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Probing trinitrotoluene (TNT) by low-energy electrons: Strong fragmentation following attachment of electrons near 0 eV

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ABSTRACT

Electron attachment to gas phase trinitrotoluene (TNT) is studied by means of a crossed electron-molecular beam experiment at high-energy resolution. TNT shows unique features in the way that electrons right at threshold (near 0 eV) generate both the non-decomposed anion and a variety of anions arising from dissociative electron attachment (DEA). While the parent anion is formed within a very narrow resonance near 0 eV, the DEA reactions extend to higher energies and are operative via several resonant features in the energy range 0–10 eV. They involve remarkably complex reaction sequences associated with multiple bond cleavages and formation of new bonds. By far the dominant DEA reaction generates an ion formed by the loss of a neutral OH radical from the precursor ion. Further strong ion signals arise from the loss of up to three neutral NO units. The remarkable instability of TNT following attachment of electrons with virtually no energy underlines the explosive nature of this compound.

1. Introduction

Trinitrotoluene (TNT) belongs to the group of aromatic nitro compounds which have extended use in industrial applications, in particular as explosives or additives to explosives [1]. The molecule has been industrially synthesised for more than 100 years and TNT still serves as a measure for the strength of an explosive. An explosive is characterised by the presence of the elements H, N, C and O *within* the molecule. Stable reaction products like N_2, CO, CO_2 and H_2O can then *intrinsically* be formed as opposed to the usual combustion of hydrocarbons which requires the addition of O_2 with the consequence that the velocity of the reaction is limited by diffusion.

Electron attachment to nitrobenzene (NB), nitrotoluene (NT) and some other aromatic nitrocompounds was studied rather early by means of swarm and electron beam techniques [2,3]. It was found that these compounds form long-lived molecular anions and also undergo dissociative electron attachment yielding NO_2^-. Different subsequent studies considered the potential of NO_2^- to serve as a fingerprint for the identification of the neutral compound [4–6]. The potential of DEA to identify different structural isomers by recording the ion yield curves of the various fragments was recently demonstrated in the case of the three isomers of NT [7] and dinitrobenzene (DNB) [8].

For TNT we find an early mass spectrometric study demonstrating that the negative ion mass spectrum recorded at about 2 eV substantially differs from that recorded at an electron energy of about 6 eV [9] in the way that the spectrum recorded at lower energy shows considerably more fragment anions. A further mass spectrum obtained at essentially zero energy [6] showed that the parent anion but also fragment anions are generated.

In this contribution we explore negative ion formation following electron attachment to TNT by recording the ion yield curves at high electron energy resolution. We find that by far the dominant signal is due to an anion which is formed by the loss of a neutral OH molecule from the transient negative ion. This is in striking contrast to other aromatic nitrocompounds, where it was found that formation of the parent anion with low energy is the dominant signal [7,8]. In TNT the parent anion is also formed, but at a comparably low intensity.

2. Experimental

Electron attachment to TNT was studied by means of a crossed electron-molecular beams device which has previously been described in detail [10]. In brief, the electron beam is formed in a custom built hemispherical electron monochromator, in the

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course of the present experiments operating at an energy resolution between 80 and 100 meV (FWHM) and an electron current of ≈20 nA. TNT is a solid under normal conditions but with sufficient vapour pressure so that at moderately elevated temperatures an effusive molecular beam can be generated. The beam emanates from a source consisting of a temperature regulated oven and a capillary. Experiments have been performed in the range around 60 °C which is well below the melting temperature. At that temperature one can safely assume that the molecules are transferred as intact entities into the gas phase. Negative ions formed in the crossed beams collision zone are extracted by a weak electric field towards the entrance of the quadrupole mass spectrometer. The mass-selected negative ions are detected by a channeltron multiplier using a single pulse counting technique. The intensity of a particular mass-selected negative ion is then recorded as a function of the electron energy.

The electron energy scale is calibrated using the well-known SF_6^- signal near 0 eV. TNT was purchased from Sigma–Aldrich at a stated purity of 99.5% and used as delivered.

