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New Micro-Method for Prediction of Vapor Pressure of Energetic Materials

by Rose A. Pesce-Rodriguez and Elizabeth Klier

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New Micro-Method for Prediction of Vapor Pressure of Energetic Materials

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14. ABSTRACT

A new indirect method for estimating vapor pressures of organic materials, including energetic materials, has been developed. The method provides an estimate that appears to be good to within an order of magnitude. The method relies on the availability of reliable experimental vapor pressure measurements at the temperature of interest. These vapor pressure values are correlated against corresponding thermogravimetric analysis (TGA) weight-loss onset temperatures to yield a line whose slope and intercept may be used to calculate the vapor pressure of an organic material. While less accurate than direct methods to determine vapor pressure, the new predictor is useful for quickly obtaining estimates for new compounds that might be available in only milligram quantities. Since the method can be used to predict vapor pressure at elevated temperatures, it is useful for predicting behavior of energetic materials to be subjected to vacuum stability testing. The method has been applied to approximately 30 energetic high-nitrogen compounds whose vapor pressures have not previously been reported.

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1. Introduction

Knowledge of a substance's vapor pressure is critical to calculations related to any material's processing, use, long-term aging, and environmental fate/transport. Rigorous measurement of a substance's vapor pressure may be obtained by several proven direct methods, including the following:

- Direct pressure measurement methods rely on sensitive pressure gauges that directly measure the pressure exerted by a material. These methods cannot distinguish impurities from test materials and require long equilibration times (*1–3*).
- Effusion methods require high vacuum and a micron-scale orifice that permits escape, but not re-entry, of volatilized material. Weight loss of a material held at a certain temperature is determined collecting vaporized material that has passed through the orifice on a cold trap. Mass loss is usually followed as a function of time. This method requires long equilibration times, cannot distinguish between impurities and test materials, and is subject to typical problems associated with high vacuum systems (*4–6*).
- Gas saturation (also known as transpiration) methods require establishing an equilibrium concentration of vapor in a carrier gas above a test material. The test material is then separated from the carrier gas and its mass determined. The method is subject to typical problems associated with high vacuum systems (*6–8*).
- Thermogravimetric methods measure mass loss and correlate to vapor pressure by use of Langmuir theory. The method requires a uniform surface area that is most easily obtained by melting/freezing a test material. While this approach may not be feasible for some energetic materials that decompose on melting, it has been successfully applied to a number of energetic materials (*9–10*).
- Differential scanning calorimetry (DSC) methods offer the advantage of observing phase changes, but require that the material exhibits a sharp melting point. Also required are the use of a pressure/vacuum chamber and samples in DSC pans with pin holes to allow material to escape as the material is heated. Pressure is recorded during observance of the boiling endotherm, and the boiling temperature is recorded as the extrapolated onset temperature (*11–12*).
- Gas chromatography (GC) headspace analysis requires the establishment of an equilibrium concentration of vapor in the headspace above a test material. Samples are then collected and analyzed by GC, which is calibrated in advance using known masses/volumes of standard test material (*13–15*).

There is no single direct vapor pressure measurement method that is applicable to the entire range of vapor pressures and temperatures. Several methods are therefore recommended for measuring vapor pressure. The reader is advised against accepting vapor pressure data quoted in non-primary sources because values are often extrapolated from data collected at higher temperatures and may not be accurate at the desired temperature. For this study, accurate values for vapor pressure at 25 °C were sought out for a number of energetic and non-energetic compounds. Very little data found on material data sheets for vapor pressure at 25 °C, for example, are reliable.

Indirect measures of vapor pressure involve the correlation of some property of a material with experimentally determined direct vapor pressure measurements. The correlation is then used to calculate the vapor pressure of a material whose vapor pressure is not known. An example of an indirect method is given in figure 1 (left) (*16*). Figure 1 (right) shows what appears to be an excellent correlation of data for four energetic materials at 370 K from the plot on the left. An attempt to extend the correlation to include additional energetic materials from the current study is shown in figure 2 and illustrates that molecular weight is actually not a good predictor for vapor pressure.

