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Effective atomic number and electron density determination using spectral x-ray CT

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ABSTRACT

We present Spectral X-ray Computed Tomography (SCT) estimations of material properties directly from energy-dependent measurements of linear attenuation coefficients (LAC). X-ray Computed Tomography (CT) is commonly utilized to characterize the internal properties of an object of interest. Dual-Energy X-ray CT allows material characterization into energy-independent physical properties such as Z_e and electron density ρ_e . However, it is not robust in presence of dense materials and metal artifacts. We report on the performance of a method for system-independent characterization of materials that introduces a spectroscopic detector into X-ray CT, called spectral ρ_e/Z_e estimation (SRZE). We benchmark the SRZE method against energy-integrated measurements in material classification tests, finding superior accuracy in the predictions. The advantage of this technique, over other methods for material characterization using x-ray CT, is that it does not require a set of reference materials for calibration. Moreover, the simultaneous detection of spectral features makes it robust to highly attenuating materials, since the energy intervals for which the attenuation is photon limited can easily be detected and excluded from the feature estimation.

Keywords: Spectral X-ray CT, X-ray Characterization, Effective atomic number, Electron density, MULTIX-ME100, Threat Detection, Security Screening

1. INTRODUCTION

For decades, X-ray Computed Tomography (CT) has been adopted as one of the standard techniques for non-destructive tests and evaluations, for example in the screening of luggage for threats.¹ Since laboratory-scale X-ray sources generate a polychromatic beam (Fig. 1), conventional CT does not measure a single-energy value of the linear attenuation coefficient (LAC), but measures but its weighted average through multiple energies. Therefore, using this technique the characterization of a material's LAC is complicated by polychromatic effects such as beam hardening² and photon starvation from metals or dense materials,³ and require an accurate model of the detector's spectral response. Moreover, different materials yield different contrast, in terms of intensity values in the reconstructions, when probed at different mean energies; therefore their classification might be not optimized depending on the choice of the source parameters of kilovoltage peak and filtration.

To overcome these limitations, researchers have recently developed methods to estimate energy-independent physical parameters of the materials, using Dual-Energy CT (DECT).^{4,5} With a DECT acquisition, the LAC of materials is probed at two different X-ray spectra (as the low- and high- energy pair in Fig. 1) and converted into the energy-independent physical parameters of electron density ρ_e and effective atomic number Z_e , as in the System-Independent ρ_e/Z_e (SIRZ) method proposed by Azevedo et al.⁶ and further developed by Champley et al.⁷ This can be technically achieved, for example with a consecutive scan with different source filtration and kilovoltage peaks, or using dual-energy sandwich detectors.⁸ However, the performance of these techniques depend on the choice of the pair of spectra used for the DECT acquisitions and the estimation of their respective detector spectral responses. These techniques will be accurate and precise for a group of materials within a limited range of Z_e , but will have lower performance for materials outside this range. This limitation can be overcome using spectral X-ray CT (SCT). SCT can be considered as an extension of DECT where the signal is simultaneously collected in multiple non-overlapping energy ranges. This would extend the range of materials for which the characterization is accurate.

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With the advent of single photon counting detectors (PCD) able to discriminate the energy of the detected photons (Fig. 1), the interest towards spectral X-ray CT (SCT) has grown significantly, for the superior contrast to noise ratio^{9–13} and for enabling k-edge CT.^{14,15} In this work we use an extension of the SIRZ method for SCT, called Spectral ρ_e/Z_e Estimation (SRZE),¹⁶ to estimate the physical parameters of a large dataset of innocuous materials commonly found in checked-in luggage, and threat materials which we want to be able to detect. The SRZE characterization's impact on the classification task accuracy is benchmarked against more direct methods for a set of different samples with including both innocuous and threat materials in a random order. For all cases studied in this work, we found superior accuracy in the classification task when using SRZE method for material characterization.

Figure 1: Left. In conventional X-ray CT, the signal is integrated over all energies. Center. In Dual-Energy X-ray CT, two different spectra are used to probe the sample attenuation at a low- and high- mean energy. Right. In Spectral X-ray CT, single photon counting detectors discriminate the incoming radiation in distinct energy bins with mean energy depending on the set energy thresholds.

2. THEORY AND METHODS

In this section, we define the system-independent physical properties we have used to characterize materials and the methods we have adopted in this work to estimate them from SCT measurements.

