

## Further insights into the discolouration of TATB under ionising radiation

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## Further insights into the discolouration of TATB under ionising radiation

To determine degradation products formed by exposure of TATB to ionising radiation, a computational and experimental study is presented. Thermochemical and spectral data have been calculated using DFT at the MH06-HF/aug-cc-pVTZ level which suggest the formation of the cation radical derivative of TATB. Irradiated TATB samples showed the widely reported yellow-to-green discolouration, with measured CIE L\*, a\*, b\* and RGB values correlating with total dose. Trace quantities of a mono-furazan derivative were detected by HPLC-MS; the discolouration is not attributed to this, but rather to the presence of a paramagnetic species (i.e. the cation), as detected by ESR measurements. Recrystallised irradiated TATB samples reverted to their original colour, further suggesting it is the cation radical that is responsible for colour change.

**Keywords:** TATB; radiation; DFT; Explosives; sensitiveness

**Subject classification codes:** N/A

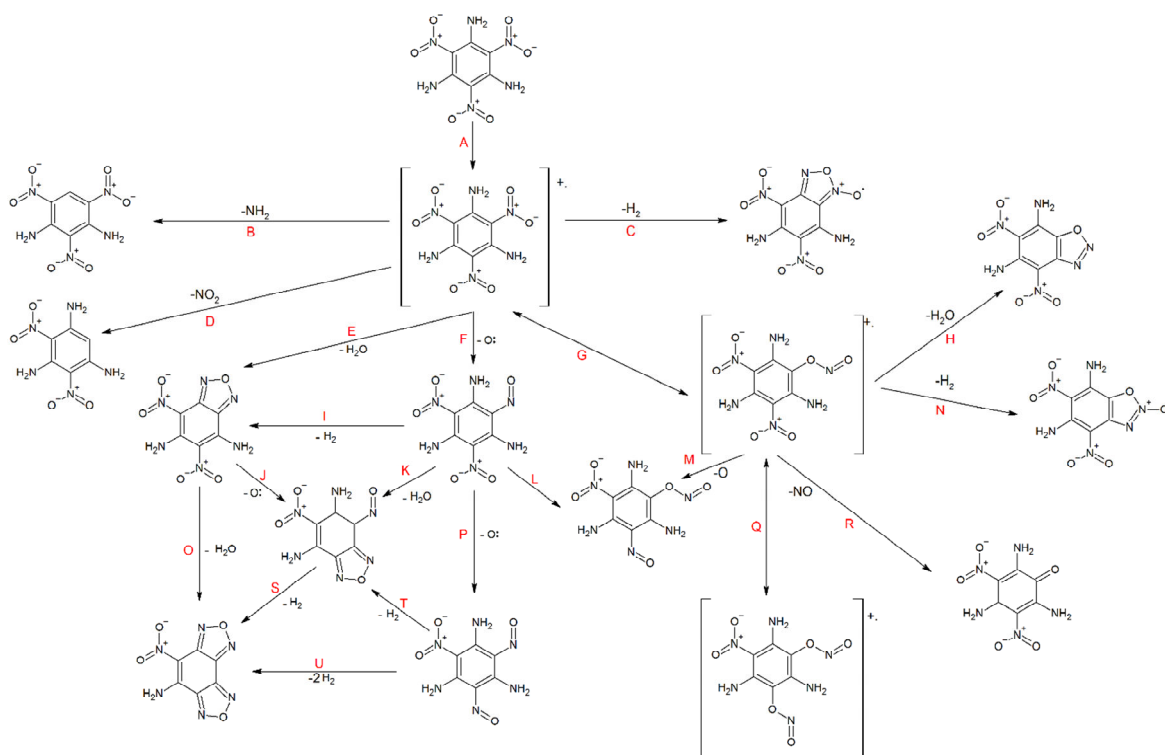
## **Introduction**

TATB (1,3,5-Triamino, 2,4,6-trinitrobenzene) has received significant attention since its discovery mainly due to its comparative insensitiveness, but also due to an optical phenomenon where the material alters colour from yellow to green upon exposure to radiation (Tian et al. 2017; Xiong et al. 2014; Firsichand and Guse. 1984; Britt et al. 1981; Skidmore et al. 1998; Avrami 1980; Golubev 2010; Manaa et al.; Connors 2014). There have been several works looking at the source and the consequence of this change to the material, with three key decomposition products being reportedly responsible, namely the mono-furazan (Connors 2014), mono-nitroso (Manaa 2002) and mono-phenoxy radical (Xiong 2002) derivatives. In order to elucidate the cause of the discolouration, and ultimately the effect that ionising radiation has upon the material, a joint computational and experimental study has been undertaken.

## **Computational thermodynamics**

The available literature was reviewed and, by its consideration, a selection of possible decomposition products resultant from the ionisation of TATB was derived. Additional molecules were also added where no literature evidence was available, if their generation was thought to be credible. The resultant decomposition map is shown in Figure 1.

Figure 1. Purported degradation products of TATB.



Each molecule within the decomposition map was optimised and analysed vibrationally at the unrestricted Density Functional Theory (DFT) MH06-HF level of theory with the augmented triple-zeta correlation-consistent basis set, aug-cc-pVTZ. All calculations were undertaken with the Gaussian 16a.03 software (Frisch et al. 2016). All optimisations were achieved at the ‘very tight’ criteria and no negative frequencies were observed during the subsequent vibrational analysis of the molecules, indicating a global minimum on the potential energy surface.

The thermodynamics resultant from the vibrational analysis of each molecule were then interrogated to provide an insight into the energetically favourable decomposition pathways TATB may follow upon irradiation (Ochterski 2000). Consideration was made as to the electronic state of the molecules within the decomposition pathways; for example, ionised TATB was analysed as a cation radical, i.e. as a double state with a charge of +1. In cases where fragmentation occurs, it is not known which species will remain ionic, as charge must be conserved. In such instances,

all fragments were considered in every perceivable electronic state, in order to ascertain which is the most favourable fragmentation mechanism (Nguyen 2015).

In an attempt to improve the accuracy of the computational investigation, an implicit solvent method (polarisable continuum model) was employed to approximate the solid state; gas phase calculations were also undertaken as a comparison.

Ground state TATB was also considered computationally alongside its cation radical equivalent, affording a value of the ionisation potential and its equivalent wavelength, derived using the Planck-Einstein relationship. This is presented within Table 1.

