaks at *m/e* 205, 351, and 462. The peak at 205 is simply $[K_2I]^+$ and was expected, as the quench involved iodine. The 351 peak can be accounted for by the positive ion of a system with five phenyl and one NO_2 moieties (i.e., structure I or one of its isomers), and the peak at *m/e* 462 may represent $[KC_6H_5(C_6H_4)_4NO_2^+]$. At any rate, it is clear that polymeric material is produced, which is consistent with the H_2 formation.



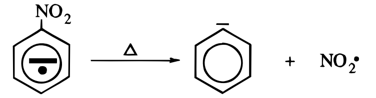
I

Indeed, the IR spectrum of the water-soluble portion of the solid reaction residue reveals the characteristic broad peak from the asymmetric NO_2^- stretch at 1640 cm^{-1} and the other characteristic bands for NO_2^-. This is consistent with an initial rupturing of the C−NO_2 bond as in reaction 1 but with the negative charge following the nitro group as shown in Scheme 2, which accounts for the formation of the polymer, hydrogen, and nitrite.

In view of the formation of nitrite ion, the fact that NO_2 was found in the dry ice cooled U tube (no. 1 in Figure 1) was somewhat surprising. There are, however, two possible explanations for the formation of neutral NO_2: (1) reaction 4 is taking place simultaneously with the first step in Scheme 2, and (2) the NO_2 comes from residual neutral $C_6H_5NO_2$ remaining in the anion radical salt. This neutral material would simply react as de-

Table 1. IR-Active Gasses Evolved from the Detonation of $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$, the Thermolysis of $C_6H_5NO_2$ at 748 K and the Detonation of TNB

	rel abundance, %		
gas	$K^+C_6H_5NO_2^{\bullet -}$ detonation	$C_6H_5NO_2$ thermolysis[4]	TNB detonation[1]
CO_2	40	1	6
CO	30	5	94
CH_4	30	not found	not found
N_2O	not found	0.4	not found
NO_2	not found	81	not found
NO	not found	12	not found
NH_3	not found	not found	not found

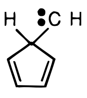


(4)

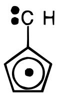
scribed in reaction 1.[3] To test these two possibilities, samples of nitrobenzene were reduced with a slight excess of K to ensure full reduction to anion radical. Under these conditions, neither NO_2 nor N_2O was found in the postexplosion gasses. All of the remaining products proved to be identical to those produced when the solid anion radical salt was contaminated with a small amount of neutral nitrobenzene. Thus, the NO_2 and N_2O were produced from the pyrolysis of neutral nitrobenzene present during the explosion of the anion radical salt.

In the absence of neutral $C_6H_5NO_2$ contamination, the IR measurements of the noncondensable (−78 °C) gasses revealed the presence of only CO, CO_2, and CH_4. It should be kept in mind that H_2 is also present as mentioned above. The IR-active gasses evolved during the $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$ detonation are similar to those evolved during the pyrolysis of neutral TNB, Table 1. The notable exception is methane, which is a major product of the $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$ detonation, yet is not observed at all during the pyrolysis of neutral $C_6H_5NO_2$ or the explosion of TNB. Methane is a surprising product, as there are no carbons bonded to more than one hydrogen in $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$. Thus, CH_4 formation must involve the capture of hydrogen by a carbon fragment. The methane does not come from residual solvent or other impurity, as is evidenced by the fact that the detonation of $K^+C_6D_5NO_2^{\bullet -}{}_{(solid)}$ yields CD_4 and no CH_4.

It is possible that the methane is formed from the methyl radical, but this would still require three protons to gather on a single carbon. Another possible mechanism for the methane formation can be taken from an analogy with a mechanism proposed by Scott and coworkers for the high temperature automerization of 1,2-di-^{13}C-benzene, which involves a carbene intermediate, Structure II.[14] Here, the cyclopentadiene moiety is replaced by a cyclopentadienyl radical, structure III.