3. Results and discussion

3.1. Negative ion mass spectrum

Fig. 1 shows the negative ion mass spectrum of TNT obtained at an electron energy close to 0 eV. The 210 amu fragment by far dominates the mass spectrum. It is formed from the precursor anion by the loss of OH and is assigned as $(M—OH)^-$. The second intense ion signal belongs to the series at 197, 167 and 137 amu which can be assigned to fragment ions arising from the precursor by the loss of one, two, and three neutral NO units, respectively, and the ions are correspondingly assigned as $(M—nNO)^-$, $n = 1–3$. At a lower intensity level the peaks at 180 and 181 amu are assigned to ions arising from the loss of HNO_2 and NO_2, respectively, that at 151 amu due to the loss of $NO + NO_2$ (N_2O_3) and that at 123 amu due to the loss of $CO_2 + 2NO$.

The peaks at the lower side of the mass spectrum are identified as the loss of fragment ions from the precursor. The signal at 46 amu is assigned as NO_2^- and that at 45 amu to an anion of the stoichiometry HCO_2^- representing either $HCOO^-$ or $HOCO^-$. By exploring the quite complex potential energy surface of that system it appears that the formyloxylanion ($HCOO^-$) is the most stable configuration [11,12]. The 26 amu signal can arise from the isobaric fragments CN^- and/or $C_2H_2^-$. The latter is a well-known anion having the vinylidene structure $CH_2{=}C^-$ [13]. From experiments in DNB and its deuterated analogues [8], however, it followed that formation of the vinylidene anion can be excluded, and it is hence very reasonable to assign the present signal also to CN^-.

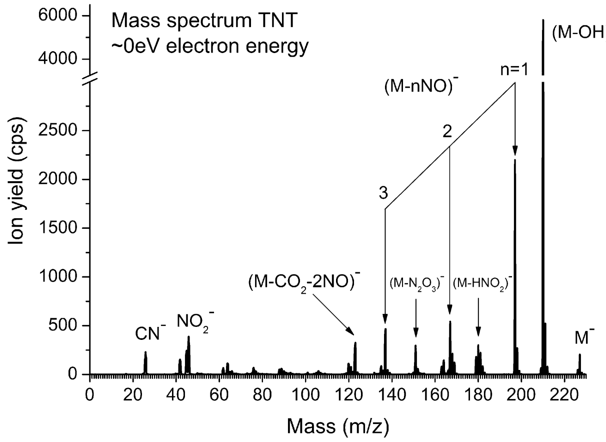

Fig. 1. Negative ion mass spectrum recorded at an electron energy close to 0 eV.

The striking difference to other aromatic nitro-compounds is the rich fragmentation pattern at energies already at 0 eV and the fact, that formation of the metastable parent anion is comparatively weak. Electron attachment to nitrobenzene (NB) exclusively generates the parent molecular anion at energies near 0 eV while a variety of DEA reactions take place at higher energies [14] and the same holds for the three isomers of nitrotoluene (NT) [7]. Electron attachment to the three isomers of dinitrobenzene (DNB) generates the parent anion as the dominant signal [8] from a narrow feature close to 0 eV. The DEA reactions generally occur via resonances at higher energies and only in 1,4-DNB the DEA reaction associated with the loss of a neutral NO radical has an onset close to 0 eV. As can be seen from Fig. 1, the ion due to the loss of neutral OH is by far dominant signal in TNT. The analogue DEA reaction (loss of OH) is also observed in the isomers of NT, but from resonances located near 3.8 eV. The presence of the methyl group in the aromatic nitro-compounds obviously triggers this rather complex reaction.

Concerning the molecular orbitals (MOs) involved in electron attachment to TNT, one can expect a situation similar to that explored in DNB. *Ab initio* calculations for the three isomers of DNB revealed [8] two low lying anionic states associated with extended wavefunctions for the extra electron which are delocalised over the ring and the two NO_2 groups. It is hence likely that the low lying electronic states (<1 eV) involved in electron attachment to TNT can accordingly be characterised as shape resonances with the excess electron delocalised over the ring and the three NO_2 groups.