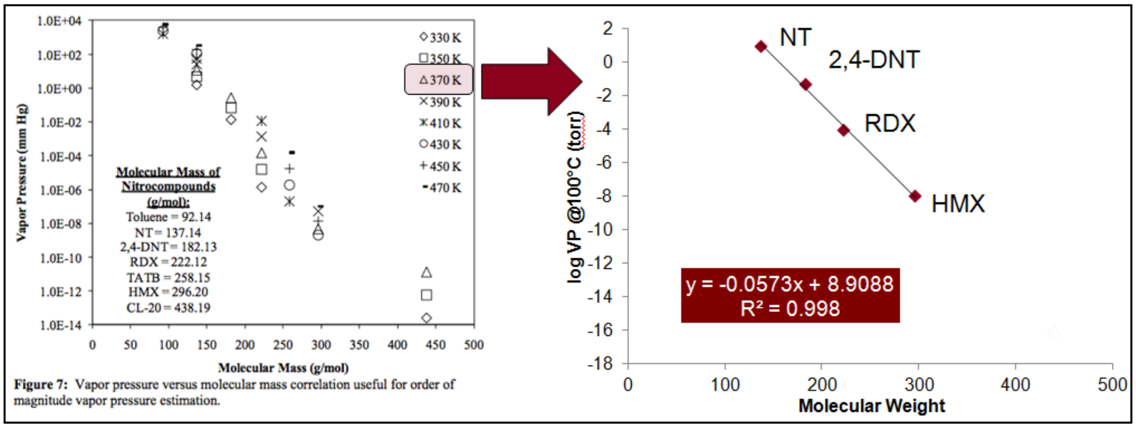

Figure 1. Vapor pressure vs. molecular weight at eight temperatures for seven energetic materials, from reference 16 (left). Log vapor pressure (at 370 K, from left) vs. molecular weight (right).

GC can also be used for indirect prediction of vapor pressure. The method is based on the correlation of the inverse of GC retention time to vapor pressure and has been found to give reasonable results for non-polar organic compounds (*17*) and polychlorobiphenyl (*18*). No references to the method's use for predicting the vapor pressure of energetic materials was found in the literature.

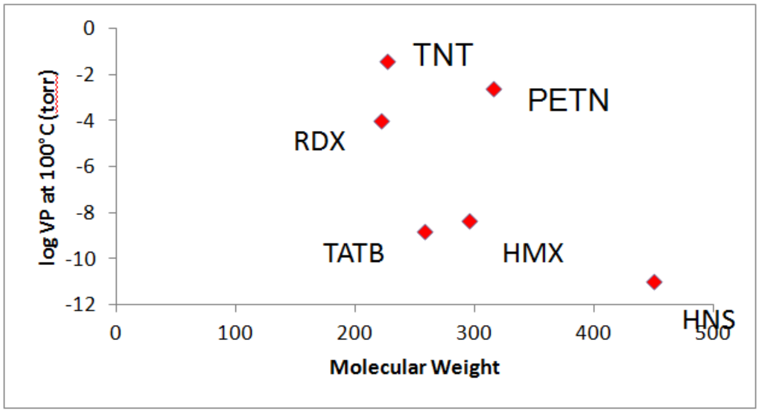

Figure 2. Log vapor pressure at 100 °C (373 K) vs. molecular weight for six energetic materials.

The vapor pressure of a material will vary with crystal form (*19*), as well as with temperature for a given crystal form. While results are often cited at specific temperatures, results may also be reported for a range of temperatures in the form of the Clausius–Clapeyron equation (equation 1), the slope of which may be used to calculate the heat of sublimation (for a solid) or vaporization (for a liquid).

$$3\log P = A - B/T \tag{1}$$

where

P - pressure

T - temperature (K)

A - species-specific constant

B - $\Delta H_{(\text{sublimation or vaporization})}/2.303R$

R - gas constant [8.314 J/(mol-K)]

For a critical review of vapor pressures of energetic material, the reader is directed to a recent publication by Ostmark et al. (*20*), which presents data for 23 energetic materials. The reference includes coefficients for the Clausius–Clapeyron equation, the temperature range at which measurements were made, and vapor pressure values at 25 °C (usually extrapolated).

The subject of the current work is a new indirect method for prediction of the vapor pressure of organic materials (energetic or non-energetic) that is based on the correlation of reliable experimental vapor pressure measurements at the temperature of interest with the temperature at which weight-loss begins in a thermogravimetric analysis (TGA) at a fixed heating rate. The method has been found to be applicable across a wide range of temperatures and vapor pressures.

While the method will not replace rigorous, direct measurements of vapor pressure, it is seen a potentially useful tool for those in the chemical propulsion community who need vapor pressure values for a variety of applications.

