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Sublimation kinetics and diffusion coefficients of TNT, PETN, and RDX in air by thermogravimetry

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ABSTRACT

The diffusion coefficients of explosives are crucial in their trace detection and lifetime estimation. We report on the experimental values of diffusion coefficients of three of the most important explosives in both military and industry: TNT, PETN, and RDX. Thermogravimetric analysis (TGA) was used to determine the sublimation rates of TNT, PETN, and RDX powders in the form of cylindrical billets. The TGA was calibrated using ferrocene as a standard material of well-characterized sublimation rates and vapor pressures to determine the vapor pressures of TNT, PETN, and RDX. The determined sublimation rates and vapor pressures were used to indirectly determine the diffusion coefficients of TNT, PETN, and RDX for the first time. A linear log–log dependence of the diffusion coefficients on temperature is observed for the three materials. The diffusion coefficients of TNT, PETN, and RDX at 273 K were determined to be 5.76×10^{-6} m^2/sec, 4.94×10^{-6} m^2/s, and 5.89×10^{-6} m^2/s, respectively. Values are in excellent agreement with the theoretical values in literature.

1. Introduction

One of the most promising technologies in security applications is the vapor detection of explosives [1]. Vapor detection is a common approach to detect traces of energetic materials for anti-terrorism purposes. Traces of explosives on passengers' belongings are usually collected using varieties of sampling techniques that are, in turn, analyzed using various analytical techniques. In an explosive vapor detection system, the explosive vapor is first pre-concentrated on a surface and later released for detection [2]. In order to develop a reliable explosive vapor detection device, the explosive sublimation or evaporation rates, as well as an estimate of their lifetimes, must be determined [3–5]. However, most high explosives are nitroaromatic and nitroamine compounds with vapors known to be highly difficult to detect due to their extremely low vapor pressures [6,7].

The diffusion coefficient is an important factor required when modeling explosives alkaline hydrolysis treatment. The mass transfer rate-limiting step is most often controlled by diffusion. Therefore, to determine the rate of diffusion, it is necessary to measure diffusion coefficient. In addition, the sublimation rates of explosives in air are limited by the diffusion process. The diffusion coefficient/diffusivity and vapor pressure are required for sublimation rate estimation in the diffusion model [3,4].

2,4,6-Trinitrotoluene (TNT), pentaerythritol tetranitrate (PETN), and cyclotrimethylenetrinitramine (RDX) are three of the most widely used secondary explosives in detonators, main charges boosters, and plastic explosives [8–10]. Due to their low volatility, large discrepancies in their enthalpies of sublimation, sublimation rates and vapor pressures are found in literature [1–4,11–21]. Experimental values of diffusion coefficients of TNT, PETN, and RDX have not been reported. An attempt to predict the values of the diffusion coefficients of the three materials using the sublimation rates determined by a quartz crystal microbalance (QCM) and the different vapor pressure values reported in literature have been made [3,4]. However, according to the authors, the prediction made lacks accuracy due to the limited data on vapor-in-air diffusion coefficients, the discrepancy in vapor pressure data available in literature, and the deviation of the samples morphology from the shapes used in the diffusion model.

The sublimation rates, enthalpies of sublimation, and vapor pressures of powders of TNT, PETN, and RDX have not been updated for over three decades. However, unlike TNT and RDX, PETN, in large single crystals form, has been recently extensively investigated for doping effects on its sublimation rates and vapor pressures to increase the long term stability [22–24]. The only recent works in literature were performed using non-isothermal

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thermogravimetry on powders which usually results in inaccurate estimations [17] and isothermal absorbance spectroscopy on nanofilms which is not an industrial form of these energetic materials [5,10,25].

In this article isothermal thermogravinetric analysis (TGA) is used to directly determine the sublimation rates of powders of TNT, PETN, and RDX, in air, below their melting/decomposition points. The instrument was calibrated using ferrocene as a standard material with well-characterized sublimation rates and vapor pressures along with the Langmuir equation to estimate the vapor pressure of TNT, PETN, and RDX powders. The measured sublimation rates and their estimated vapor pressures are then used to experimentally determine the diffusion coefficients in air for the first time. In addition, the dependence of diffusion coefficients of the three explosives on temperature is determined.