3.2. Ion yield curves

In the following we shall consider the ion yields as a function of the electron energy for the more intense ions as seen in the mass spectrum (Fig. 1). By just looking at the spectra (Figs. 2–6) one can see that formation of the parent ion is restricted to a narrow feature near 0 eV (Fig. 2) while all fragment ions show more

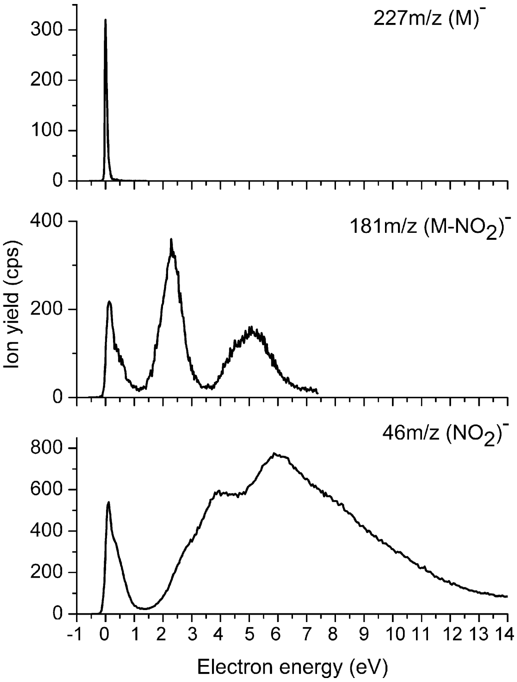

Fig. 2. Ion yield for the parent negative ion (M^-) and the complementary DEA reactions due to the cleavage of a $C—NO_2$ bond leading to the ions NO_2^- and $(M—NO_2)^-$, M = TNT.

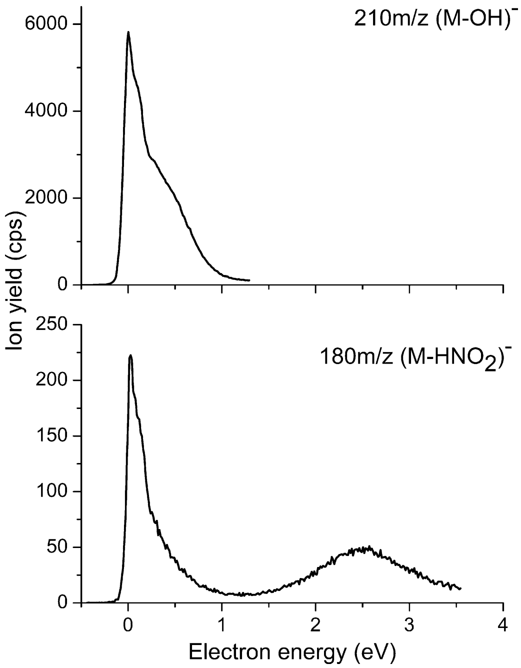

Fig. 3. Yield for the product ion arising from the loss of a neutral OH radical ($(M—OH)^-$), and the loss of a neutral HNO_2 molecule ($(M—HNO_2)^-$).

extended resonance profiles indicative of DEA. Within the variety of resonant structures in the entire energy range between 0 and 10 eV it appears that most of the fragment ion intensity is concentrated within three main areas, namely in the range below 1 eV, near 3–4 eV and a higher broader feature in the range around 6–8 eV.

While the transient negative ions (TNIs) generated at low energy (below 1 eV) are assigned as shape resonances involving the π^* system, it is likely that the resonance features at higher energies can be characterised as core excited resonances with possible contributions of high-energy shape resonances.