Table 1. Calculated Ionisation potential for TATB

| Phase | $E_1$ (eV) | $\lambda$ (nm) |
|-------|------------|----------------|
| Gas   | 9.56       | 129.71         |
| Solid | 8.01       | 154.81         |

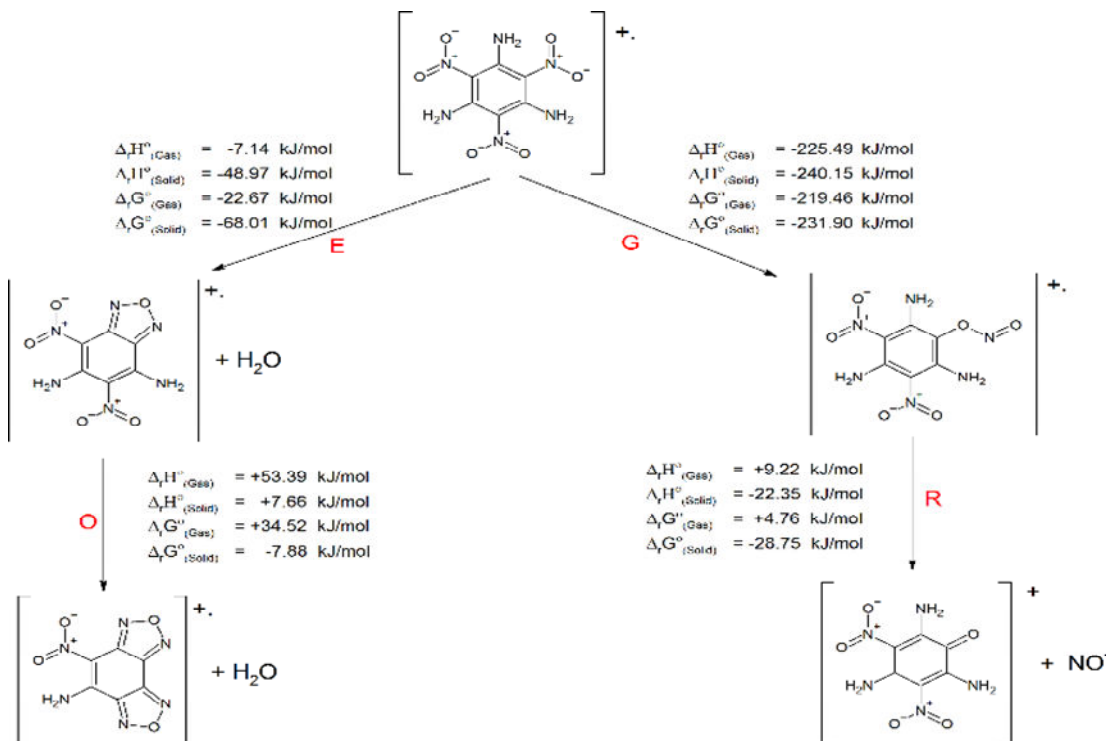
The calculated ionisation potentials suggest that the energy required to ionise TATB is within the mid ultraviolet range, indicating that the material behaviour under UV light will likely be similar to that of higher incident energies. This is perhaps unsurprising considering the reported discolouration of TATB, from UV, X-ray and gamma ray sources. Consideration of the thermodynamics of the decomposition pathways suggested that six subsets of the twenty initial pathways were energetically favourable, these are detailed within Table 2 and shown in Figure 2.

Table 2. Calculated Thermodynamic favourable properties for TATB degradation

| Pathway | Gas Phase             |                     | Solid Phase           |                     |
|---------|-----------------------|---------------------|-----------------------|---------------------|
|         | $\Delta H_f$ (kJ/mol) | $\Delta G$ (kJ/mol) | $\Delta H_f$ (kJ/mol) | $\Delta G$ (kJ/mol) |
| E       | -7.14                 | -48.97              | -22.67                | -68.01              |
| G       | -225.49               | -240.15             | -219.46               | -231.90             |
| K       | 36.33                 | -6.81               | 15.67                 | -26.02              |

|   |        |        |        |        |
|---|--------|--------|--------|--------|
| L | -34.27 | -37.07 | -23.35 | -25.55 |
| O | -5.46  | -49.16 | -10.70 | -54.24 |
| R | 9.22   | -22.35 | 4.76   | -28.75 |

Figure 2. Thermodynamically favourable decomposition products

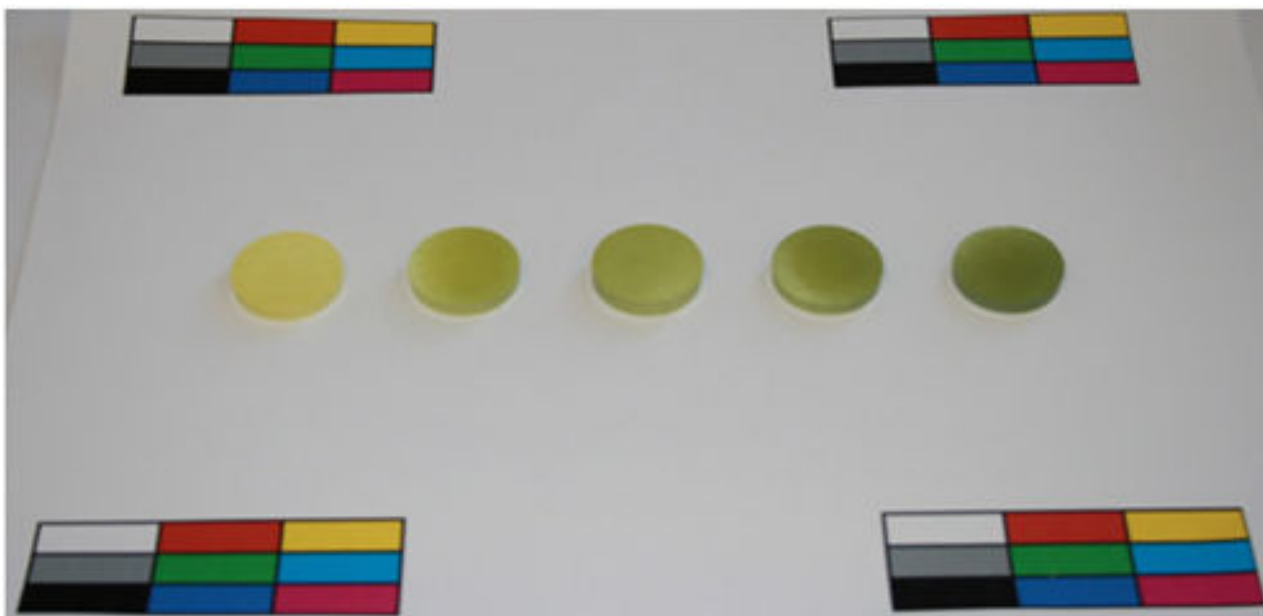


Of the six energetically favourable pathways, only paths E, G, R and O are credible due to a lack of energetically favourable preceding reactions for the remaining pathways. This suggests that a mono-furazan, di-furazan, mono-nitrite cation radical and mono-phenoxy radical are potential decomposition products of ionised TATB.