2. Experimental

Pentaerythritol tetranitrate (PETN) powder of high purity was supplied by Lawrence Livermore National Laboratory and used without further purification. 2,4,6-Trinitrotoluene (TNT) powder (Austin explosives) was purified by crystallization of TNT by ultrasonication in 2-isopropanol. TNT single crystals were then carefully grinded and used as a powder. Cyclotrimethylenetrinitramine (RDX) powder of high purity was supplied by Sandia National Laboratory and used without further purification. ACS reagent grade ferrocene (98% purity) was obtained from Sigma-Aldrich (St.Louis, MO) and used without further purification.

Thermogravimetric analysis was carried out using a Q50 (TA Instruments, Delaware, USA) TGA instrument. The TGA was calibrated using Alumel (Curie point transition temperature is 154 °C) as a standard reference material. Powder samples were pressed in the TGA pan of radius of 0.275 mm to form a cylindrical shaped disk. Preliminary TGA experiments on PETN show that there is no significant mass loss observed on isothermal heating until 100 °C. The PETN samples were heated from 110 to 135 °C in steps of 5 °C and were maintained for 1–3 h at each temperature. TNT samples were isothermally heated from 55 °C to 75 °C in steps of 5 °C and were maintained for 6–15 h at each temperature. The RDX samples were heated from 100 to 145 °C in steps of 10 °C and were maintained for 2–6 h at each temperature. The mass of the samples used were chosen such that the mass loss does not exceed 20% of the starting mass such that the sample maintains its cylindrical shape indicating a nearly constant surface area throughout the experiment. The rate of heating between isothermal steps is 5 °C/min. Nitrogen is used as the purge gas for both sample and the balance at 10 cm^3/min. Gas purge rate was found to have a minimal effect on the sublimation rate where a purge rate of 40 cm^3/min increases the sublimation rates by ~10%. During the isothermal heating, the weight of the sample is measured as a function of time allowing calculation of the rate of mass loss. The calculated rate of mass loss at each temperature was normalized to the surface area of the disk-shaped sample.

3. Theoretical background

The diffusion coefficient of TNT, PETN, and RDX can be determined indirectly in three steps. First, we determine the sublimation rates of the materials using TGA. The rate of mass loss per unit area due to sublimation/evaporation from a sample of surface area S at temperature T in Kelvin is given by Arrhenius relation in the form [6,7]:

$$\frac{dm}{Sdt} = f\ \exp\left(-\frac{E_a}{K_B T}\right) \tag{1}$$

where f is the pre-exponential/frequency factor, E_a is the activation energy of sublimation, and K_B is Boltzmann's constant. The sublimation from the surface is usually considered to be a homogenous process. Thus, a plot of $\text{Ln}\left(\frac{dm}{Sdt}\right)$ versus the inverse of temperature in Kelvin yields a straight line with a slope of $-E_a/K_B$ that can be used to determine the activation energy of sublimation.

Second, we indirectly estimate the vapor pressure of the materials by calibrating the TGA using a standard volatile material. Starting from the Langmuir equation for free evaporation/sublimation, the vapor pressure of any volatile material can be determined [26]. Using a standard material of a well-characterized vapor pressure, a calibration procedure can be used to estimate the vapor pressure of other materials to a good accuracy [27]. For vapor pressure determination, the Langmuir equation is usually written in the form [27]:

$$P = k\upsilon \tag{2}$$

where $\upsilon = \frac{1}{S}\frac{dm}{dt}\sqrt{\frac{T}{M}}$ and $k = \left\{\frac{\sqrt{2\pi R}}{\alpha}\right\}$where $\frac{1}{S}\frac{dm}{dt}$ ($\text{kg}\,\text{s}^{-1}\,\text{m}^{-2}$) is the rate of mass loss per unit area, T is the absolute temperature (K), M is the molecular weight ($\text{kg}\,\text{mol}^{-1}$), R is the universal gas constant ($\text{J}\,\text{K}^{-1}$), and α is the unitless instrument-dependent evaporation constant.

