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Optical absorption in polycrystalline PETN, RDX, HMX, CL-20 and HNS and its possible effect on exploding bridgewire detonator function

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Abstract

Exploding bridgewire (EBW) detonators work by bursting a thin conducting wire as a result of a high voltage discharge. This process is known to produce a strong UV emission. The roles of optical absorption, photochemistry, shock sensitivity, and impact sensitivity are assessed with respect to the relative roles each plays in the operation of an EBW detonator.

The optical absorptivity and penetration depth have been measured using dilute polycrystalline samples of PETN, RDX, HMX, CL-20 and HNS in KBr between 190 and 1100 nm. The results show strong absorption at UV wavelengths with a gradual decline at longer ones. It is found that while strong UV absorption appears to be necessary, it is not sufficient to make an effective EBW detonator.

Introduction

Relatively little has been published on the polycrystalline optical properties of important commonly used pure pressed explosives. This sparsity became obvious to us when looking for data about the relative absorption of PETN (Pentaerythritol tetranitrate) and HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazoctane) as a function of wavelength. PETN was of interest because of its use in EBW (exploding bridgewire) detonators and the possible roles that photochemical breakdown and radiative heating play in the functioning of detonators [1]. Studies on the processes that occur during the deflagration-to-detonation (DDT) in granular explosives have also been undertaken by our group for many years. The optical absorptivity of HMX is currently of interest to us, both because of the proposed radiative pre-heating that may occur in

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powder ahead of the deflagration front, and also the effect that selective wavelength absorption may have on multi-channel optical pyrometry.

These tools are currently being used to understand the temperature buildup processes in DDT. For example, a typical peak flame temperature of a deflagrating explosive is 3000-3500K and the front advances at speeds ranging between 10^{-3} and 10^2 ms^{-1} . The Planck distribution for that temperature results in maximum emission intensity occurring at a wavelength of 800-900 nm. If the penetration depth δ_p (the depth at which the input energy has decayed to $\frac{1}{e}$ of the incident energy) for an explosive is a few millimeters at those wavelengths, then significant radiative heating of the material just ahead of the flame front position may occur rapidly and be relevant for DDT processes occurring in short propagation distances. However, if the penetration depth is on the order of 100 mm then radiative heating effects will likely be negligible except for very large DDT events with long propagation distances and deflagration times, e.g., production plant-sized events rather than DDT events in munitions. Attempts to make short propagation distance DDT based detonators do not appear to have been successful suggesting that the shortest practical DDT distance is 15-30 mm, but in most regular DDT scenarios a much longer distance is required [2].

Smit [3] appears to have made the most in-depth study of both solution phase and polycrystalline solid explosives. Unfortunately, while the plots are qualitatively very helpful, there are insufficient experimental parameter data to allow fully quantitative results to be extracted. Specifically, the common method of solid sample measurement was used, wherein a dilute mixture of the test compound (explosive) is made with potassium bromide (KBr) and pressed into a transparent disc [4, 5]. The absorption of a comparable thickness of a pure KBr pellet is then made to extract just the effects of the test compound. To allow quantitative data to be extracted from the plots both the specific dilution and exact sample thickness are required and these are lacking in Smit's paper. However, Smit does conclusively demonstrate that in the case of the organic molecular crystals studied (explosives in this case), the absorption spectra for the same molecule is significantly altered when dissolved in acetonitrile compared with the solid polycrystalline absorptivity.

Cooper [6] has reported the experimental and theoretical absorptivities of several common high explosives (HEs), but the quantitative experimental measurements were made in acetonitrile solutions. Since acetonitrile solutions of explosives are not used in practice, the results are of limited use for our intended applications. Aluker has published a number of papers related to the effects of near infra red (IR) light on the initiation of PETN; see for example [7] and references therein. In [7] the ultraviolet through visible (UV-Vis) absorptivity of a single PETN crystal is reported. Typically absorptivity spectra are not generated from single crystals owing to the difficulty of correcting for the surface reflection and refraction effects that occur. Qualitative studies of RDX [8] and HMX [9] have also been reported.