## Irradiation Experiments

Pressed discs of TATB (Type B batch AD/5/101, as provided by AWE Plc. with no binder), were irradiated to a total dose (equivalent to water) of 50, 100, 200 and 400 kGy, at a dose rate of  $1.8 \text{ kGy hr}^{-1}$  using the 1.17 and 1.33 MeV quanta from a cobalt-60 source. As expected, when compared to the baseline material, a significant colour change that correlated with total dose resulted, as shown in Figure 3.

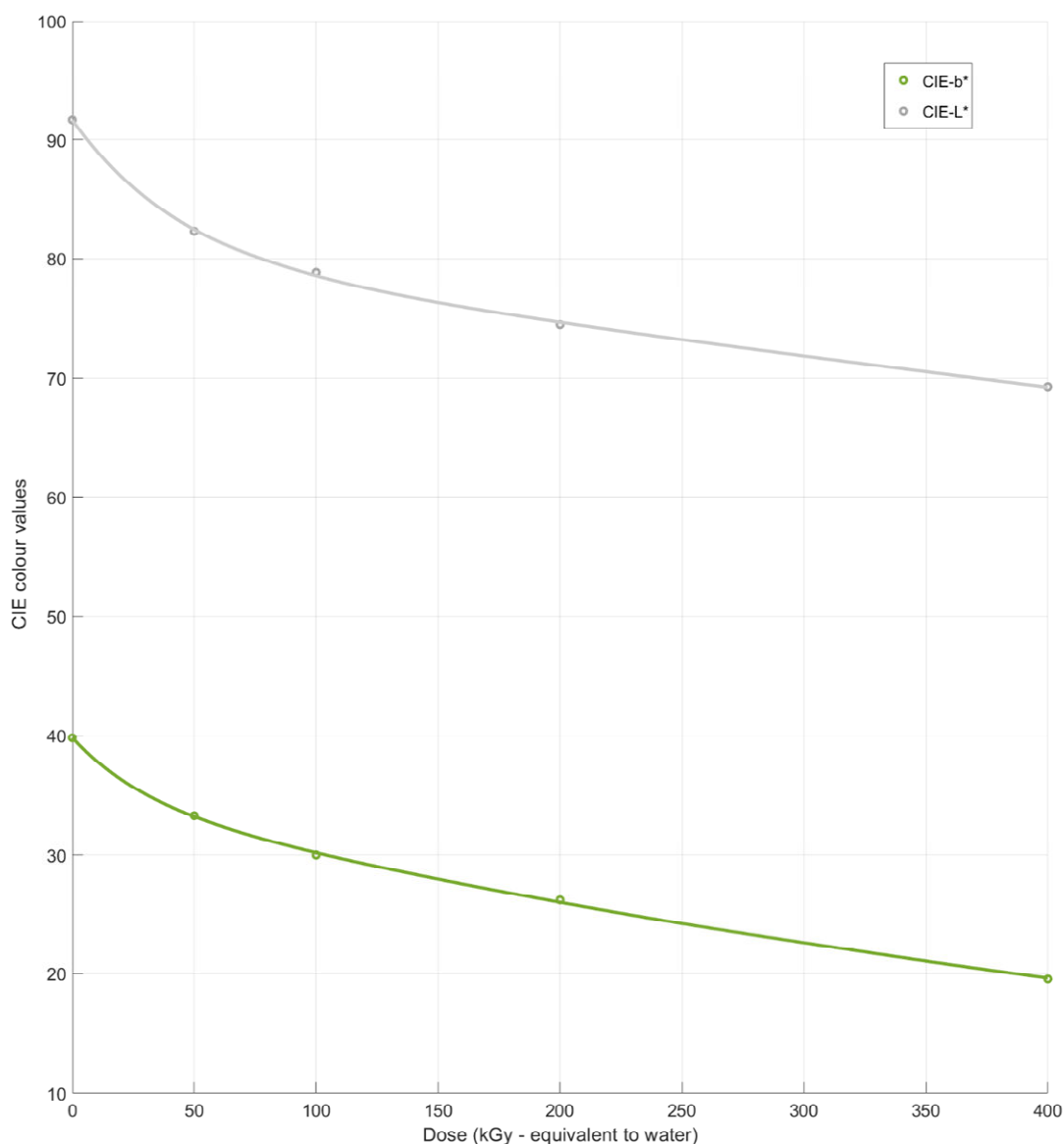
Figure 3. Colour change of TATB upon Irradiation exposure



### Colour Measurement Experiments

The colour change of the irradiated TATB was quantified using a PCE Instruments colour meter, and CIE  $L^*$ ,  $a^*$  and  $b^*$  values were recorded. The  $L^*$  and  $b^*$  values, indicating a colour change from lighter to darker (decreasing  $L^*$ ), and towards green (decreasing  $b^*$ ), showed a good correlation with total dose, as shown in Figure 4;  $a^*$  values remained essentially constant.