2.1 Dual-Energy X-ray CT Characterization

As described in the Lambert-Beer's law,¹⁷ X-ray CT measures the Linear Attenuation Coefficient (LAC) of materials. However, LAC is a function of the energy and therefore conventional CT, which use acquisitions with energy integrating detectors, is not a robust method for the characterization of materials since it depends on the source spectrum and polychromatic effects such as beam hardening that cause distortions in the reconstruction. Alvarez and Macovski showed in 1976 that the LAC could be approximated as linear combination of a dual set of basis functions:⁴

$$\mu(E) = a_1 f_{ph.abs.}(E) + a_2 f_{KN}(E), \quad (1)$$

where $f_{ph.abs.}(E) = 1/E^3$ models the photoelectric absorption interactions of photons with matter, and $f_{KN}(E)$ is the Klein-Nishina function, which approximately models the incoherent (Compton) scattering interactions of photons with matter:

$$f_{KN}(E = E'/511\text{keV}) = \frac{1+E}{E^2} \left[\frac{2(1+E)}{1+2E} - \frac{1}{E} \ln(1+2E) \right] + \frac{1}{2E} \ln(1+2E) - \frac{1+3E}{(1+2E)^2}. \quad (2)$$

The coefficients a_1 and a_2 are proportional to the physical parameters of bulk density ρ and atomic number Z , which are energy-independent. Based on this concept, Azevedo et al. presented a method⁶ using Dual-Energy X-ray CT for the system-independent characterization of materials into their features of electron density (ρ_e)

and effective atomic number (Z_e). For a compound material, consisting of a number n_i of N distinct elements i , the electronic density is defined as:

$$\rho_e = \frac{\sum_{i=1}^N n_i Z_i}{\sum_{i=1}^N n_i A_i} \rho, \quad (3)$$

where $A(Z)$ is the atomic mass (g/mole) of the element Z . To approximate the atomic number of such a compound Azevedo et al.⁶ used the effective atomic number, Z_e , defined as a non-integer atomic number that corresponds to an artificial element, for which the interactions are assumed to be modeled by the X-ray attenuation cross sections. The cross sections for the artificial element Z_e are obtained by a linear interpolation between the cross section of the two adjacent elements in the periodic table:

$$\sigma_e(Z_e, E) = (1 - \epsilon)\sigma_e(Z', E) + \epsilon\sigma_e(Z' + 1, E). \quad (4)$$

Therein, Z' is the lower adjacent element, $Z' = \text{floor}(Z)$ and ϵ is the difference, $\epsilon = Z' - Z$. In terms of the effective atomic number and electronic density presented above, we express the LAC of a material m as:

$$\mu^m(E) = \rho_e^m \sigma_e(Z_e^m, E). \quad (5)$$

In their study, Azevedo et al.⁶ demonstrated system-independence of the method and very good accuracy and precision for a set of standard materials with $Z_e < 15$ with well-known physical parameters.

2.2 Spectral X-ray CT Characterization

We briefly describe the method presented in detail by Busi et al.¹⁶ to estimate the effective atomic number and electron density from SCT acquisitions. The measured raw data undergoes a spectral detector correction algorithm presented by Dreier et al.,¹⁸ which corrects for the spectral distortions caused by the interactions between photons and the PCDs. This step is followed by the spectral scattering corrections method, from Monte Carlo X-ray simulations, presented by Busi et al.¹⁹ The energy resolved sinograms are converted into attenuation using Lambert-Beer's law, and reconstructed using Livermore Tomography Tools (LTT) software²⁰ using the filtered back projection algorithm. The energy-dependent LACs are obtained by taking the mean values in the manually segmented regions respective to each material, for each energy bin. The respective variance of the mean values in the segmented regions is calculated as well, as it will be used in the feature estimation step. At this stage, an automated energy thresholding is used to disregard energy bins in which the reconstructions are corrupted by photon starvation caused by highly dense materials. The estimation of the physical parameters is performed by solving a constrained minimization of the squared distance between the measured LAC, $\tilde{\mu}(E)$, and its relative theoretical definition $\mu(E)$, parametrized by ρ_e and Z_e as in eq. (5) :

$$\arg \min_{\{\rho_e, Z_e\}} \sum_{k=i}^f \lambda_{E_k} |\tilde{\mu}(E_k) - \rho_e \sigma_e(Z_e, E_k)|^2. \quad (6)$$

Therein, λ_{E_k} are the energy weights, computed as the reciprocal of the variance (s^2) of each material's LAC in their ROI, $\lambda_{E_k} = 1/s^2(\tilde{\mu}_{E_k})$. These can be interpreted as the weight given to each energy bin E_k into the estimation of the material's features. The minimization process in this work was performed with MATLAB[®]'s routine function FMINCON with solution boundaries $\rho_e = 0 - 15 \text{ e}^- \text{ mol/cm}^3$ and $Z_e = 1 - 99$ and initial guesses $\rho_e^0 = 1 \text{ e}^- \text{ mol/cm}^3$ and $Z_e^0 = 7$. No particular dependency on the starting values was observed.