II



III

The compound depicted in structure III would react with hydrogen, which has been found to be present, to

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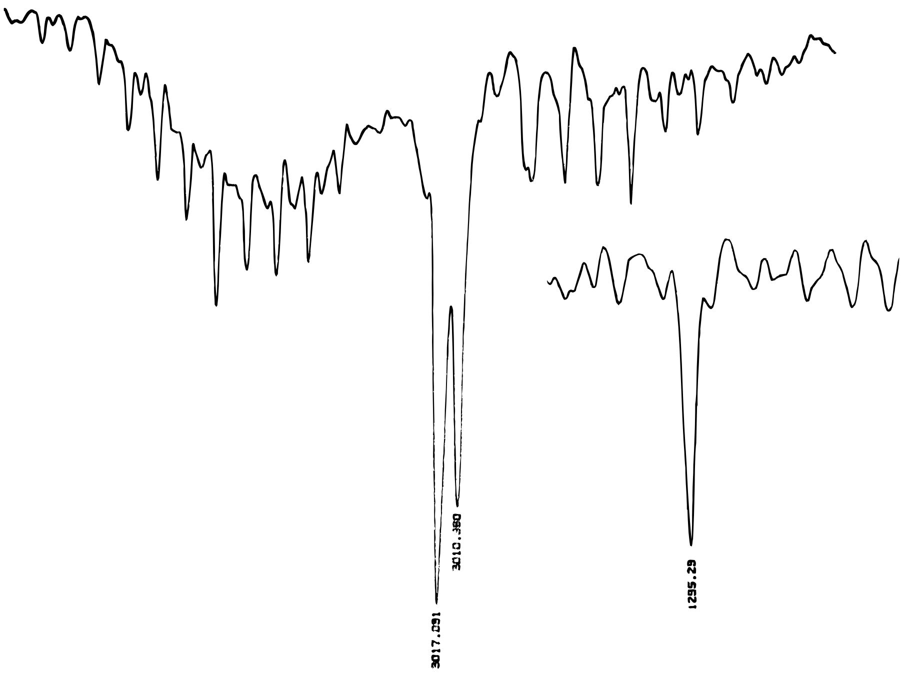
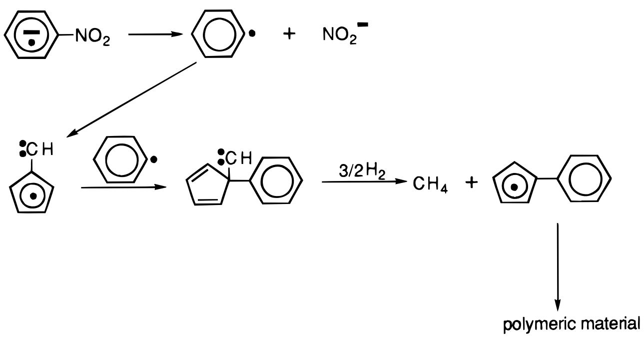


Figure 2. FT-IR spectrum of the gaseous reaction products resulting from a detonation of a mixture of $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$ and $K^+C_6D_5NO_2^{\bullet -}{}_{(solid)}$. Note the strong peak at 1295 cm^{-1} (inset) due to the symmetrical bending mode of CHD_3 and the band at 3017 due to the asymmetrical stretch in CH_3D. The peak at 3011 is due to the asymmetrical stretch in CH_2D_2.

Scheme 3



yield methane. To test this idea, we introduced deuterium gas into the reaction vessel prior to initiating the explosion. Indeed, IR analysis proved CH_2D_2 to be present along with CHD_3 and CH_3D in the postexplosion gasses. The presence of CHD_3 strongly favors a mechanism involving a carbene over a methyl radical. Scheme 3 involves the very stable cyclopentadienyl moiety and accounts for the methane formation. Also consistent with Scheme 3 is the fact that the explosion of a mixture of $K^+C_6D_5NO_2^{\bullet -}{}_{(solid)}$ and $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$ yields all four CH_xD_{4-x}'s, Figure 2.