A selection of literature is referenced that speculates about the photochemical

effects that may result when high-intensity light falls on explosive crystals [10–20]. In particular, references [12, 13, 15] demonstrate that the photochemistry occurs on a timescale relevant to detonator function and imply that it may play a role in regular detonation. The absorptivity of such materials is important to understand if the extent of localization of that energy source is to be understood, e.g., UV laser illumination of a polycrystalline powder bed.

The Beer-Lambert law describes the absorbance, A , of a compound (solid, liquid or gas) as,

$$A = \log_{10} \frac{I_o}{I} = \epsilon t c, \quad (1)$$

where I_o is the initial intensity of light at a given wavelength and I is the transmitted intensity, ϵ is the molar absorptivity of the compound, t is the thickness of the sample and c is the concentration of the compound of interest [4,21]. The penetration depth, δ_p , may be calculated from,

$$\delta_p = \frac{t}{\ln 10 A}. \quad (2)$$

Plots for PETN, HMX, RDX (1,3,5-Trinitro-1,3,5-triazinane), HNS (Hexanitrostilbene) and CL-20 (Hexanitrohexaazaisowurtzitane) are given and both absorptivity plots and transmission depth are presented to allow a quantitative understanding of the material response in a specific application.

Experimental

For this study we used UV/visible spectroscopy to examine five commonly used explosives: PETN, HMX, RDX, HNS and CL-20. High specific surface area powders of α -RDX and α -PETN were obtained from Teledyne RSI, CA, USA. The β -HMX and HNS were obtained from Holston Army Ammunition Plant, TN, USA. The HMX was a bimodal distribution of three parts class 1 (coarse) and one part class 2 (fine) [22] and the HNS was class IV. The ϵ -CL20 was obtained directly from ATK Thiokol, USA. All of the powders were used as received from the manufacturer.

A Thermo Scientific UV/Vis spectrophotometer (Evolution 220) was used in the collection of all spectra. The Evolution 220 is a double beam spectrophotometer with sample and reference pellet positions utilizing dual silicon photodiodes. The settings used for the final scans are as follows: spectral bandwidth 1 nm, scan speed 30 nm/min, and a data interval of 0.05 nm. Initial range finding scans were performed at a scan speed of 1000 nm/min. KBr blanks were prepared fresh, scanned, and subtracted prior to analyzing each sample. Thicknesses of blanks were matched to that of the sample pellets.

Master sample stocks were prepared at 2% by weight explosive/KBr (potassium bromide, Sigma Aldrich FT-IR grade, 221864). These were pulverized using a mortar and pestle and then stored in a vacuum desiccator until use. Dilutions were made to 0.2% explosive/KBr for all 5 explosives using the master stocks to test maximum

absorbance and gain insight into the ideal concentration and thickness for each explosive. This initial range finding series allowed for the appropriate conditions for each powder to be established. The final sample values determined from these initial scans can be found in Table 1.

Explosive	% EM/KBr	Weight(mg)	Thickness(μm)
Range Finding	0.2%	250	750
HMX	0.2%	250	740
PETN	0.1%	250	710
RDX	0.1%	200	580
HNS	0.01%	150	420
CL-20	0.1%	200	560

Table 1: Optimized pellet conditions used for this paper. These conditions were determined via initial range finding scans performed on each powder.

KBr pellets with a diameter of 13 mm were pressed using a PIKE Technologies evacuable pellet press (PIKE PN:161-1900). Pellets were pressed under vacuum using the following procedure, Segment 1: 6000lbs force, 3s; Segment 2: Release, 3s; Segment 3: 14,000lbs, 30s; Segment 4: Release, 30s; Segment 5: 20,000lbs, 120 s. Pellets were then scanned immediately after ejection from the die.

Results

Figure 1 contains detailed information from the 5 explosives investigated. As previously mentioned, sporadic accounts of single explosives or narrow scan widths can be found in the literature. However, for the first time, both absorptivity and precise thickness are documented for solid thin pellets. This allows for more rigorous analysis to be performed such as penetration depth calculations. As can be seen in Table 2, the absorbance maximums (Abs_{max}) for all of the materials investigated are very similar and can be found in the UV. Full tabular absorbance information is provided in the supplementary information.