Third, we use the determined sublimation rates and the vapor pressures to determine the diffusion coefficients. Consider the quasi stationary steady state diffusion process from the sample surface into the open space. The diffusive flow considerably depends on the sample morphology. Analytic solutions were derived for the cases of a disk shaped source. The diffusive flows from a disk shaped sample is given by [3,4,28,29]:

$$\frac{dm}{dt} = 4r_d D C_{sat} M \tag{3}$$

where dm/dt is the diffusive flow from the source to open space in units of kg/s which is equal to rate of mass loss, r_d is the radius of the disk, D is the diffusion coefficient, C_{sat} represents the concentration of the saturated vapor, and M is the sample molecular mass.

Assuming an ideal gas behavior ($P_{sat}=C_{sat}\ RT$) and a circular disk ($S=\pi r_d^2$), the diffusion coefficient D can be determined by

$$D = \left(\frac{\pi r_d RT}{4MP_{sat}}\right)\ \left(\frac{1}{S}\frac{dm}{dt}\right) \tag{4}$$

where R is the universal gas constant, T is the absolute temperature in Kelvin, and P_{sat} is the saturation vapor pressure.

4. Results and discussion

The mass loss/sublimation rates of ferrocene, TNT, PETN, and RDX at different temperatures below their decomposition and melting temperatures are determined isothermally using TGA. The sublimation rates were determined from at least three samples of each material.

Fig. 1 represents a plot of the logarithm of the sublimation rates per unit area of ferrocene versus the inverse of the absolute temperature in Kelvin according to Eq. (1). The plot is linear with excellent R^2 value and the error bars are too small to be seen indicating excellent data reproducibility. The activation energy of sublimation of ferrocene is calculated from Fig. 1 to be 71.97 ± 0.3 kJ/mol. Ferrocene has a low discrepancy with values of enthalpy of sublimation in the range 69.5–75.5 kJ/mol [30–34]. The value determined in this work is in excellent agreement with those reported using a recently developed static apparatus [32] and the value recommended by ICTAC (73.42 ± 1.08 kJ/mol) [30] indicating reliable data. The sublimation rates are also in excellent agreement with the recently reported values in literature [35,36].

The sublimation rates of ferrocene shown in Fig. 1 were used to calibrate the TGA instrument using the most recent average vapor pressure data reported by Monte et al. [35] and Ribeiro da Silva et al. [36]. Fig. 2 shows a plot of the reported vapor pressure values in Pascal versus our experimental ν values of ferrocene. The plot is linear with excellent R^2 value, and the instrument calibration constant (k) is calculated to be 1.08633×10^5.

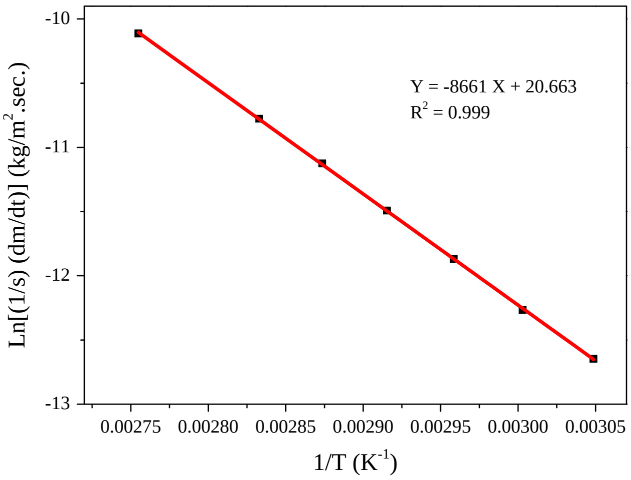

Fig. 1. A plot of the logarithm of the sublimation rates per unit area of ferrocene versus the inverse of the absolute temperature, slope determines the enthalpy of sublimation.