2. Experimental

Samples used in this work are listed in table 1 along with any available identifying information.

Table 1. Samples used in this work.

Material	**Available Identifying Information**
Benzoic acid	Sigma Aldrich (for calorimetric determination)
Adipic acid	Mettler certified thermometric standard
Anthraquinone	Mettler certified thermometric standard
Naphthalene	Mettler certified thermometric standard
Caffeine	Arthur R Thomas Co thermometric standard
Acetanilide	Arthur R Thomas Co thermometric standard
Melamine	Sigma Aldrich
Urea Nitrate	Matt Sherrill (U.S. Army Research Laboratory [ARL])
RDX	Class 5; Lot HOL88M675079
HMX	Class 5; Lot BAE09D082-03J
HNS	Class 1?; Lot 208130110D
PETN	Class 5?; Lot 96-34
TATB	Class 5?; Lot BAE06K298-002
TNT	Flake; CIB91H003-090
CL-20	Class 5; EX-9405294
NTO	BAE0713305-001
DNAN	Provided by the U.S. Army Armaments Research and Development Engineering Center (ARDEC)
Fox-7	Naval Surface Warfare Center, Indian Head Division (NSWC-IHD); LLFOX7000; 50L-02
Fox-12	NSWC-IHD; LL9440Q03; 20047012
TAGZT	NSWC-IHD; IH23003M-0613
BTAT	Synthesized by ARDEC
HAO-TAF	Synthesized by ARDEC
ABTOX	Synthesized by ARDEC
TKX-50	Synthesized by ARDEC
All other high-nitrogen compounds	Synthesized by Klapötke’s group at the Ludwig-Maximilian University of Munich. Stored at ARL since 2007. Analyzed as received.

Note: All abbreviations of defined on the List of Symbols, Abberivations, and Acronyms at the end of the report.

All samples were subjected to TGA using a TA Systems Q500 TGA. Analyses were conducted by first allowing the sample to equilibrate at 40 °C for 5 min and then heating at 10 °C/min to 400 °C. All analyses were run under an inert atmosphere (nitrogen flowing at 60 mL/min). Sample mass generally ranged from 1 to 2 mg. No effort was made to use a constant mass. All samples were powders or crystals, and were dispersed in disposable aluminum pans that were then placed on a standard platinum TGA hanging pan. No effort was made to control the distribution of the sample in the aluminum pan other than to gently tap the aluminum pan before placing on the platinum pan. Weight-loss onset temperatures were determined by identifying the temperature at which the starting mass-% has decreased by 0.3 wt.%. Given a sample that starts out at 100.0 wt.%, the weight-loss onset temperature therefore corresponds to the temperature at which the mass decreased to 99.7 wt.%. There is no physical significance to this mass loss; the 0.3% loss was arbitrarily selected and appears to result in a useful correlation with experimentally determined vapor pressures from the literature.

An example of TGA data and weight-loss onset temperatures for a number of energetic materials is given in figure 3. Table 2 presents data on the reproducibility of determining the TGA weight-loss onset temperature for RDX. Reproducible values were readily obtained using the process described above despite the variation in sample size.