Significantly, the results agree and greatly expand upon the limited qualitative dataset provided by Smit [3]. However, when comparing to the single crystal work reported in [7], neither the band gap absorption at 1060 nm nor the absorption increase at 890 nm are observed in our polycrystalline PETN data. Whether this is due to a different measurement method or the use of powdered material rather than a single crystal is unclear.

The measurements made in this paper allow for a more precise calculation of the deposition of photon energy as a function of depth. However, further investigation is needed to fully determine the scattering/reflectance effects in these powders. The scattering effects are likely to be minimal due to the close match in refractive index between the KBr ($\eta=1.55$) [23] and HMX ($\eta=1.59$), RDX ($\eta=1.58$) and PETN

($\eta=1.55$) [24] (Refractive indices for HNS and CL-20 have not yet been reported). As such, we hypothesize that once scattering/reflectance are properly accounted for, the short wavelength data will be relatively unaltered while the IR absorption will be lowered resulting in an increased penetration depth.

Explosive	Abs_{max}	$\delta_{p(Abs_{max})}$	$\delta_{p(1064)}$
HMX	237.4	645	8400
PETN	209.7	187	14100
RDX	206.4	210	5900
HNS	210.5	11.6	454
CL-20	212.4	114	1700

Table 2: Absorbance maximum and penetration depths for explosives. For comparison penetration depths at the commonly used laser initiation wavelength of 1064nm is provided. All values given in nanometers.