3. EXPERIMENTS

3.1 Instrumental setup

The instrumentation used for the characterization of the materials into their physical properties was designed for SCT measurements and briefed in Table 1. The X-ray beam was generated by a Hamamatsu source with a tungsten anode and the acceleration voltage and filament current set to 160kV and 0.5mA, respectively. For these operating parameters the focal spot was $75 \mu\text{m}$. The detector was made up of two 1D PCD Multix-ME100²¹ modules, composed of 1×128 pixels of size $0.8 \times 0.8 \text{ mm}^2$ and each with 128 energy bins of width 1.1 keV, evenly

distributed between 20 and 160 keV. The energy resolution of the detector under high X-ray fluxes is 6.5% (8 keV at 122 keV).²² A 2-mm-thick aluminum filter was placed in front of the source to reduce the beam hardening effects and to suppress the photons with energy below the spectral range of the detector. The characteristic X-ray peaks of the tungsten target are smeared due to the limited detection energy resolution,^{18,23} resulting in a smoother spectrum compared to what is theoretically expected. For all the SCT scans performed, the total acquisition time per scan was 30 minutes with the rotation stage continuously rotating. Each scan was rebinned into 5 seconds frames to form 360 projections evenly distributed between 0° and 359°. The source to detector distance (SDD) was set to 1115 mm whereas the source to object distance (SOD) was set to 575 mm.

Table 1: Experimental parameters.

Source parameters	160 keV, 0.5 mA
Focal spot	75 μm
Number of pixels	1×256 1D array
Pixel size	$0.8 \times 0.8 \text{ mm}^2$
Detector's resolution	6.5%(8 keV) at 122 keV
Number of energy bins	128 (1.1 keV width)
Number of projections	360
Exposure time per projection	5 seconds
SDD	1115 mm
SOD	575 mm

3.2 Characterization results

We used the SCT characterization method described in Section 2.2 to estimate the physical parameters of a set of 73 different materials listed in Table 3 in Appendix A. The results are displayed in a ρ_e/Z_e chart, in Fig 2. The choice of the materials in this work focus on the threat detection in airport luggage. It consists of a varied selection of organic innocuous compounds, mostly in water solutions, and a selection of explosive or precursor threat materials. We found a good contrast in the two physical parameters of ρ_e and Z_e for threat and innocuous materials, except for a few materials. Ethanol 96% (index: 25) for example, will have a high chance of being detected as a false positive for its proximity to acetone (index: 3). Among the threats, the hydrazine solution in water (index: 7) and nitromethane (index: 12) are also challenging, due to their similarity with water (index: 48).

3.3 Singular Value Decomposition analysis

We estimate material physical parameters from their LAC using the model in Eq. 5. To confirm that this model matches with the experimental findings, we performed a Singular Value Decomposition (SVD) analysis procedure, similar to the one proposed by Eger et al.²⁴ for synthetic data. We constructed a matrix $\mathcal{M}$ with the linear attenuation coefficients measured of all the materials listed in Appendix A. The matrix $\mathcal{M}$ has dimensions ($E_b \times N_{mat}$) where E_b is the number of energy bins for which the LAC is probed and N_{mat} is the number of materials. The SVD decomposition aims to find a set of linearly independent vectors that can express the LAC, and can be expressed as:

$$\text{SVD}(\mathcal{M}) \equiv \mathcal{M} = \mathcal{U} \mathcal{S} \mathcal{V}^T, \quad (7)$$

where $\mathcal{U}$ is a ($E_b \times N_{mat}$) matrix where each column i compose the set of linearly independent vectors $U_i(E)$, $\mathcal{S}$ is a ($N_{mat} \times N_{mat}$) diagonal matrix where the magnitude of each element $S_{i,i}$ describes the relative contribution of the corresponding vector U_i to the model. The first singular values $S_{i,i}$ and the first six singular vectors U_i are shown in Fig. 3. A qualitative look at these vectors indicate the two dominant singular vectors, U_1 and U_2 are corresponding to the basis functions for incoherent scattering and photoelectric absorption, as in Eq. 1. These observations were confirmed by finding a linear proportionality between U_1 and the Klein-Nishina function f_{KN} , and a linear trend of the inversion $1/\sqrt[3]{U_2(E)}$. The remaining singular vectors are dominated by noise components and the oscillations in the measured LAC due to the poor spectral resolution of the detector around