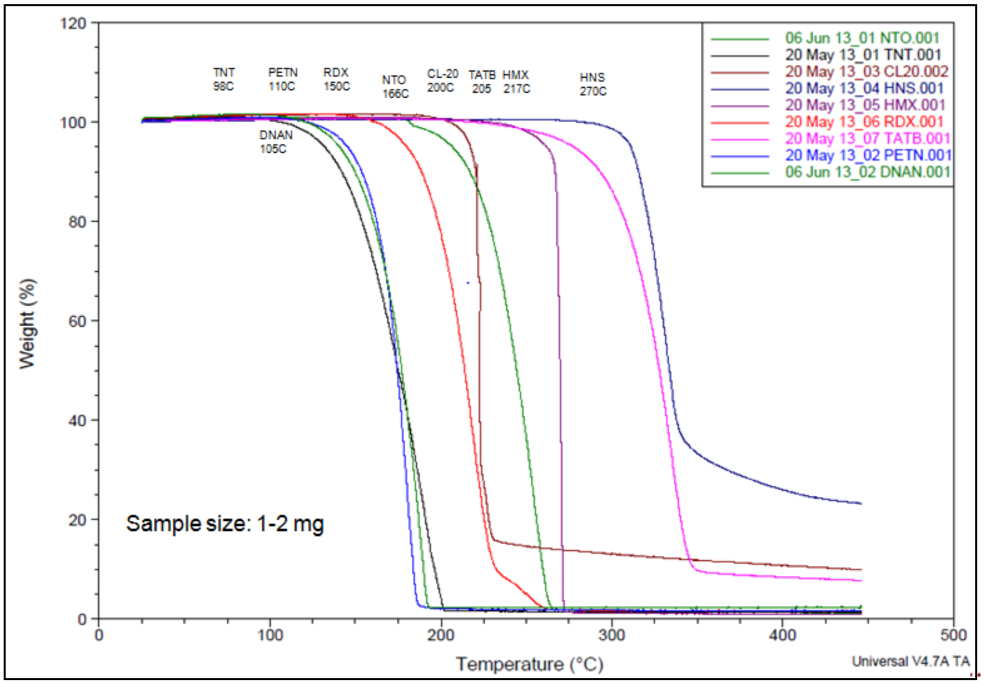

Figure 3. TGA traces for nine energetic materials heated at 10 °C/min.

Table 2. Repeatability of TGA weight-loss onset determination.

RDX – Trial #	**Sample Mass (mg)**	**TGA Weight-loss Onset Temperature (°C)**
1	0.838	149
2	0.615	151
3	0.481	149
4	0.451	152
5	0.536	151
6	0.523	148
average	-----	150 ± 1.4

3. Results and Discussion

Figure 4 shows a correlation of log vapor pressure at 100 °C versus TGA weight-loss temperatures for 14 materials (energetic and non-energetic). The two data points in red are both for caffeine; values for vapor pressures measured by two different groups differ by about two orders of magnitude. It is clear that any indirect prediction method can only be as good as the direct measurements used in establishing the correlation.

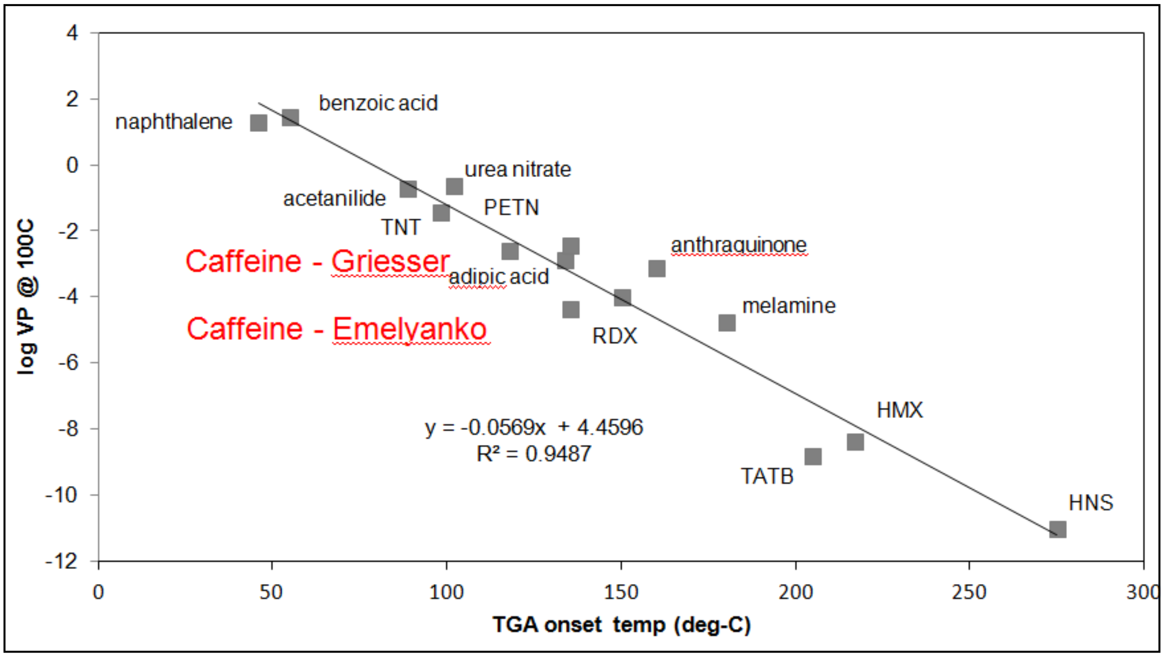

Figure 4. Log vapor pressure at 100 °C versus TGA weight-loss temperatures for 14 compounds (mix of energetic and non-energetic materials). References for vapor pressures: TNT, urea nitrate, PETN, RDX, HMX, TATB, and HNS (*20*), caffeine (*19*, *21* both values used in linear regression), naphthalene (*22*), benzoic acid (*23*), adipic acid (*24*), anthraquinone (*25*, *26*, *27*), melamine (*28*).