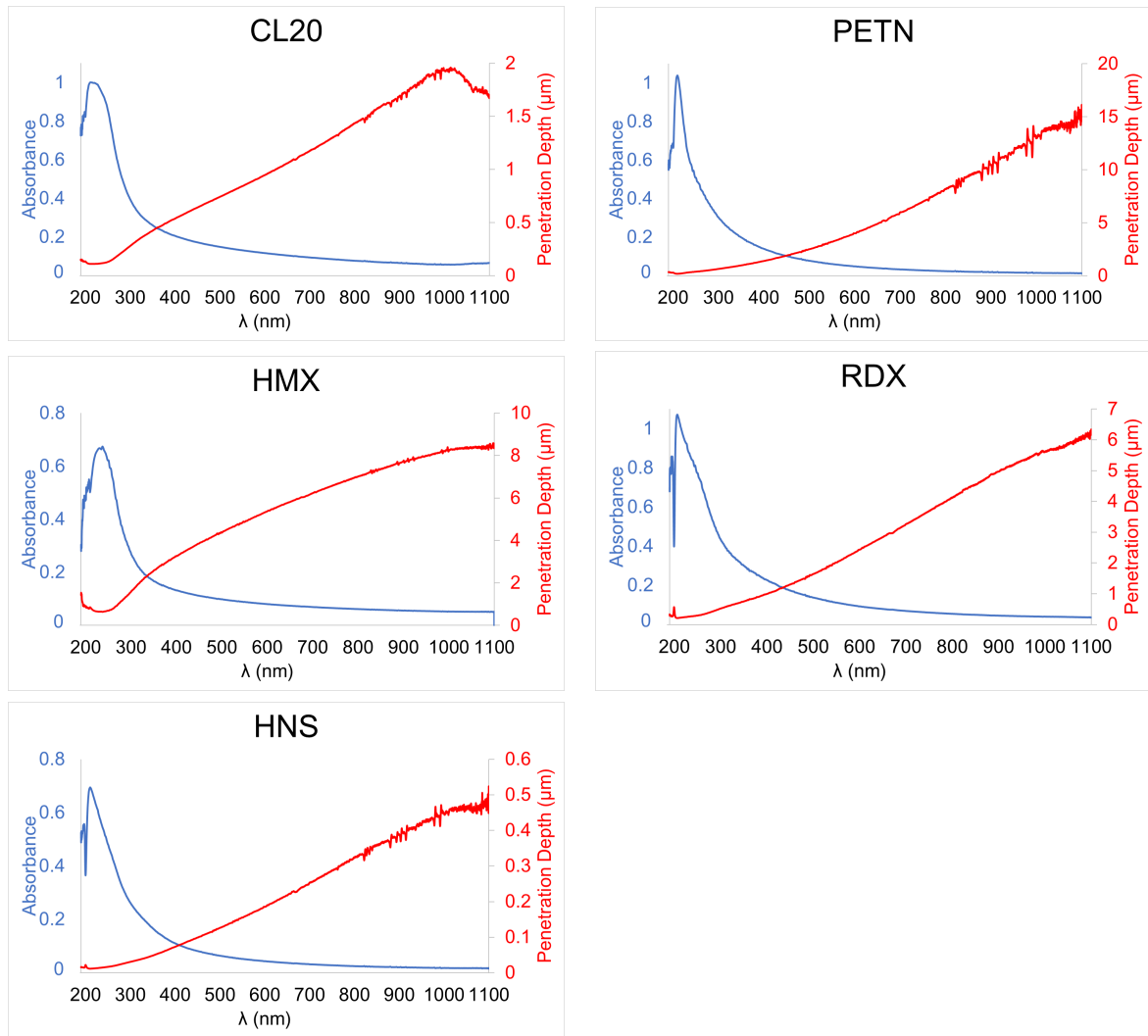


Figure 1: The absorbance and penetration depth of investigated HE powders as a function of wavelength

Discussion and Conclusions

This research provides absorbance measurements and an estimate for the penetration depth of five commonly used powdered explosives. As might be anticipated, all of these organic molecular crystals are highly absorbing at short wavelengths (UV) and less so at longer wavelengths. Visual inspection of the powders reveals that only HNS is reasonably opaque and colored (a light yellow) while the rest are translucent with no apparent color tinge. The spectrophotometer confirms this observation of no strong band absorbances at short, visible and longer wavelengths for all of the materials studied.

It is widely agreed that UV photons can produce photochemical effects in nitramine and similar nitrated explosives [6,9–15,18–20,25–27]. Specifically, of the many potential degradation products, the X–NO₂ bond is extremely susceptible to radical cleavage by high energy photons, a process that occurs in picoseconds. Once a sufficient number have been cleaved, the •NO₂ can become autocatalytic leading to runaway reaction and energy release. The UV-induced lability of the X–NO₂ bond of a particular HE appears to be an important determining factor in ability to function within an EBW detonator. Bond disassociation energies (BDE) and therefore resistance to radical cleavage by UV irradiation for X–NO₂ are reported to increase as follows: O–NO₂ < N–NO₂ < C–NO₂ [28]. While this general trend can be seen to hold true for many of the common explosives, i.e., PETN < HMX < TNT, one must use caution when using only BDEs to determine susceptibility to UV irradiation. Multiple other factors including molecular strain and conjugation can lead to extreme outliers like HNAB, which, while containing the less reactive C–NO₂ bonds, is found to function reliably in EBW detonators.

Reference [1] demonstrates that the mechanism of operation of EBW detonators is highly unlikely to be either shock-to-detonation (SDT) or deflagration-to-detonation (DDT) in the strict scientific definition of those terms. Instead the mode of operation is a volumetric thermal explosion [29]. If this is accepted, the remaining questions are about the mechanism of volumetric heating and how the resulting explosion transitions to a detonation so quickly. It is hypothesized that one significant mechanism is direct UV photochemistry of the explosive powder resulting in a combustion radiating in the IR that is absorbed by the explosive kernel. It is the purpose of most of the remainder of this discussion section to investigate this hypothesis.

UV susceptibility of HEs is important as electrical bursting of the wires in EBW detonators has been shown to produce large amounts of UV radiation [30]. The extreme absorption of UV light in the explosives examined here suggests that photochemical breakdown of the material, and heating, will therefore occur extremely close to the bridge location. Indeed, it is observed in PETN-based EBWs that detonation in the low-density pressing occurs approximately 1 mm in front of the bridge and is a volumetric thermal explosion with a delay of approximately 1 μ s after bridge burst [1].