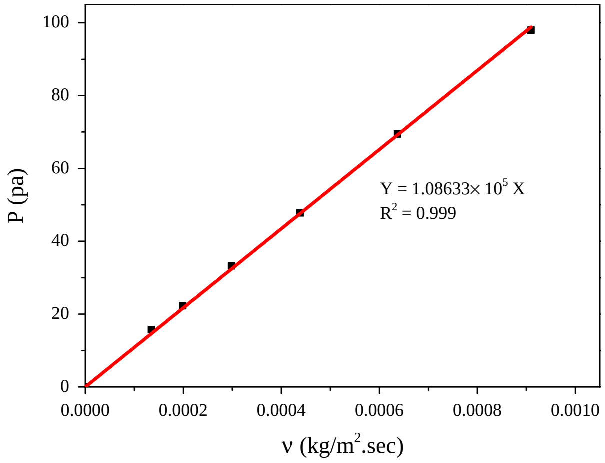

Fig. 2. A plot of vapor pressure of ferrocene versus the determined ν values to determine the calibration constant (k) value of the TGA instrument.

The experimental sublimation rates of TNT, PETN, and RDX along with the extrapolated sublimation rates values at temperatures below their melting points down to 273 K are shown in Fig. 3. The sublimation rates per unit area of TNT determined here are about 20% larger than those determined recently for nanofilms of TNT using absorbance spectroscopy [5]. Unfortunately, no further comparison could be made since all the other sublimation data on TNT found in literature were not normalized to the surface area of the sample [1,2–4]. The sublimation rates of PETN per unit area determined here are about 1–2 orders of magnitude larger than those previously determined using the same technique on large single crystals of PETN. This difference can be attributed to the low sublimation from the two prominent faces (110) and (101) of PETN crystals [6,7,18–20]. On the other hand these sublimation rates per unit area are one order of magnitude larger than those determined for nanofilms of PETN using absorbance spectroscopy [10]. At the microscale, two data sets on PETN sublimation rates have been recently reported [4,6,7]. The values reported by Pitchmani et al. [6] and Burnham et al. [7] on PETN microcrystals and microislands on single crystals of PETN are one order of magnitude larger than the values determined here. However, according to the authors, these inaccurate results are due to the expected PETN molecular migration on the PETN crystal surface and surface quality [7]. The values reported by Zeiri et al. are not normalized to the sample surface area thus no comparison is achievable here [4]. The sublimation rates per unit area of RDX are about one order of magnitude larger than those determined recently for nanofilms of RDX using absorbance spectroscopy [5,25].

Fig. 4 shows a plot of the logarithm of the sublimation rates per unit area of TNT versus the inverse of the absolute temperature in Kelvin. The plot is linear with an excellent R^2 value. The activation energy of sublimation of TNT is calculated from Fig. 4 to be 95.94 ± 1.1 kJ/mol. There is a large discrepancy in the activation energy value of TNT in literature (90–141 kJ/mol) [3–5,11–14,37–39]. Our value is in a very good agreement with the reported results using the most sensitive techniques used in measuring sublimation rate of TNT: QCM, absorbance spectroscopy, and Knudsen effusion methods giving activation energy of sublimation of 97 ± 7, 99.6 ± 5, and 103 kJ/mol, respectively [3,5,13]. However, a larger value of 131 kJ/mole has been reported using QCM [3]. Thus, our results support the lower end values for TNT activation energy of sublimation that have been determined at the nano/micro-scale [3,5,13].

Fig. 5 represents an Arrhenius plot of the logarithm of the sublimation rates per unit area of PETN versus the inverse of the absolute temperature in *Kelvin*. The activation energy of sublimation of PETN is calculated from Fig. 5 to be 140.2 ± 2.3 KJ/mol. The discrepancy in the activation energy of sublimation of PETN lies in the range of 122–150 KJ/mol [6,7,10–22–24]. The value determined here is in excellent agreement with the recently reported value for single