Figure 2: Charts of the effective atomic number and electron density (Z_e, ρ_e) of the materials scanned, estimated through the SRZE method. The numbers labeling the data points are referring to the index in Table 3 in Appendix A. Note that to avoid overlap of the material labelled indexes, a magnified version of the left frame is displayed in the right frame.

the characteristic peaks of the X-ray source, as indicated by the wiggles around the energy of the K_{α_1} (59.3 keV) and K_{β_1} (67.2 keV) tungsten emission lines. The third singular vector U_3 , displays a sharp rise and consecutive relaxation, and is required to fully represent all the materials LACS. One would find the same behavior of the third significant singular vector, when running the same procedure on standard reference LAC curves from NIST database.²⁵ We found, however, that the first two vectors are sufficient to approximate all the materials studied. This was confirmed by calculating the autocorrelation values of the singular vectors, which were below the value of 0.5²⁶ except for $U_{1,2,3}$ and a few more $U_{4,5,6}$, as seen in Fig. 3 (b), with the same behavior as U_3 but different modulation of the peaks.

Figure 3: Singular Value Decomposition analysis of the reference materials LACs. (a) Singular values of the diagonal i -elements (blue-squares). Note logarithmic scale in the y -axis. (b) Singular vectors U_i respective of the diagonal singular values s_i . The scale is in arbitrary units.

4. CLASSIFICATION BENCHMARKING

4.1 Materials and prediction models

In this work, we have tested three different methods for the material classification from SCT data acquisitions. In the first method, we used as the material's feature the energy integrated LAC, $\tilde{\mu}(E')$, obtained by summing the signal over all the 128 energy channels of the detector. The effective energy (E') corresponding to $\tilde{\mu}$ was calculated using the source spectrum as measured by the flat field acquisition (i.e. without the sample) as a model for the detector's response. The second method, utilizes as the material's feature the energy-dependent LAC, i.e. the attenuation coefficient probed at the 128 energy values corresponding to the specifics of the detector ($\mu(E_k)$ with $k = 1, 2, 3, \dots, 128$). In the third method, we used the SRZE characterization method described in Section 2. For each of these methods, a look-up table library of materials features such as the one in Appendix A, has been built by using single slice fan-beam SCT of individual materials in ideal condition (i.e. without metal artifacts and center-offset).

In the following scans, we have measured 30 samples composed of four glass bottles filled with different materials (found in Appendix A) and aluminum pin of 4mm diameter placed in a sample holder. Of these samples, 10 of them were with the sample holder centered with the sample's rotation stage, 10 of them were with an offset between the sample holder and rotation stage centers, and the remainder 10 with an aluminum slab of 10×30 mm as well. Examples of the CT reconstructions of the different groups are shown in Fig. 4.

Figure 4: Reconstruction examples of the three types of dataset reproduced. Left: the samples are placed centered in respect to the center of rotation. Center: the samples are placed offset in respect to the center of rotation. Right: the samples are placed offset in respect to the center of rotation and an aluminum plate 10×30 mm wide is inserted to provoke metal artifacts and photon starvation.

For each of the four materials in the samples, we have benchmarked the classification accuracy, as the ratio between successful predictions and total cases, of the three methods. The prediction models in the equations below have been used for the material classification to find the labels (i.e. the type of materials) from the ground truth library obtained using SRZE method listed in Table 3 in Appendix A. A similar library has been constructed for the other two methods.

- Integrated LAC discrimination:

$$label = \arg \min_{label} \sqrt{(\mu^{est} - \hat{\mu}^{label})^2}. \quad (8)$$

- Spectral LAC discrimination:

$$label = \arg \min_{label} \sqrt{\sum_{k=1}^{128} (\mu_{E_k}^{est} - \hat{\mu}_{E_k}^{label})^2}. \quad (9)$$

- SRZE discrimination:

$$label = \arg \min_{label} \sqrt{w_{Z_e} \left(\frac{Z_e^{est} - \hat{Z}_e^{label}}{\langle \hat{Z}_e^{label} \rangle} \right)^2 + w_{\rho_e} \left(\frac{\rho_e^{est} - \hat{\rho}_e^{label}}{\langle \hat{\rho}_e^{label} \rangle} \right)^2}. \quad (10)$$

The hat sign refers to the values stored in the libraries whereas the $\langle \rangle$ operator corresponds to the mean, applied to all reference values of Z_e and ρ_e . That is done to have the physical parameters in the same scale and with same importance. The weights w_{ρ_e} and w_{Z_e} are assigned to the individual features to tune the significance given to each of them. In this work both have been set to $w = 0.5$.