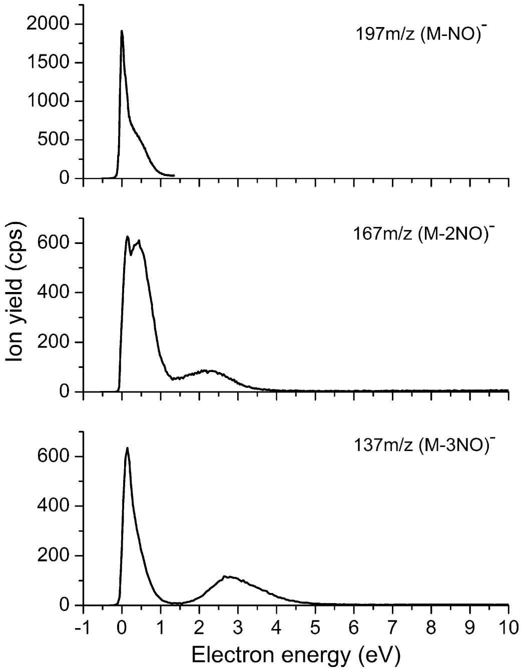

Fig. 4. Ion yield for the fragment arising from the loss of one, two and three neutral NO units ($(M—nNO)^-$, $n = 1–3$.

3.2.1. Parent molecular anion (associative attachment) $M^-/C_7H_5N_3O_6^-$ (227 amu)

Under the present experimental conditions the signal due to the parent molecular anion is comparatively weak with respect to the abundant ion signals arising from DEA and also weak compared to the other aromatic nitrocompounds [7,8,14]. It is exclusively formed within a narrow resonant feature at low energy (Fig. 2). The width is essentially instrumental, with a noticeable asymmetry towards higher energies. The common picture to rationalise the formation of metastable parent anions under collision free conditions is that the electronic energy of the electron attaching system (comprised of the energy of the incoming electron and the electron affinity of the molecule) is effectively dispersed over the vibrational degrees of freedom in the molecule, thereby delaying autodetachment [15].

A prototype system of associative attachment is SF_6 which possesses one of the highest attachment cross sections [16]. In SF_6, all DEA channels are endothermic and hence not accessible at 0 eV provided that the temperature of the target molecule is low (no thermal activation). The fact that in TNT the signal of the parent anion (M^-) is comparatively weak can then be interpreted by the fact that already near zero electron energy a variety of DEA channels are operative thereby strongly competing with the detection of the metastable anion on a mass spectrometric time scale.

3.2.2. The complementary ions NO_2^- (46 amu) and $(M–NO_2)^-/C_7H_5N_2O_4^-$ (181 amu)

These ions arise from the cleavage of one of the three C—N bonds leading to the complementary DEA reactions:

$$e^- + M \rightarrow (M—NO_2) + NO_2^- \quad (1a)$$

$$e^- + M \rightarrow (M—NO_2)^- + NO_2 \quad (1b)$$

with respect to the extra charge (M = TNT). The thermodynamic threshold for the DEA reaction (1a) is given by the C—NO_2 bond dissociation enthalpy minus the electron affinity NO_2. Taking the average value of D(C—NO_2) in aromatic nitro compounds (3.1 eV [1]) and the well-known electron affinity of NO_2 (2.27 eV, Table 1) one arrives at thermodynamic thresholds of 0.8 ± 0.2 eV. The uncertainty of this value is based on the variation of the D(C—NO_2) binding energy in the different in aromatic nitro compounds [1]. The fact that NO_2^- is already observed close to 0 eV may then be due to rearrangement in the neutral system generating more stable compounds than the dinitrotoluene radical. It may also be due to *hot band transitions*, i.e., DEA reactions involving vibrationally excited neutral TNT molecules. Due to the particular situation for a DEA reaction at very low energies, such transitions can lead to appreciable signals in spite of an only weak population of excited vibrational levels [15,17].