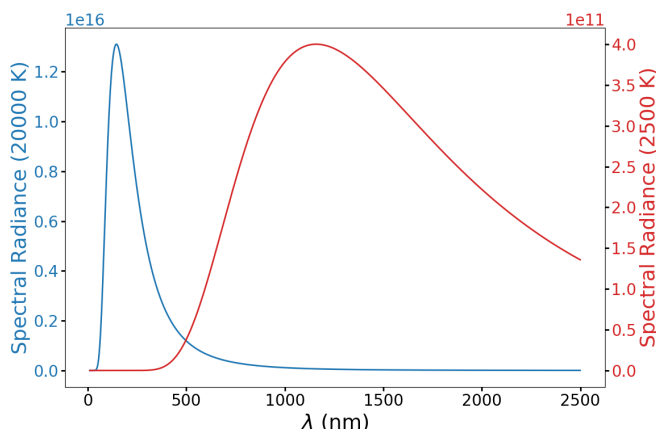


Figure 2: Plank blackbody radiation expected from a bursting bridgewire ($\approx 20000\text{K}$) compared to that of the average HE flame temperature ($\approx 2500\text{K}$).

If the energy produced from thermal and photochemical breakdown of the PETN was at a normal spatially dependent flame temperature for burning explosives (800–3000K) [31,32], the peak emission wavelength would vary greatly from 3600–965 nm. Because the low density PETN is close to 50% of the theoretical maximum density (TMD) the greater penetration depth would place the region of maximum heating some distance in front of the bridge. That is, the PETN powder exposed to UV would absorb almost all of it within a few microns, but the ensuing chemical breakdown would occur at a much lower temperature, have a spatial component and transfer thermal energy in front of the bridge location where thermal explosion and transition to detonation events could then occur some short time later. Reference [1] discusses that observation that a thermal explosion would result in PETN in approximately a microsecond of a volumetric thermal explosion kernel were heated by 700K.

Therefore, an argument can be made that there is both a UV and thermal element contributing to the initiation of a low density PETN pressing. Figure 2 contrasts the expected blackbody radiation for a bridge burst with that of a burn front, and as can be clearly seen, the bursting bridgewire contributes 10^5 more radiance to the sample. What is more, the vast majority of that energy is in the UV which leads to a rapid increase in radical decomposition products within the short absorbance depth.

To define the contributions of UV to HE initiation we found that while PETN, CL-20, RDX and HMX have all been used successfully in EBW detonators (burst energy required to operate increases in the order listed), HNS has never been reported to have detonated in an EBW configuration. Interestingly, HNS has the greatest absorbance at all wavelengths of any of the materials studied here and has been reported to undergo similar photochemical breakdown under UV illumination to the others studied here [18]. This leads us to deduce that UV absorbance may not be the sole determining factor in an explosive’s ability to function in an EBW, but is still

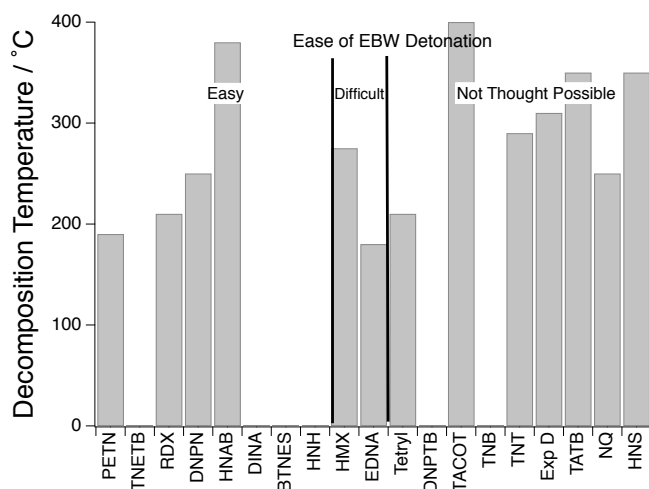


Figure 3: A comparison of the decomposition temperature of some explosives and their ease of detonation in an EBW detonator and shows little correlation. The acronyms are listed in appendix A.

important nevertheless.