4.2 Results

The results of the benchmarking are reported in Table 2 for the different prediction methods and sample groups. In the material classification, the prediction is successful when the individual material label is found correctly,

Table 2: The accuracy results (%) obtained for the different sample groups. In the exact material classification, the prediction is successful when the specific materials are classified correctly. In the binary classification, the discrimination is only performed between threats and innocuous materials.

Material classification			
	Integrated LAC ($\tilde{\mu}$)	Spectral LAC ($\mu(E)$)	SRZE (ρ_e/Z_e)
Centered	24.0%	72.0%	72.0%
Offset	28.0%	68.0%	72.0%
Offset with Al plate	40.0%	38.3%	58.3%
Mean	30.7%	59.4%	67.4%

Binary classification (Threat/Innocuous)			
	Integrated LAC ($\tilde{\mu}$)	Spectral LAC ($\mu(E)$)	SRZE (ρ_e/Z_e)
Centered	60%	100%	100%
Offset	64%	98%	100%
Offset with Al plate	75%	66.7%	78.3%
Mean	66.3%	88.2%	92.8%

whereas in the binary classification the discrimination is only done between innocuous and threat materials. Both the spectral characterization methods (LAC and SRZE) show an overall improved prediction accuracy when compared to integrated LAC method (which is corresponding to conventional integrating detectors). Samples with metal artifacts induced by the aluminum plate show a significant decrease in the accuracy of the direct LAC discrimination method, whereas the accuracy increases with the SRZE method. That is due to the energy thresholds selection step of the SRZE method, which allows data affected by photon starvation induced by the Aluminum plate to be disregarded. We remark that such a relatively low accuracy in the exact material classification was expected as most of the innocuous materials in the library are water-based compounds and some of them are varieties of the same specimens (e.g. 5 types of beer, 4 sun lotions etc.). On the other hand, the SRZE method shows perfect accuracy in the binary classification for samples without the aluminum plate. Nevertheless, the relatively low result obtained in the presence of metal artifacts suggests a demand for a further optimization of the data pre-processing step, possibly with the introduction of a metal artifact removal step.

5. CONCLUSIONS

We have demonstrated feasibility of material characterization into system-independent physical parameters (ρ_e , Z_e) using spectral X-ray CT. We have shown that the spectral methods have overall superior accuracy in the material classification, when compared to the conventional CT techniques. Spectral LAC method shows a 28.7% and 21.9% increase in material and binary overall mean classification, respectively. The SRZE method shows a

36.7% and 26.5% increase in material and binary overall mean classification, respectively. The SRZE method is free of calibration steps and system-independent, which makes it suitable for a standard method estimation of a material's physical properties ρ_e , Z_e . Moreover, the SRZE method presents higher robustness in the presence of high-Z materials due to the capability to omit photon starved data. Further developments in the metal artifact removal algorithms for SCT, and advances in the hardware technologies of the PCD, decreasing their spectral distortions, should increase the screening of threats even further, using this method.

APPENDIX A. MATERIALS ESTIMATED FEATURES LIBRARY

The library of materials, for which the physical parameters were estimated, includes innocuous materials, which are commonly found in checked-in luggage, and explosive or precursor materials, which are aimed to be screened by the SCT inspection. Note that it is composed of mostly organic and liquid materials without a k-edge discontinuity and with $6 \leq Z_e \leq 10$. Table 3 provides a summary of all the materials scanned by themselves, their type and their estimated physical parameters, using the SRZE method described in Section 2. This table was used as the ground truth for material classification when the materials are scanned in groups of 4.

Table 3: The list of all the 73 materials scanned and processed through the SRZE method, and their estimated physical parameters ρ_e (e⁻ mol/cm³) and Z_e .