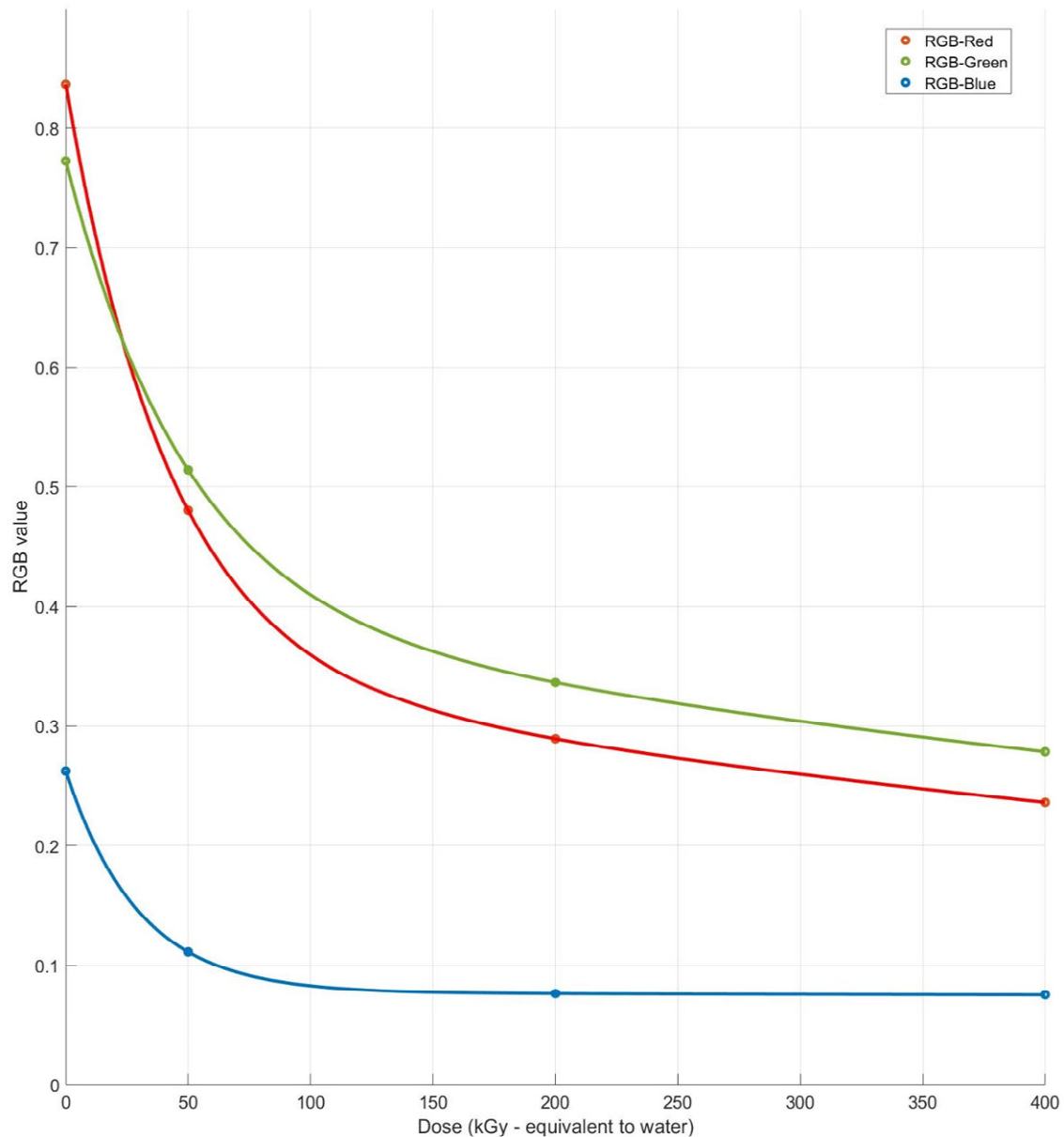
Figure 4. CIE  $L^*$  &  $b^*$  values of irradiated TATB



In addition, the UV-vis reflectance properties of the irradiated samples were measured against a Spectralon® reflectance standard using a Thermo Scientific Evolution 220 UV-Visible Spectrophotometer.

The UV/Vis reflectance spectra were converted to CIE RGB values using the technique described by Williams (Williams et al. 2007). As with the L\* and b\* values, good correlation of the R, G, and B values with radiation dose were obtained (Figure 5).

Figure 5. Colour change of Irradiated TATB CIE-RGB

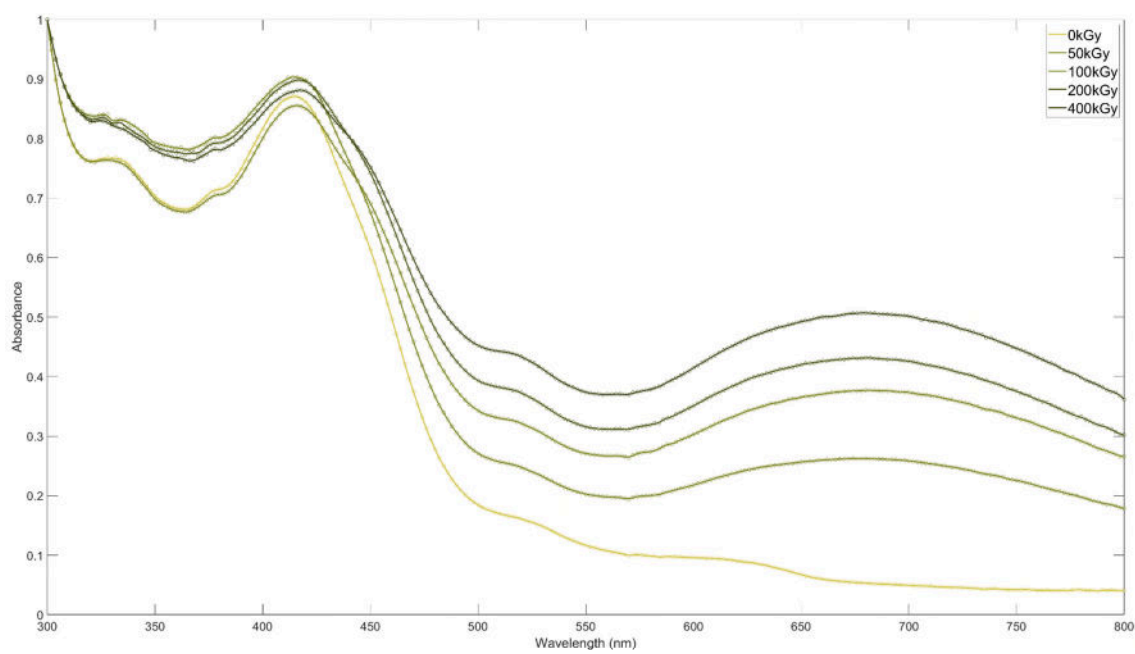


Both techniques, use of a colour meter to measure CIE  $L^*$   $a^*$  and  $b^*$ , or measurement of UV/Vis reflectance with a spectrometer and subsequent conversion to CIE RGB values, have been demonstrated to be effective methods for estimating with good accuracy the total radiation dose received by sample of TATB.

The reflectance spectra was also converted to absorbance (Figure 6 – coloured according to RGB values) which agreed with that observed by Xiong (Xiong et al. 2014) who saw a similar growth in the red absorption area of the spectra as a function of exposure time from a UV source. Absorptions below 300 nm are believed to be

minimal, however the image suggests that they are significant due to scattering of the low wavelength light and the conversion to absorbance from reflectance.

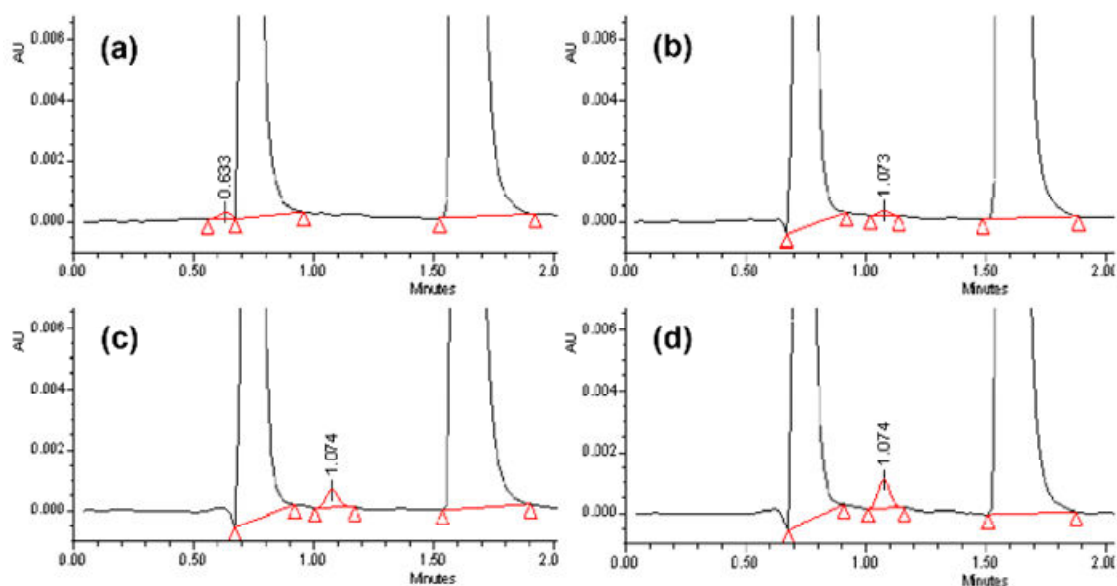
Figure 6. UV-Vis reflectance spectra converted to absorbance