It is interesting to note that the NO_2^- signal extends to much higher energies than that of its larger complement $(M—NO_2)^-$ (Fig. 2). This behaviour is a mirror of the possibility to distribute the excess energy within the dissociating system which is much different between reactions (1a) and (1b). Assuming a statistical behaviour in the unimolecular decomposition of the TNI one expects that the large fragment receives about 92% of the available excess energy (owing to the number of vibrational degrees of freedom). Since both reactions have thresholds close to 0 eV, the excess energy should approximately correspond to the electron energy. In the case when the small ion NO_2^- is detected, the larger neutral counterpart ($M—NO_2$) will become increasingly unstable towards further decomposition beyond a certain electron energy (which is in the order of the binding energy). One can thus expect that along the high-energy side of the NO_2^- feature (beyond about 6–7 eV) the neutral system ($M—NO_2$) will further dissociate. In contrary, when the excess charge is localised on the large fragment $(M—NO_2)^-$, it will accordingly become increasingly unstable beyond a certain

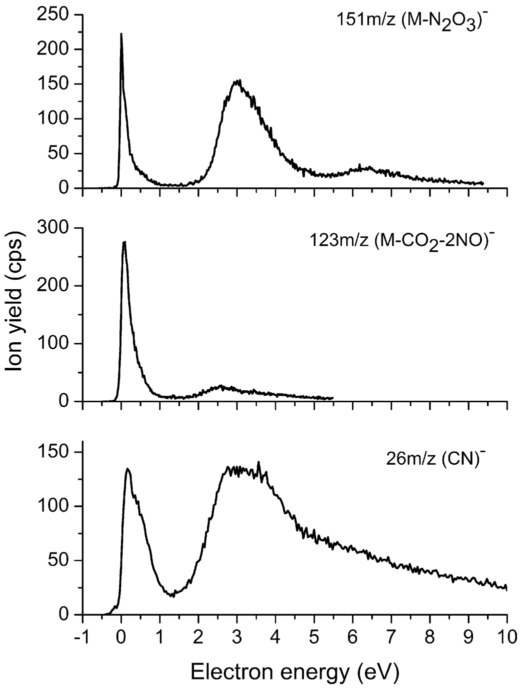

Fig. 5. Yields for the product ions due to the loss of (NO + NO_2) or N_2O_3 (151 amu), the loss of one CO_2 and two NO units (M–CO_2–2NO)$^-$ (123 amu) and the excision of the cyanide anion CN^- (26 amu).

electron energy with respect to both autodetachment and dissociation. This explains that (M—NO_2)$^-$ is no longer detected above 7 eV.

3.2.3. *Ion yields of (M—OH)$^-$/$C_7H_4N_3O_5$ (210 amu) and (M—HNO_2)$^-$/$C_7H_4N_2O_3$ (180 amu)*

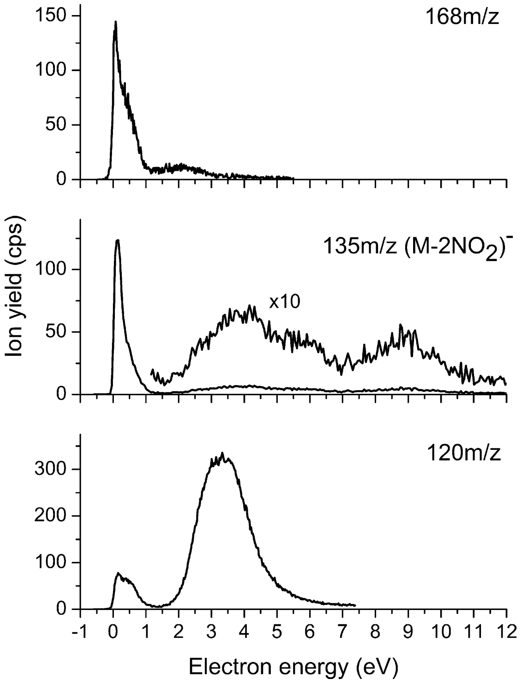

Fig. 6. Three selected yields for ions of lower intensity at 168 amu, 135 amu, and 120 amu. For possible assignments see the text.