To give further support to the existence of carbene as a reactive intermediate, we carried out explosions under an atmosphere of methane. Since there is no reasonable means of formation of ethane from methane other than carbene insertion into the H_3C-H bond, we thought that the presence of ethane would represent significant evidence for the involvement of carbene. Indeed, ethane was found in the postexplosion gasses, Figure 3.

The pyrolysis of o-nitrotoluene (o-$CH_3C_6H_5NO_2$) follows a different mechanism than that of $C_6H_5NO_2$ as evidenced by the formation and destruction of anthranil during the decomposition of the former (Scheme 4).[15] Anthranil (a stable intermediate) provides a pathway with a lower energy of activation. Thus, *o*-methyl substitution increases the rate of decomposition over that of nitrobenzene by 1 order of magnitude[3] and provides anthranil, *o*-cresol, and cyanocyclopentadiene as products.[15] The solid anion radical salts of *o*-, *m*-, and *p*-nitrotoluenes can be formed and detonated in a manner identical to that of $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$. For all three of these materials CH_4, CO, CO_2, and H_2 make up the gas phase products, and as in the case of $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$ no liquid or low molecular weight solid products were formed. Further, the K^+o-$CH_3C_6H_5NO_2^{\bullet -}{}_{(solid)}$ did not exhibit any extra shock sensitivity when compared to those of K^+p-$CH_3C_6H_5NO_2^{\bullet -}{}_{(solid)}$, K^+m-$CH_3C_6H_5NO_2^{\bullet -}{}_{(solid)}$, or $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$. This suggests that all three of these methyl-substituted systems undergo detonation in a manner that is analogous to that of $K^+C_6H_5NO_2^{\bullet -}{}_{(solid)}$, and the mechanism of decomposition of K^+o-$CH_3C_6H_5NO_2^{\bullet -}{}_{(solid)}$ does not involve anthranil or an anthranil radical.

Summary and Conclusions

Highly explosive anion radical salts of nitroaromatics are efficiently formed via electron transfer from potassium metal in liquid ammonia followed by evaporation of the ammonia. These anion radical solid salts were found to be very shock- and impact-sensitive explosives that emit a number of gasses including CO, CO_2, CH_4, and H_2, upon detonation. It is proposed that the initiation step is the cleavage of the $C-NO_2$ bond, which is easier to disrupt (forming potassium nitrite) due to the presence of the extra electron. The electron apportionment follows the "regioconserved" or heterolytic (mesolytic) mode, as observed for other anion radical sys-

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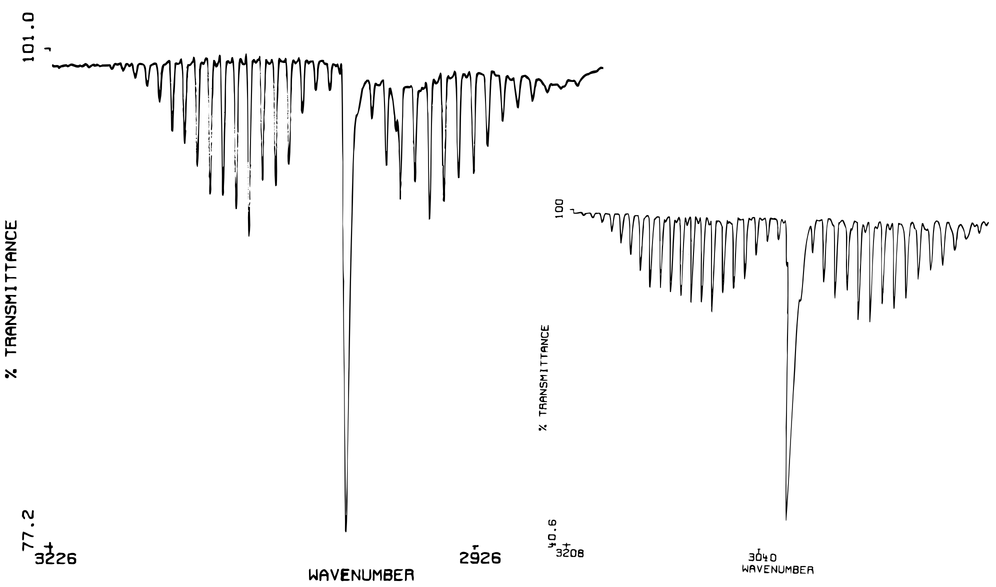
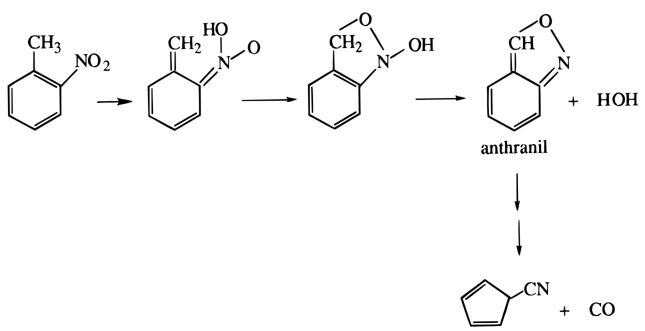