### Other Experimental Analysis

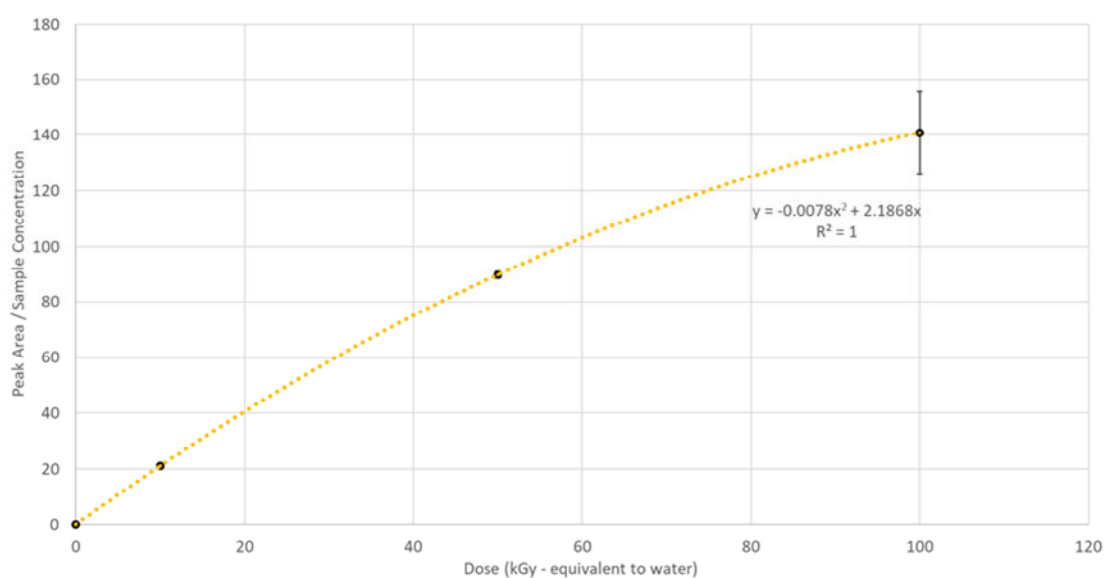
Samples of baseline (a), 10 (b), 50 (c) and 100 (d) kGy gamma irradiated TATB were submitted for HPLC analysis, which showed a peak eluting at approximately 1.074 minutes that was not in the baseline sample, as shown in Figure 7.

Figure 7. HPLC Chromatograms



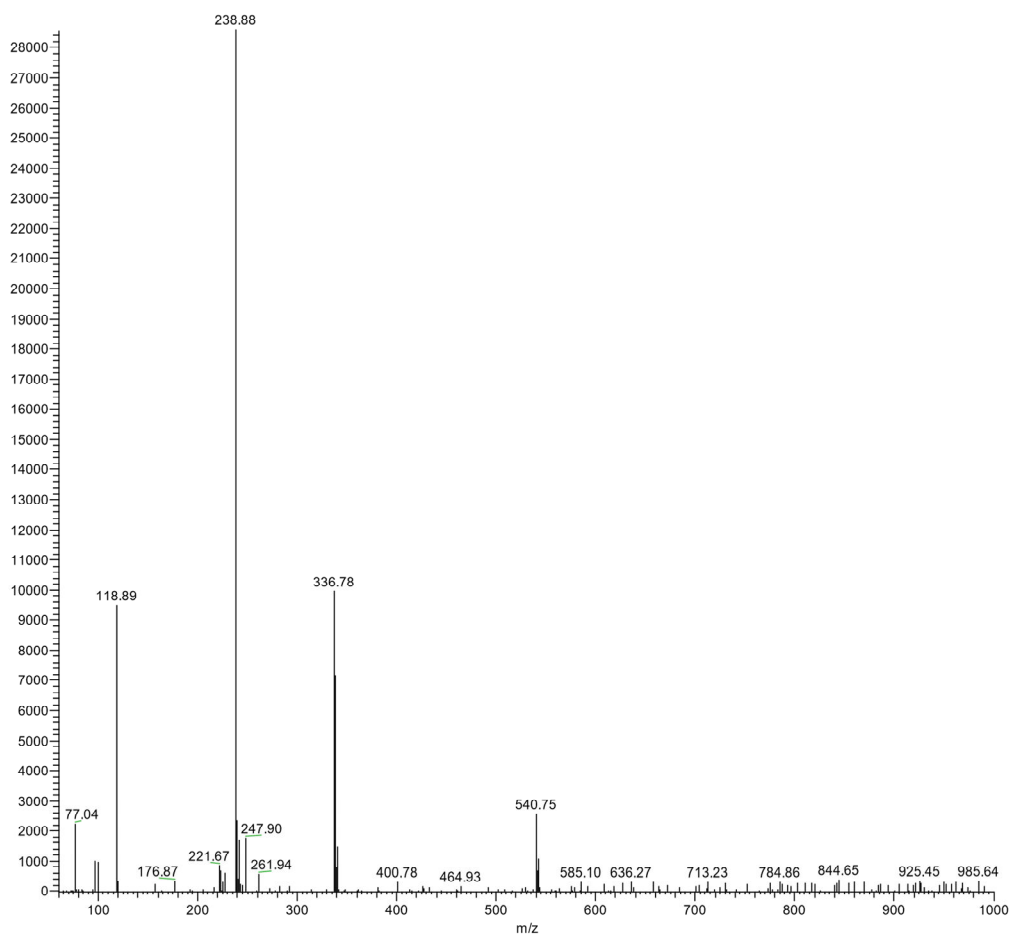
In agreement with the UV/Vis results, the area of the additional peak also correlated with the total dose as shown in Figure 8.

Figure 8. Peak area correlated radiation dose



Negative electrospray mass spectroscopy was undertaken on the eluate from the additional peak, where a species with neutral atomic mass of 240, 18 less than TATB was identified, as shown in Figure 9.