Table 1
Gas phase standard heats of formation (ΔH_f°) und electron affinities relevant in dissociative electron attachment to TNT (taken from Ref. [19])

Compound	ΔH_f° (kJ mol^{-1})
$C_7H_5N_3O_6$ (trinitrotoluene, TNT)	24.1
$C_6H_5NO_2$ (nitrobenzene, NB)	68.53 ± 0.67
$C_7H_5NO_2^-$ (1,4-nitrobenzaldehyde anion)	−216 ± 9.2
OH	40.0
NO_2	33.1
NO	90.29
N_2O_3 (dinitrogentrioxide, ONNOO)	82.84
HNO_2	−76.73
CO_2	−393.51
CN	435.14
Compound	**Electron affinity (eV)**
$C_7H_5NO_2$ (1,4-nitrobenzaldehyde)	1.69 ± 0.09
$C_6H_5NO_2$ (nitrobenzene, NB)	1.000 ± 0.010
NO_2	2.27
CN	3.8620 ± 0.0050

Formation of the fragment ion due to the loss of a neutral OH radical ((M—OH)$^-$) is by far the dominant process in electron attachment to TNT. Fig. 3 shows that the DEA reaction has a steep onset which is essentially controlled by the energy resolution of the electron beam. No such corresponding ion ((M—OH)$^-$) is observed from nitrobenzene [14] or from any of the isomers of dinitrobenzene [8]. It is, however, observed from nitrotoluene (NT) [7] suggesting that only the presence of the methyl group enables OH abstraction. In the three isomers of NT the loss of OH proceeds via a resonance located near 3.8 eV and at comparatively lower intensity.

Obviously, the location of the methyl group between the two NO_2 groups provides particular favourable conditions for the formation of a neutral OH radical. The reaction requires the cleavage of two bonds (N—O and C—H) and formation of the O—H bond. Since it proceeds already at threshold, the electron affinity of the species (M—OH) must be sufficiently high to compensate for the difference between the energy required to break the two bonds and the energy gain in forming the O—H bond.

Accordingly, formation of the fragment ion (M—HNO_2)$^-$, i.e., loss of a neutral HNO_2 requires cleavage of a C—H bond, cleavage of a C—NO_2 bond and formation of the H—NO_2 bond. From Fig. 3 it can be seen that the steep onset of this reaction is close to zero and from energy balance one can estimate a lower limit of the electron affinity of the (M—HNO_2) radical. With D(C—H) = 4.5 eV [18], D(C–NO_2) = 3.1 ± 0.2 eV from above and D(H–ONO) = 3.40 eV obtained from the data in Table 1 we arrive at EA(M–HNO_2) ≥ 4.2 ± 0.3 eV. For the C—H binding energy we used the value of methane which may slightly be altered for the methyl group of TNT yielding the estimated accuracy for the electron affinity. The equality sign refers to a situation when the reaction proceeds without excess energy (no activation energy). It has to be noted that such a treatment neglects rearrangement in the negative ion fragment following loss of neutral HNO_2. We also note that loss of OH is restricted to the low-energy feature while formation of HNO_2 (HONO) additionally proceeds via a resonance located near 2.4 eV.

3.2.4. *Fragment ions due to the loss of neutral NO units (M—nNO)$^-$, n = 1–3*

The yields of the fragment ions due to the loss of one to three neutral NO are plotted in Fig. 4. In the isomers of DNB the loss of one and two NO units was also observed, however, from resonant features located in the range 3–4 eV (depending on the isomers) while in TNT the reactions have steep onsets right at zero energy. It is surprising that the loss of multiple NO units can be triggered by an excess electron with essentially no extra energy. The structures of the final neutral and ionic products formed along these reactions remain under question. Energetically the formation of N_2 + O_2 is more favourable than two NO radicals (see Table 1). Loss of three NO radicals yields an ion with stoichiometric composition $C_7H_5O_3^-$ which could represent the OH–benzoate anion ($HO–C_6H_4–COO^-$). The three isomers are well-known anions possessing appreciable electron binding energies in the range of 4 eV [20]. Such a reaction would require a series of rearrangements in the transient negative ion involving hydrogen and oxygen transfer.

It must be noted that from the present experiments we cannot extract information to which degree the above reactions are concerted or sequential (see below).