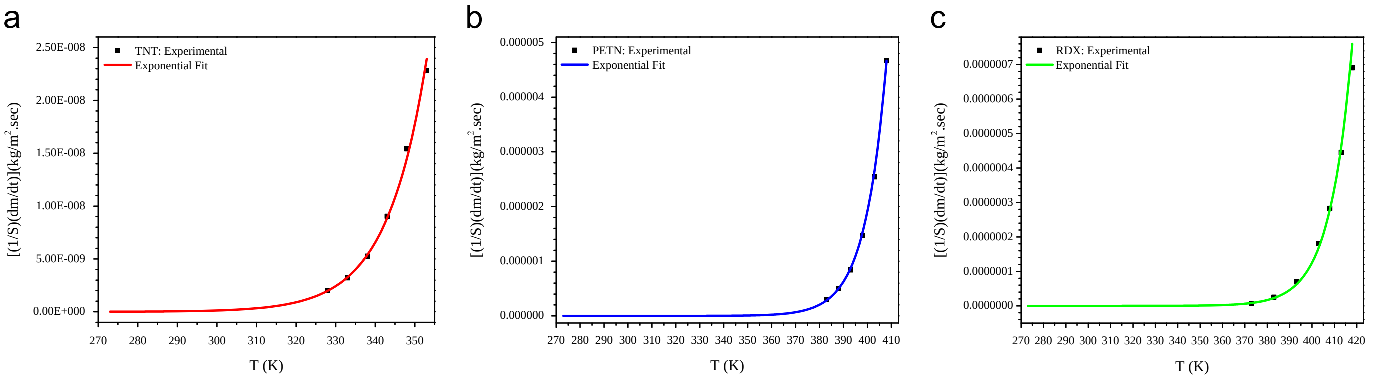

Fig. 3. (a) sublimation rates of TNT, (b) sublimation rates of PETN, and (c) sublimation rates of RDX: squares represent experimentally determined values and lines represent the exponentially extrapolated values from the Arrhenius equation.

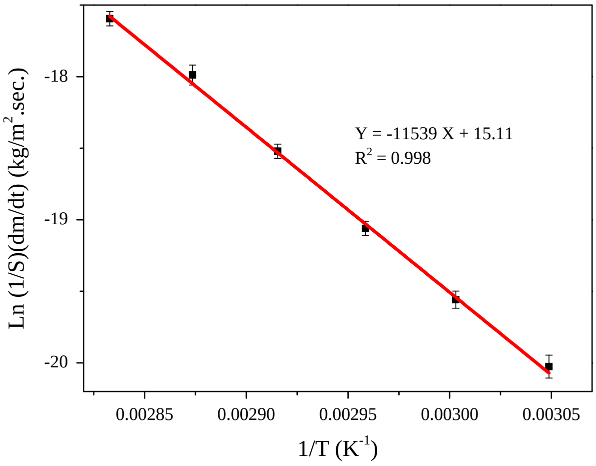

Fig. 4. A plot of the logarithm of the sublimation rates per unit area of TNT versus the inverse of the absolute temperature, slope determines the enthalpy of sublimation.

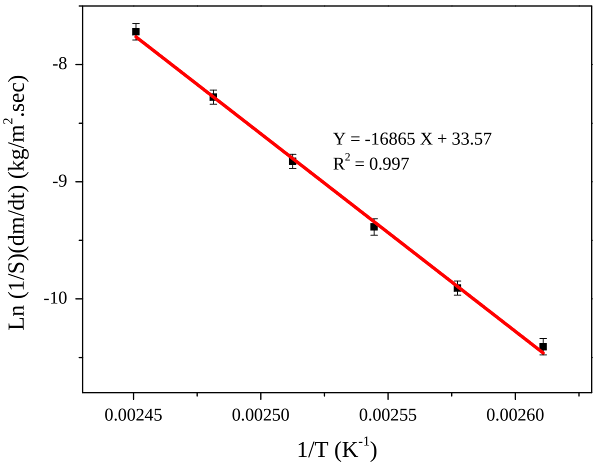

Fig. 5. A plot of the logarithm of the sublimation rates per unit area of PETN versus the inverse of the absolute temperature, slope determines the enthalpy of sublimation.

crystals of PETN (E_a = 140 kJ/mol) using the same technique [7,22–24]. However, the value is slightly higher than those of microcrystals of PETN (E_a = 125 kJ/mol and 137.5 kJ/mol) using QCM [4] and atomic force microscopy AFM [6,7], respectively, and continuous nanofilms of PETN using absorbance spectroscopy (134.4 ± 4 kJ/mol) [10].