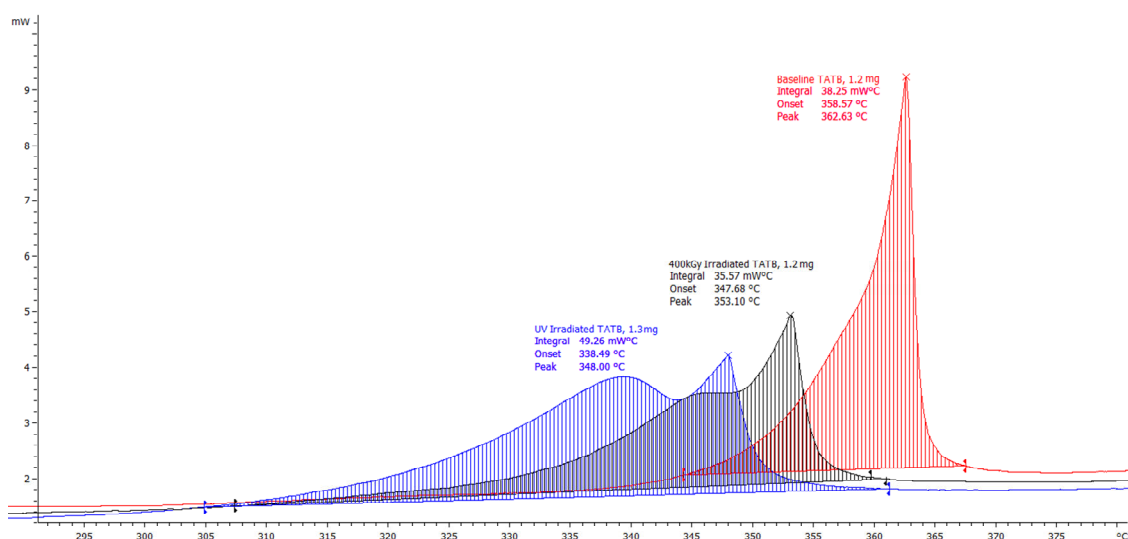
Figure 9. Mass spectra of 1.074 minute elute



The species was attributed to a loss of water from TATB and the subsequent generation of a mono-furazan derivative of TATB, as shown in Figure 2, resultant from path E.

Samples of irradiated TATB were submitted for thermal analysis by differential scanning calorimetry (2 °C per minute) which yielded a marked change in the thermal behaviour of the decomposition peak. An example for 400 kGy irradiated TATB is shown in Figure 10, however a correlation with dose could not be ascertained, attributed to sampling variability. A sample of 120 day UV irradiated TATB, which showed the greatest decolouration of all available samples was also run showing the most altered thermal behaviour.

Figure 10. DSC thermograms



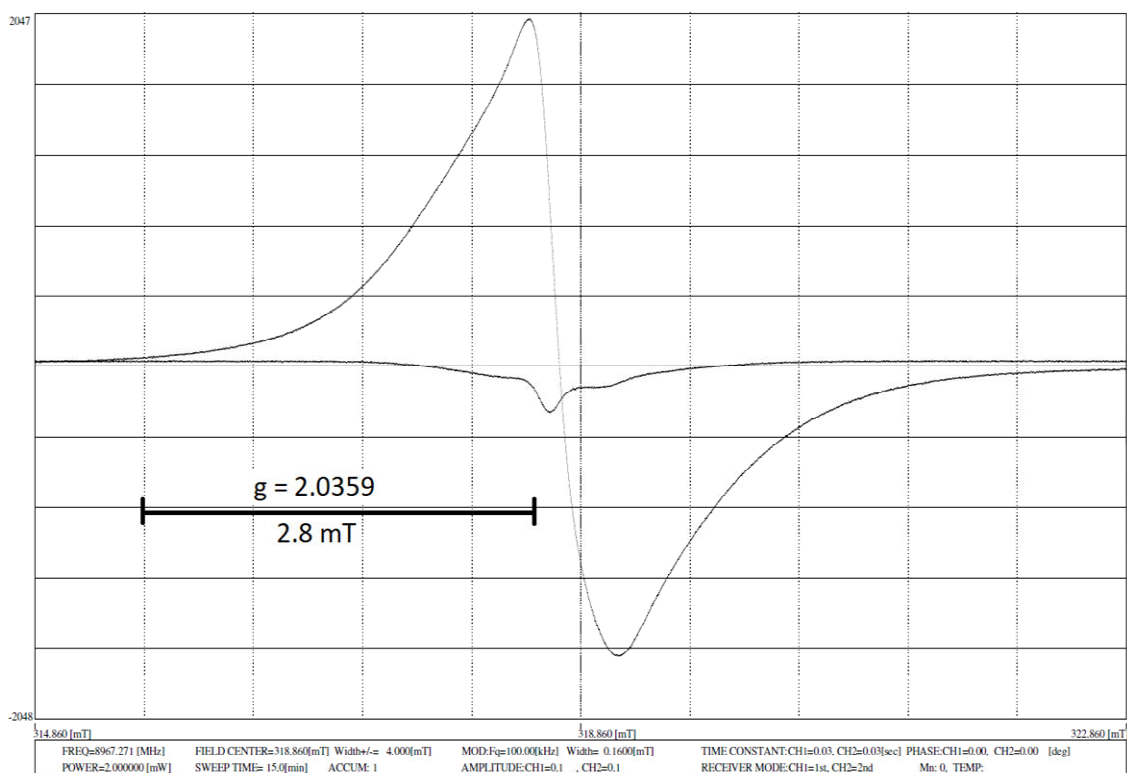
Where sample availability permitted (0, 50 and 200 kGy), the sensitiveness to impact of the irradiated samples was assessed by a 10 shot Langlie Rotter impact test (STANAG 4489). A marked increase in the sensitiveness to impact was noted from the Rotter results as detailed in Table 3.

Table 3. Small scale hazard properties

| Dose (kGy) | Rotter – Langlie (F of I) |
|------------|---------------------------|
| 0          | 165                       |
| 50         | 141                       |
| 200        | 87                        |

Electron spin resonance analysis was undertaken on baseline, 50, 100, 200 and 400 kGy irradiated specimens approximately 7 years after the initial irradiation took place. All samples, including the baseline, produced a non-complex spectra as shown in Figure 11, similar to that observed by Tian (Tian et al. 2017) and Britt (Britt et al. 1981). As with the UV/Vis and HPLC-MS analysis, the strength of the signal appeared to correlate linearly with the total absorbed dose.