Index	Material label	Type	Z_e	ρ_e
1	2-Butanone	Threat	6.64	0.440
2	2,4-Dinitrotoluene	Threat	8.16	0.316
3	Acetone	Threat	6.12	0.442
4	Ethylenediamine	Threat	6.31	0.506
5	H ₂ O ₂ 50%	Threat	7.24	0.661
6	Hexamethylenetetramine	Threat	5.59	0.461
7	Hydrazine solution	Threat	7.07	0.575
8	Methanol	Threat	7.17	0.439
9	N,N-Dimethylhydrazine	Threat	6.36	0.454
10	Nitric acid 65%	Threat	7.21	0.744
11	Nitrobenzene	Threat	6.70	0.621
12	Nitromethane	Threat	7.09	0.586
13	Wine	Innocuous	7.16	0.557
14	Cream Liquor	Innocuous	7.19	0.580
15	Balsamic Vinegar	Innocuous	6.98	0.640
16	Bromhexin DAK	Innocuous	7.24	0.608
17	Baby Shampoo	Innocuous	7.39	0.614
18	Aftersun Lotion 1	Innocuous	6.69	0.560
19	Brandy	Innocuous	7.51	0.537
20	Hand cream	Innocuous	7.01	0.545
21	Sun Lotion 1	Innocuous	6.74	0.579
22	Body Lotion 1	Innocuous	6.93	0.566
23	Beer 1 (Wheat)	Innocuous	7.14	0.566
24	Ethanol 40%	Innocuous	6.81	0.541
25	Ethanol 96%	Innocuous	6.08	0.463
26	Shampoo	Innocuous	7.36	0.589
27	Beer 2 (Brown Ale)	Innocuous	7.35	0.564
28	Porto Wine	Innocuous	7.26	0.568
29	Aftersun Lotion 2	Innocuous	6.95	0.567
30	Sun Lotion 2	Innocuous	6.61	0.572
31	Neutral Hand Soap	Innocuous	6.50	0.585
32	Sun Lotion 3	Innocuous	7.19	0.580
33	Sun Baby Lotion	Innocuous	8.73	0.606

Continued on next page

Table 3 – Continued from previous page

Index	Material label	Type	Z_e	ρ_e
34	Antiperspirant	Innocuous	6.05	0.340
35	Beer 3 (Pale Ale)	Innocuous	7.55	0.556
36	Olive Oil	Innocuous	5.41	0.510
37	Alcohol Drink	Innocuous	7.27	0.583
38	Rapeseed Oil	Innocuous	5.40	0.516
39	Simple Eye Makeup Remover	Innocuous	7.00	0.576
40	Body Lotion 2	Innocuous	6.92	0.563
41	Sugar	Innocuous	6.49	0.524
42	Sun lotion 4	Innocuous	8.57	0.595
43	Hairspray 1	Innocuous	7.11	0.568
44	Beer 4 (IPA Ale)	Innocuous	7.35	0.563
45	Beer 5 (Danish Christmas Beer)	Innocuous	7.42	0.560
46	Whiskey	Innocuous	7.27	0.524
47	Beautifying Anti-Blemish Care	Innocuous	7.15	0.582
48	Water	Innocuous	7.05	0.562
49	Energy Drink	Innocuous	7.10	0.586
50	Hairspray 2	Innocuous	8.10	0.391
51	Shaving Foam	Innocuous	8.12	0.542
52	Toothpaste 1	Innocuous	8.19	0.665
53	Ammonia Nitrate	Threat	6.73	0.490
54	Book	Innocuous	9.74	0.419
55	C4 Simulant	Threat	8.02	0.855
56	C4	Threat	6.44	0.497
57	Chocolate	Innocuous	6.68	0.700
58	Comp B	Threat	6.54	0.897
59	Crystal Sugar	Innocuous	6.63	0.531
60	DVD Bomb Simulant	Threat	7.49	0.878
61	Hard Cheese	Innocuous	7.41	0.619
62	Marzipan	Innocuous	6.47	0.648
63	Nitromethane	Threat	6.86	0.575
64	PETN Simulant	Threat	7.72	0.719
65	Peanut Butter	Innocuous	6.94	0.636
66	PETN	Threat	6.73	0.839
67	Shampoo	Innocuous	7.37	0.582
68	Soap Bar	Innocuous	6.13	0.595
69	Soft Cheese	Innocuous	7.35	0.604
70	Sun Cream	Innocuous	7.32	0.571
71	TNT (chunks)	Threat	6.63	0.434
72	Toothpaste 2	Innocuous	8.26	0.678
74	Vinegar	Innocuous	7.13	0.639

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