3.2.5. Ion yields $(M–N_2O_3)^-/C_7H_5NO_3$ (151 amu), $(M–CO_2–2NO)^-/C_6H_5NO_2$ (123 amu) and CN^- (26 amu)

The signal at 151 amu (Fig. 5) can be identified as the ion arising from the loss of a neutral NO and NO_2 unit which may arise from the unimolecular decomposition reaction as N_2O_3 (dinitrogentrioxide, ONNOO) which is thermodynamically more stable (Table 1). From the present experiment, we do not have direct information on the neutral products. With the stoichiometric composition of the corresponding anion ($C_7H_5NO_3^-$) a possible structure is the radical anion of nitro-benzaldehyde ($H(O)C–C_6H_4–NO_2^-$) [19]. Like above, such a reaction would require substantial rearrangement including oxygen and hydrogen transfer. From Fig. 5 it can be seen that it has a threshold near 0 eV and also proceeds via two higher energy resonances located at 3.0 and 6.3 eV. With the thermochemical data from Table 1 (referring to the para isomer of nitrobenzaldehyde) the reaction

$$e^- + C_7H_5N_3O_6 \rightarrow C_7H_5NO_3^- + N_2O_3 \qquad (2)$$

becomes exothermic by −1.66 eV.

The signal at 123 amu can be assigned to the radical anion of nitrobenzene ($C_6H_5NO_2^-$) arising from the loss of a CO_2 molecule and two NO radicals (or $N_2 + O_2$). As above, such a reaction requires complex rearrangements in the precursor ion involving hydrogen and oxygen atom transfer. Based on the thermodynamic values from Table 1 the corresponding reaction

$$e^- + C_7H_5N_3O_6 \rightarrow C_6H_5NO_2^- + CO_2 + N_2 + O_2 \qquad (3)$$

is highly exothermic (−4.61 eV) which may also underline the explosive nature of TNT.

The cyanide anion CN^- represents an excision of this unit from the target molecule. CN is a well-known pseudohalogen having an appreciable electron affinity (3.86 eV, Table 1) exceeding even that of the halogen atoms. Formation of CN^- via complex DEA reactions is well-known in amino acids and other larger molecules containing C and N atoms [21–23]. Possible structures of the neutral reaction channel is nitro-aniline ($NO_2–C_6H_4–NH_2$) or dinitrobenzene and molecular hydrogen and oxygen ($(C_6H_4–(NO_2)_2) + H_2 + O_2$).

3.2.6. Fragment ions at low intensity

From the mass spectrum recorded close to 0 eV it is obvious that some more ions are formed at lower intensity and Fig. 6 presents the ion yields of a selection of them.

A possible assignment of the ion at 168 amu is dinitrobenzene (DNB) which is formed from TNT by the loss of $CHNO_2$. In electron attachment to DNB a long-lived parent anion is generated within a narrow resonance near 0 eV [7]. From that one can conclude that at least for the signal beyond zero electron energy, a contribution from DNB impurities can be excluded.

The ion formed at 135 amu can arise from TNT by the loss of two neutral NO_2 molecules thereby creating a radical anion of dehydrogenated nitrotoluene ($CH_3–C_6H_2–NO_2^-$). Accordingly, the ion at 120 amu can be assigned to a radical anion formed by a further loss of the methyl group, i.e., a radical anion of dehydrogenated nitrobenzene ($C_6H_2–NO_2^-$).

It must be emphasized that all ions are detected within the time window of the present experiment which is in the range of tens of microseconds, dependent on the mass of the ion. Ions decomposing within the quadrupole will strike the rods and will not be detected. We do not have information on the question, to which degree the corresponding DEA reactions (e.g., loss of nNO (n = 1–3)) are sequential or concerted.