Next, we utilized a study of explosives amenable for use in EBWs [33]. We attempted to use the data from this to correlate EBW function, or failure to detonate, with the explosive decomposition temperature. This correlation was anticipated to help bridge the gap between UV absorbance and the thermal properties influencing a material’s ability to function in an EBW. Some of the compounds reported are relatively unknown and literature on them is sparse. However, results for those that could be found are shown in Figure 3. HNS was not part of the study, but data from other sources has been added for comparison. Clearly, there is little correlation suggesting that decomposition temperature is not exclusively responsible for eventual successful detonation.

In addition, reference [33] also includes 50% drop-weight go/no-go thresholds for the materials studied. A plot of these data with respect to detonation in an EBW configuration is given in Figure 4. The correlation is much better for this metric suggesting that drop-weight may be a better indicator of EBW detonator function. The drop-weight is a highly integrated explosive sensitivity test that closely couples ignition sensitivity and ease of reaction propagation [34]. In an EBW, both ignition and growth to detonation must happen in very short timescales ($< 2\mu\text{s}$) and short length scales ($< 3\text{ mm}$) to be practically useful. In many materials a relatively small increase in violence is noticed at drop-weights above the 50% threshold, although this is not true for all materials such as HNS [35]. Specifically, moderately increasing the height on PETN does not greatly increase the observed violence, while for HNS it does. This suggests that PETN grows quickly to a consistent violent reaction after

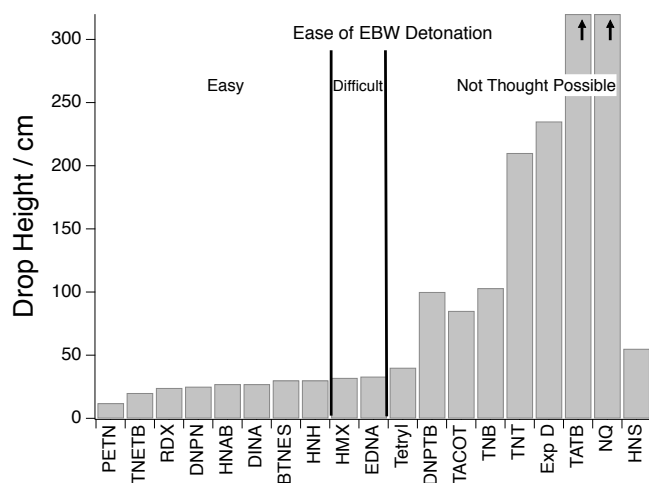


Figure 4: A comparison of the 2 kg type 12 tooling drop-weight sensitivity of some explosives and their ease of detonation in an EBW detonator showing strong correlation. The acronyms are listed in appendix A.

ignition while in HNS reaction builds with greater difficulty.

It is important to realize that the drop-weight test is not a detonation sensitivity test, but that there is undoubtedly a strong correlation between materials that SDT easily and those that are observed to be sensitive to the drop-weight stimulus. In the drop-weight only true primary explosives are observed to detonate, while secondary explosives may violently deflagrate. Indeed, damage to the drop-weight anvils often results when detonations occur while none is observed even when violent responses are recorded in secondary explosives. It is perhaps significant that the drop height for HNS is second only to Tetryl in terms of sensitivity for materials that cannot be used in EBW detonators. Such a ranking, in the absence of other factors, would suggest that HNS could be used if a sufficiently large fire-set and bridgewire were used. To our knowledge this has not been achieved suggesting that perhaps there is something else different about the material that makes it unsuitable for EBW detonators.