Figure 11. Measured ESR spectra



The ESR results suggest that a radical species is present within the material and is particularly long lived. Up until this piece of evidence, the discolouration had been attributed to the mono-furazan, however, the molecule does not have any unpaired spin and would therefore not yield an ESR signal. The signal itself is non-complex and is typical of signals seen in the solid state where hyperfine coupling is lost due to degeneracy, therefore little to no chemical information could be ascertained from the signal other than the fact that a radical is present in the irradiated, but also the baseline material. The small, almost unobservable, signal in the baseline material is attributed to laboratory exposure to sunlight causing small ionisations.

### Additional Investigations

Investigations continued in the attempted synthesis of the mono-furazan derivative of TATB, with the ultimate aim of positive confirmation of the HPLC results. Synthesis

was successful (Entwhistle 2015) and a pure sample isolated and confirmed by NMR analysis. However, the resultant material, dissolved in DMSO, was a ‘deep red-orange’ colour and not blue, indicating that the molecule is not responsible for the widely reported discolouration of TATB. As a further observation, the material appears to be unstable and decomposes readily, possibly to the di-furazan derivative which is energetically favourable, but this is still to be confirmed. Unfortunately, the synthetic product was produced at a different site to where the irradiated TATB samples were kept and the sample would decompose before transport could be completed, affording no comparative HPLC analysis.

Synthesis of the mono-nitroso derivative was also performed successfully, resulting in an off-yellow/green product that was markedly less green than even the most mildly irradiated specimen at 50 kGy, suggesting that this was also not the cause of the discolouration, this was later supported by DSC analysis.

These results coupled with the ESR signal, began to suggest that the discolouration of TATB may be attributed to a paramagnetic species rather than the mono-furazan or mono-nitroso species. This agrees with Xiong’s (Xiong et al. 2014) suggestion that a phenoxyl derivative could be the cause of the discolouration. However, the computational investigation suggested that in the case of the nitrite cation derivative fragmenting, the energetically favourable path results in the phenoxyl derivative remaining positively charged and therefore would not give rise to a signal in an EPR spectrometer.

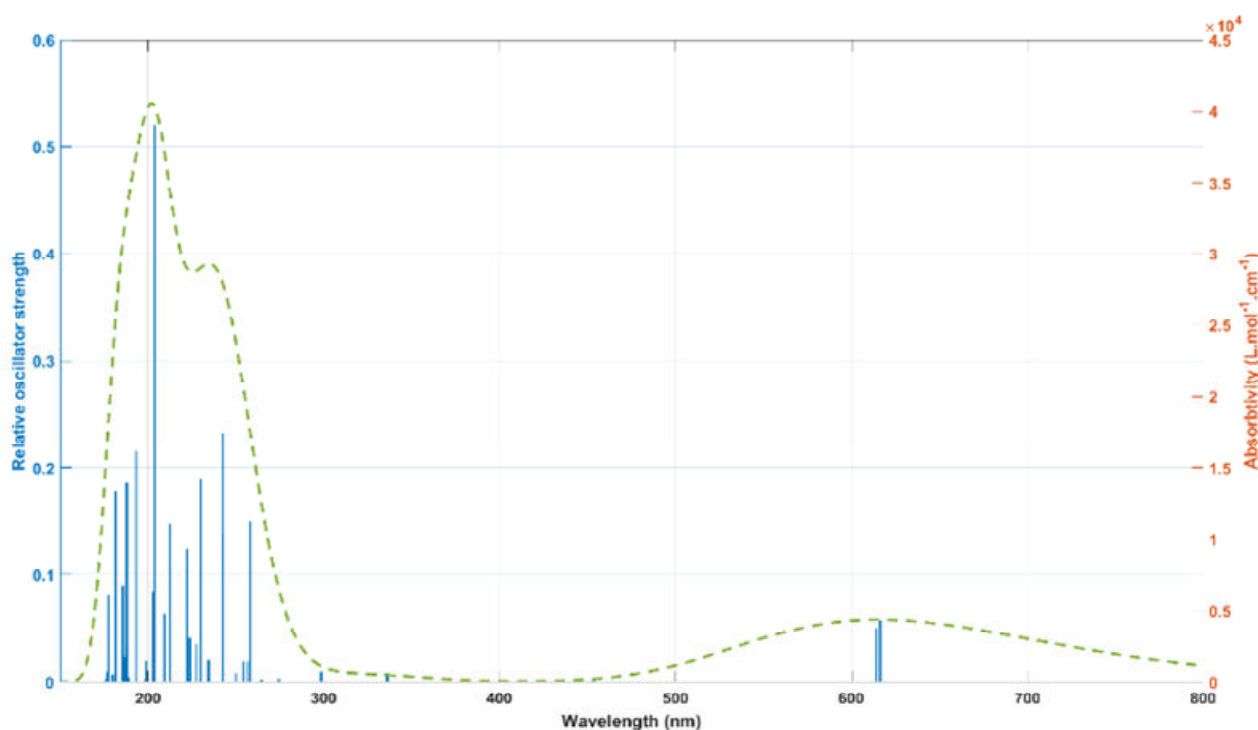
Despite this, further computational calculations were undertaken on all species within Scheme 1 in all possible electronic states in order to identify the potential source of the discolouration. Time Dependant DFT (TD-DFT) at the MH06-HF level of theory was used along with the same basis set as the thermodynamic study. In order to

generate a sufficiently detailed spectra the first fifty singlet and first fifty triplet excitations were calculated, which provided a predicted UV-Vis response of each molecule. In addition, the electrostatic properties of any paramagnetic species was also achieved at the same level of theory, but by utilising the EPR-II basis set required for such calculations.

Interestingly at this particularly high level of theory and basis set, neither the mono-nitroso, mono-furazan or the mono-phenoxy radical produced a UV-Vis spectrum that was comparable to that observed experimentally, as shown in Figure 6. This disagrees with that observed by Xiong (Xiong et al. 2014) for the phenoxy radical derivative, however those calculations were undertaken with a much less complex basis set and hybrid functional of DFT.

Only one of the species from Figure 2 showed a UV-Vis spectrum that was comparable to that seen experimentally, this was the cationic radical derivative of TATB. The resultant computational spectra is shown in Figure 12, where strong absorptions in the 600-650nm region can be seen. This suggests that light reflected from the cation derivative of TATB will be comparatively deficient in red light, making the material appear blue/green.

Figure 12. UV-Vis absorption properties of irradiated TATB



Calculation of the electrostatic properties of the cationic radical derivative of TATB yielded hyperfine coupling that, along with the electron density of the molecule, strongly suggested that the radical is carbon centred, sitting beneath one of the nitro, rather than amine, groups on the molecule. The radical appears to couple strongly to the adjacent nitrogen of the nitro group, which twists out of plane when compared to ground state TATB. The hyperfine coupling between the radical and the adjacent nitrogen can be visualised within Figure 13 (Biternas, Charnock and Kuprov 2014), by the orange mesh, where the twist can also be observed.