4. Conclusion

Capture of an excess electron with virtually no energy by TNT shows very particular features in that the metastable parent anion and a variety of DEA products are generated. While formation of the parent anion is restricted to a very narrow energy range near 0 eV, the DEA reactions extend to higher energies and involve different resonant features. In comparison with other aromatic nitrocompounds the intensity of the non-decomposed anion is weak which can be explained by the competition of the different DEA channels which are already operative near zero energy. The most dominant DEA reaction is loss of a neutral OH radical which is formed by the cleavage of two bonds (C—H and N—O) and formation of the C—O bond. Further and more complex reactions are observed like the loss of up to three neutral NO units having a steep onset at zero energy. The rich and intense fragmentation already at very low energies underlines the explosive nature of TNT.

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References

[1] T.B. Brill, K.J. James, Chem. Rev. 93 (1993) 2667.
[2] R.N. Compton, L.G. Christophorou, G.S. Hurst, P.W. Reinhardt, J. Chem. Phys. 45 (1966) 4634.
[3] L.G. Christophorou, Atomic and Molecular Radiation Physics, Wiley Interscience, London, 1971.
[4] E.C.M. Chen, E.S. Chen, M.S. Milligan, W.E. Wentworth, J.R. Wiley, J. Phys. Chem. 96 (1992) 2385.
[5] C.D. Harvey, M. Eberhart, T. Jones, K.J. Voorhees, J.A. Laramee, R.B. Cody, D.P. Clougherty, J. Phys. Chem. A 110 (2006) 4413.
[6] S. Boumsellek, S.H. Alajajian, A. Chutjian, J. Am. Soc. Mass Spectrom. 3 (1992) 243.
[7] P. Sulzer, A. Mauracher, S. Denifl, F. Zappa, S. Ptasinska, M. Beikircher, A. Bacher, N. Wendt, A. Aleem, F. Rondino, S. Matejcik, M. Probst, T.D. Maerk, P. Scheier, Anal. Chem. 79 (2007) 6585.
[8] P. Sulzer, A. Mauracher, S. Denifl, M. Probst, T.D. Märk, P. Scheier, E. Illenberger, Int. J. Mass Spectrom. 266 (2007) 138.
[9] J. Yinon, H.G. Boettger, W.P. Weber, Anal. Chem. 44 (1972) 2235.
[10] D. Muigg, G. Denifl, A. Stamatovic, T.D. Märk, Chem. Phys. 239 (1998) 409.
[11] E.H. Kim, S.E. Bradforth, D.W. Arnold, R.B. Metz, D.M. Neumark, J. Chem. Phys. 103 (1995) 7801.
[12] T.G. Clements, R.E. Continetti, J.S. Francisco, J. Chem. Phys. 117 (2002) 6478.
[13] K.M. Ervin, J. Ho, W.C. Lineberger, J. Chem. Phys. 91 (1989) 5974.
[14] A. Pelc, P. Scheier, T.D. Maerk, Vacuum 81 (2007) 1180.
[15] E. Illenberger, in: C.-Y. Ng (Ed.), Electron Attachment Processes in Free and Bound Molecules, Photoionization. Part II. Advanced Series in Physical Chemistry, vol. 10B, Wold Scientific, Singapore, 2000, p. 1063.
[16] D. Klar, M.-W. Ruf, H. Hotop, Int. J. Mass Spectrom. 205 (2001) 93.
[17] I. Hahndorf, E. Illenberger, Int J. Mass Spectrom. 167/168 (1997) 87.
[18] D.A. Lide (Ed.), Handbook of Chemistry and Physics, 78th edition, CRC Press, Boca Raton, 1997.
[19] NIST Chemistry webbok: http://webbook.nist.gov/chemistry.
[20] P. Kebarle, T.B. McMahon, J. Am. Chem. Soc. 99 (1977) 2222.
[21] S. Gohlke, A. Rosa, F. Brüning, M.A. Huels, E. Illenberger, J. Chem. Phys. 116 (2002) 10164.
[22] P. Papp, J. Urban, S. Matejcik, M. Stano, O. Ingólfsson, J. Chem. Phys. 125 (2006) 204301.
[23] I. Bald, I. Dabkowska, E. Illenberger, O. Ingólfsson, Phys. Chem. Chem. Phys. 9 (2007) 2983.