Fig. 6 represents an Arrhenius plot of the logarithm of the sublimation rates per unit area of RDX versus the inverse of the absolute temperature in Kelvin resulting in activation energy of sublimation of RDX of 130.2 ± 1.9 kJ/mol. There is a large discrepancy in the value of the activation energy of sublimation of RDX in literature (107–134 kJ/mol) [12,18–21]. Our value(s) is in a very good agreement with those reported by Edwards [18], Cundall et al. [12], Eiceman et al. [21], supporting the higher end values.

The determined calibration constant (k) was used to determine the vapor pressure values of TNT, PETN and RDX according to Eq. (2). Fig. 7 shows a plot of the logarithm of TNT, PETN, and RDX vapor pressure values versus the inverse of the absolute temperature. In terms of the Clapeyron equation, the dependence of TNT, PETN, and RDX vapor pressures on temperature can be described by the relations $\mathrm{Ln}P$ (Pa) = 30.8–11,687/T (K), $\mathrm{Ln}P$ (Pa) = 44.95–17,190/T (K), $\mathrm{Ln}P$ (Pa) = 39.16–15,860/T (K) respectively. The vapor pressure values for the three materials lie within the reported values in literature and are in excellent agreement with the data reported recently using absorbance spectroscopy [5,7,13,22–24].

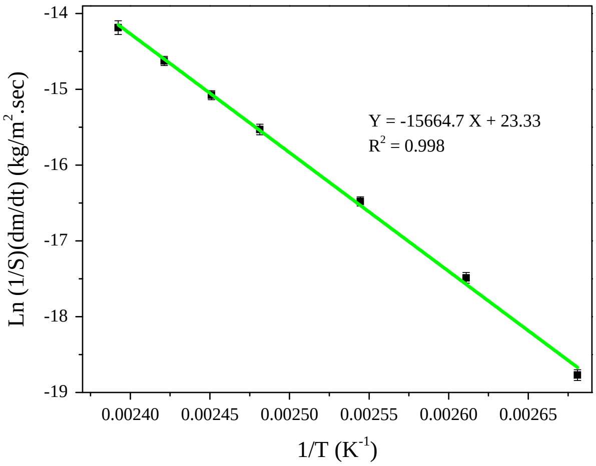

Fig. 6. A plot of the logarithm of the sublimation rates per unit area of RDX versus the inverse of the absolute temperature, slope determines the enthalpy of sublimation.

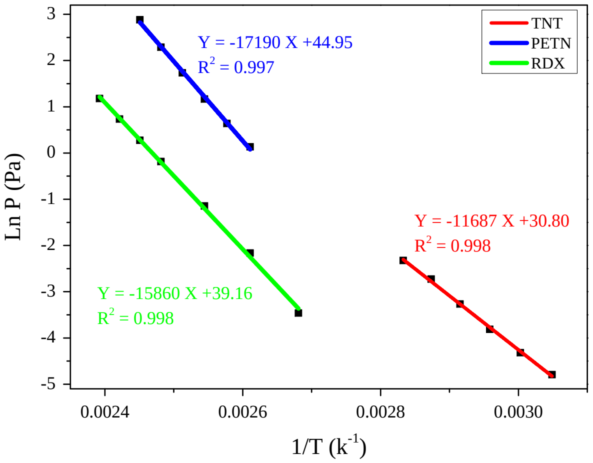

Fig. 7. Plots of the logarithms of the determined vapor pressures of TNT, PETN, and RDX using thermogravimetry versus the inverse of the absolute temperature according to Clapeyron equation.

Table 1
Diffusion coefficient of TNT, PETN, and RDX at different temperatures.