Figure 3. FT-IR spectrum of methane (inset) and the gaseous products resulting from the detonation of nitrobenzene in an atmosphere of methane. Note the presence of ethane absorptions under the P branch of the methane spectrum. This spectrum can be reproduced by mixing a small amount of ethane in methane in the IR cell.

Scheme 4



Scheme 5

	$\Delta H°$, kJ/mol	ref
$NO_2{}^\bullet{}_{(gas)} + e^- \rightarrow NO_2{}^-{}_{(gas)}$	−377	17
$C_6H_5NO_2{}^{\bullet -}{}_{(gas)} \rightarrow C_6H_5NO_{2(gas)} + e^-{}_{(gas)}$	+95.3	6
$C_6H_5NO_{2(gas)} \rightarrow NO_2{}^\bullet{}_{(gas)} + C_6H_5{}^\bullet{}_{(gas)}$	+299	18
$C_6H_5NO_2{}^{\bullet -}{}_{(gas)} \rightarrow NO_2{}^-{}_{(gas)} + C_6H_5{}^\bullet{}_{(gas)}$	+17.3	

tems.[16] Methane is formed from an intermediate carbene that, in turn, is created from the phenyl anion.

The presence of an extra electron renders the innocuous nitrobenzene, nitrotoluene, and many other nitroaromatic systems powerful explosives that are extremely more shock and impact sensitive than are TNB or TNT. The odd electron directs a different pathway for the molecular decomposition, and the extreme difference in the sensitivities of the anion radical and neutral nitroaromatics is apparently due to the fact that the C−NO_2 bond dissociation energy is considerably attenuated (by 282 kJ/mol) by the presence of the extra electron, Scheme 5. We suspect that this will be the case for the anion radicals of nitroaromatics in general.

This work indicates that the addition of an electron followed by isolation of the anion radical salt will render a large number of otherwise nonexplosive nitroaromatic materials explosive. Further, the solid anion radical salts of common nitroaromatic explosives (DNT, TNT, etc.) may be considerably more potent than their neutral analogues. These matters are under current investigation.

There is great variability in the impact and shock sensitivity of nitro aromatic explosives, and a wide number of correlations have been made, some of which have been called absurd.[1] It is important to keep in mind that since nitroaromatic anion radicals are very thermodynamically stable[9] (they persist even in water)[10] they can be easily generated via electron transfer. Further, evaporation of the solvent leaves the solid anion radicals. The presence of trace quantities of these anion radicals (e.g., $TNT^{\bullet -}$) in high energy materials can result from electron transfer from Lewis base impurities. These anion radicals could significantly contribute to the reported[1] variability in shock sensitivity and, perhaps, even to inadvertent disasters.

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