The shock-to-detonation sensitivity of HNS is comparable to RDX and HMX although the exact ranking depends on the particle size and pressing density of each specific material. It has been reported by Smit [36] that while HNS would structurally be seen as very similar to HNAB in regards to reactivity, HNS adopts a steric induced non-planar geometry leading to the loss of conjugation within the molecule. This in turn leads to HNS sharing very similar chemical properties with TNT which also does not function in EBW detonators. Specifically, we propose that it is the difficulty of propagating a combustion reaction in HNS that renders it unsuitable for use in EBW detonators rather than the difficulty of starting reaction per-se. The unusual incremental violence response of HNS in the drop weight and the relative ease of

producing decomposition products by the application of UV energy supports this conjecture [35].

Although many useful insights into the role of UV light in the function of detonators can be gleaned from the information within this paper, it is important to take into consideration outliers such as HNAB and HNS. If not accounted for, the different conformations, conjugation, and bond strengths of the common explosives can produce nonintuitive results in EBW detonators.

It is proposed that the direct optically initiated (DOI) detonations studied in [37, 38] have many similarities to EBW detonators [1]. Specifically, it was demonstrated in these references that sufficient 1064 nm laser energy could produce a detonation in PETN, but only when the powder was moderately confined in a sealed cup. In contrast, significantly less laser energy at 355, 308 and 266 nm could produce detonation in relatively unconfined cups of the same powder (similarly, EBW detonators do not require confinement to function). It is therefore clear that with DOI detonations, not all photons are equally efficacious and the authors propose that in addition to bulk heating, UV wavelength light results in photochemistry that significantly lowers the total energy requirement for detonation. Additionally, it has been discovered that the addition of small amounts of materials that increase the absorption rate of IR light, such as gold nanospheres, lower the energy threshold for detonation with 1064 nm light [39]. Finally, in neither DOI investigation could HNS be made to detonate under any conditions tried. These findings are in full agreement with the discussion presented here.

It is mentioned, although it may prove to be entirely coincidental, that the following compounds that did not detonate in the EBW tests are colored and/or opaque (HNS, Tetryl, TNB, TNT, TATB and Explosive D are all visibly opaque and yellow colored; Tacot is orange/red; nitroguanidine and EDNA are white). In contrast, the translucent and colorless compounds PETN, DINA, RDX, CL-20, HMX could all detonate in the EBW test. Two other compounds that did detonate in the EBW tests were HNAB which is a translucent red color and HNH that is a white color. We therefore speculate that a degree of translucency of the explosive may also be important to allow the transmission of initial reaction energy to be coupled forward into a building reaction kernel. Obviously, many of the explosives that did not detonate in the EBW configuration are extremely shock insensitive (i.e., TATB), although if this also is related to opacity and coloring is unclear and requires further study.

In summary, it is quantitatively demonstrated that all of the explosives tested are extremely efficient absorbers of UV light and less efficient as the wavelength increases. None of the materials showed any strong absorbance bands between 190 and 1100 nm or distinct coloring with the exception of HNS which is a pale yellow. It is suggested by the authors that the UV absorption and resulting picosecond timescale photochemistry play a strong role in how EBW detonators function and that consideration of the full chemical structure and conformation of an explosive molecule

allows a fairly reliable prediction to be made of its efficacy in such initiation schemes.

Appendix A: Acronyms used in figures 3 & 4

Acronym	Name
PETN	pentaerthritol tertrinitrate
TNETB	trinitroethyltrinitrobutyrate
RDX	cyclotrimethylene trinitramine
DNPN	dinitropropylnitramine
HNAB	hexanitrobenzene
DINA	diethylnitramine dinitrate
BTNES	bistrinitroethylsuccinate
HNH	hexanitroheptate
HMX	cyclotetramethylene tetranitramine
EDNA	ethylenedinitramine
Tetryl	methyltrinitrophenylnitramine
DNPTB	dinitropropyltrinitrobutyrole
TACOT	tetranitrodibenzo tetrazpentaline
TNB	trinitrobenzene
TNT	trinitrotoluene
Exp D	ammonium picrate
TATB	triaminotrinitro benzene
NQ	nitroguanidine
HNS	hexanitrostilbene

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