The calculated hyperfine coupling and g tensors were passed through EasySpin (Stoll and Schweiger 2005), in order to provide a calculated ESR spectra as shown in Figure 14. Once anisotropy was removed, the resultant spectra consists of three peaks which is typical for an unpaired electron coupling with a nitrogen atom. Coupling to other atoms, such as hydrogens, was negligible.

Figure 13. Hyperfine coupling tensor of cationic TATB

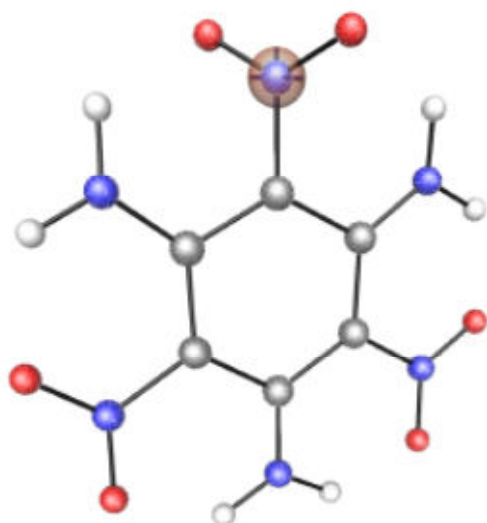
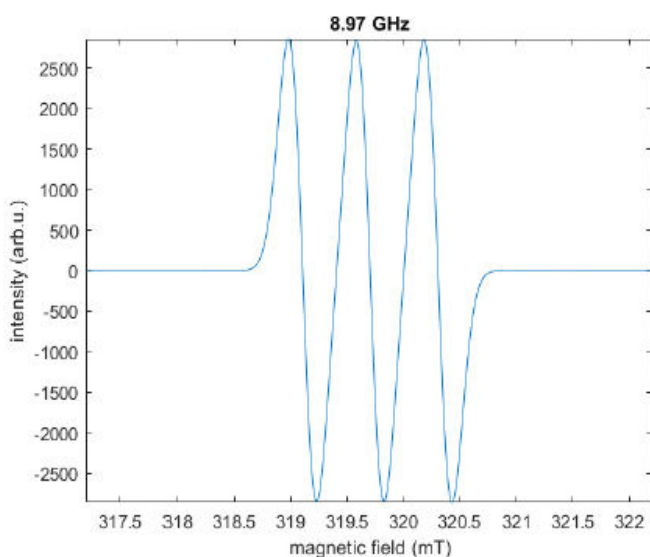


Figure 14. Predicted ESR spectra



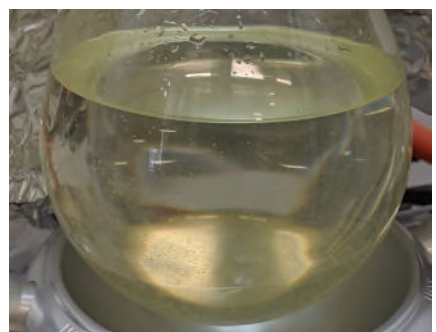
In an effort to investigate further, and also consider the possibility that the discolouration may be due to structural effects, recrystallisation of the most heavily gamma irradiated and discoloured sample of TATB was attempted. 460 mg of the 400 kGy gamma irradiated TATB was dissolved in DMSO at 80 °C for one hour. Once in solution, a marked colour change was observed from green to yellow across a period of 30 minutes.

The solution was crash precipitated into water, where a white/yellow precipitate was recovered. As analysis by DSC and ESR had proven to be the most sensitive

technique on irradiated specimens, the recovered product was analysed by these methods where it appeared indistinguishable from baseline TATB.

The recrystallisation was repeated under inert (nitrogen) atmosphere with a 42.82 mg sample of TATB that had been UV irradiated for 120 days. This material was selected as it was the most discoloured sample of TATB available. As shown in Figure 15, the same colour change of a deep green/black to yellow was observed, requiring a longer period of approximately two hours to complete. A yellow precipitate was successfully recovered after addition of water, sodium chloride and magnesium sulphate. The recovered material was washed copiously with water to remove traces of the salts, and a final recovered mass was measured at 42.86 mg indicating full recovery at  $100.09 \pm 0.29$  % yield.

Figure 15. Recrystallisation of UV Irradiated TATB



## Discussion

Through the experimental and computational investigations, it is suggested that the paramagnetic cation radical derivative of TATB is responsible for the discolouration observed within irradiated material. The discolouration and radical concentration appear to correlate linearly with dose, which is perhaps unsurprising as samples were exposed to a constant dose rate. This linearity alongside the strong ESR signal observed up to eight years after the initial irradiation suggest that the radical is particularly long lived which is likely due to stabilisation born through aromatic resonance, a known phenomenon that imbues a material with resistance to radiation.

It is this stabilisation that is believed to be the cause of the discrepancy between the observed and predicted ESR spectra. Where the computational spectra has been generated by a fixed radical location, it is likely that practically the radical will be delocalised through the molecule by means of this resonance, causing degeneracy in the measured ESR spectra.

It is thought that in the solid state, electrons or rather a deficiency of electrons are likely to be shared across molecules, much like a semi-conductor. Tian et al. (Tian et al. 2017) suggested in their research that the discolouration was resultant from changes in the crystalline structure of TATB. However, in a phenomenon also widely observed with the irradiation of gemstones (Ashbaugh 1988), it is thought that the irradiation simply alters the colour centre of the crystal. Through irradiation, the colour centre responsible for the widely reported discolouration of TATB is now believed to be the cationic derivative of TATB, rather than changes to the crystal structure. This colour centre is blue in nature and mixes with the yellow colour centre of unaltered TATB. This yields the widely reported discolouration, which appears to correlate with dose, as

well as with the concentration of the paramagnetic species, observed through ESR measurements.

The lack of an electron on a TATB molecule is likely to cause a reduction in its stability, as it is electronically unbalanced. It is hypothesised that it is for this reason that there is an increase in the sensitiveness to impact and the altered DSC thermograms, alongside the aforementioned optical properties.

The recrystallisation study does suggest that the effects that irradiation has on TATB may be reversed, as shown by the change in colour from green to yellow and the reversal of the altered thermal properties, determined by DSC and lack of an ESR signal. It is suggested that the cation radical TATB derivative is stable in the solid state and further decompositions, such as those that appear to be energetically favourable from the computational investigation, do not occur. However, once the material is no longer in the solid state, it is free to react, by either further decomposition to the monofurazan or monophenoxyl radical, or by capturing unbound electrons to re-form the parent TATB. The probability of each occurring is described by their thermodynamics, but it is significantly more favourable for TATB to reform compared to further decomposition. It is for this reason that it appears that the damage caused by irradiation may be reversed, whilst trace quantities of decomposition products are detected by HPLC.

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