TNT		PETN		RDX	
T (°C)	D (m²/s)	T (°C)	D (m²/s)	T (°C)	D (m²/s)
55	5.777×10^{-6}	110	5.751×10^{-6}	100	6.76×10^{-6}
60	5.793×10^{-6}	115	5.788×10^{-6}	110	6.86×10^{-6}
65	5.808×10^{-6}	120	5.825×10^{-6}	120	6.95×10^{-6}
70	5.823×10^{-6}	125	5.863×10^{-6}	130	7.04×10^{-6}
75	5.838×10^{-6}	130	5.899×10^{-6}	135	7.08×10^{-6}
80	5.852×10^{-6}	135	6.012×10^{-6}	140	7.13×10^{-6}

Using the determined values of the vapor pressures and the sublimation rates along with Eq. (4), the diffusion coefficients of TNT, PETN, and RDX were determined at the temperatures studied. The values are summarized in Table 1.

As mentioned, no experimental values of the diffusion coefficient (D) for TNT and PETN have been reported. However, an estimation of the diffusion coefficient of PETN using sublimation rates and modeling of the evaporative recrystallization resulted in a small value of $\sim 9.5 \times 10^{-7}$ m²/s at just 90 °C [7]. The authors explained the inaccuracy to the surface migration due to the high surface mobility of PETN. The theoretical values found in literature

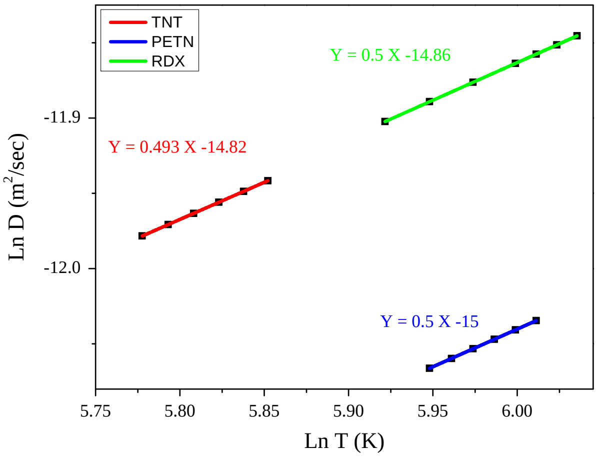

Fig. 8. Plot of the logarithm of the diffusion coefficient of TNT, PETN, and RDX versus the logarithm of the absolute temperature.

are 5.59×10^{-6} m^2/s for TNT, 5.0×10^{-6} m^2/s for PETN [40,21], and 7.4×10^{-6} m^2/s for RDX [41], respectively, at 273 K.

The diffusion coefficient of PETN has been shown to be proportional to $T^{0.5}$ [7]. To check this relation we plot the logarithm of the determined diffusion coefficients at different temperatures versus the logarithm of the absolute temperature for TNT, PETN, and RDX as shown in Fig. 8. The plots are linear and the exponents are determined from the slopes to be 0.5 are in agreement with literature [7]. The fit equations were used to estimate the diffusion coefficients of TNT and PETN at 273 K.The diffusion coefficients are found to be 5.76×10^{-6} m^2/s for TNT and 4.94×10^{-6} m^2/s for PETN at 273 K, and 6.13×10^{-6} m^2/s for RDX at 300 K which is in excellent agreement with their theoretical values [21,40].

5. Conclusions

Thermogravimetry was used to determine the sublimation rates and enthalpies of sublimation of two important energetic materials TNT, PETN, and RDX. The instrument was calibrated using a standard material, ferrocene, by using its sublimation rates and its reported accurate vapor pressures. This allowed determining the vapor pressure of the two explosives at different temperatures according to Langmuir equation. The sublimation rates and vapor pressure values were used to determine the diffusion coefficients of TNT, PETN, and RDX for the first time. The determined values at relatively elevated temperature are very reasonable. The diffusion coefficient of the two materials was found to be proportional to $T^{1/2}$, which allowed estimating the diffusion coefficient at 273 K. The values of the diffusion coefficient at 273 K are in excellent agreement with the theoretical values reported in literature.

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