Whereas the correlation shown in figure 4 includes vapor pressure data that were either obtained in the range of 100 °C or obtained outside that range and extrapolated to 100 °C, the plots shown in figure 5 are obtained using only data obtained in the range of the indicated temperatures (i.e., 100, 70, and 25 °C). The correlation for 25 °C includes just 5 points. Despite the plethora of data for vapor pressures at 25 °C available on internet, reliable data (i.e., data obtained in a range that includes 25 °C) was very hard to come by for the materials on hand in our lab. For all three temperatures, correlation coefficients are a minimum of 0.9 and are expected to yield useful predictions for materials with unknown vapor pressures at those temperatures.

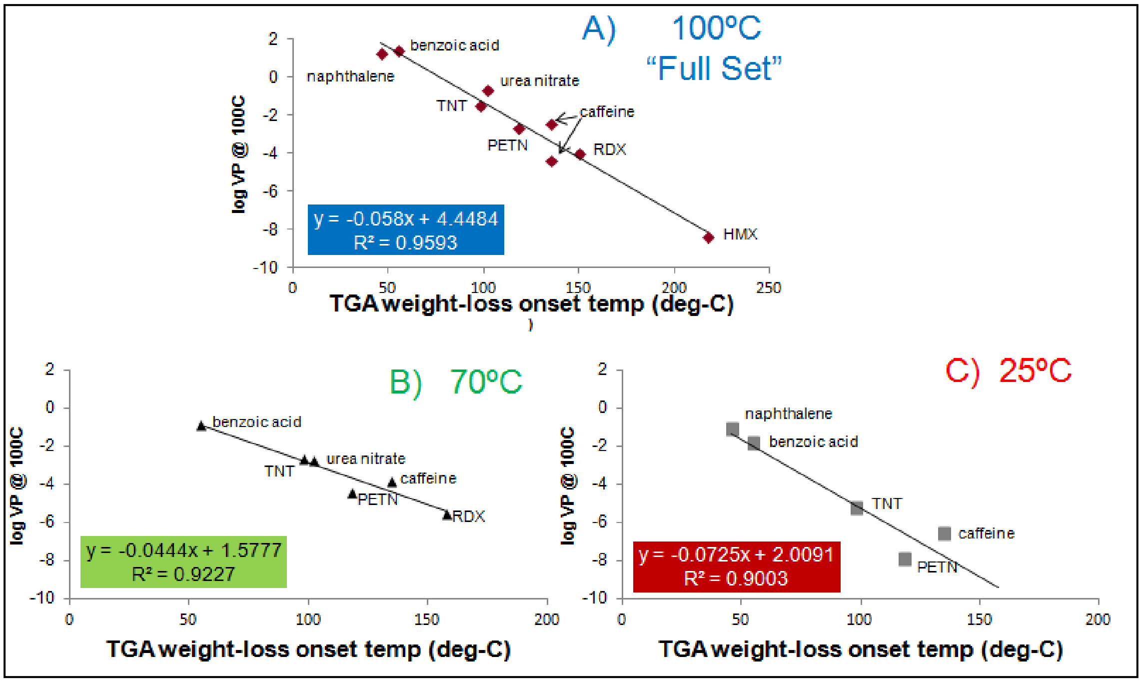

Figure 5. Log vapor pressure at (a) 100, (b) 70, and (c) 25 °C vs. TGA weight-loss temperatures for several compounds (mix of energetic and non-energetic materials).

Using the correlation plots shown in figure 5a and c, the vapor pressures of CL-20 at 100 and 25 °C were determined, and then compared with values calculated by Boddu et al. (*29*). The results are shown in table 3. ARL predictions are approximately two orders of magnitude higher than the calculated estimates by Boddu et al. At 100 °C, the ARL prediction suggests that the vapor pressure of CL-20 (log VP = –7.2) is about an order of magnitude higher than HMX (log VP = –8.3), whereas the Boddu et al. calculation (log VP = –9.2) predicts it to be about an order of magnitude lower than HMX. In either case, it is clear that CL-20 has a relatively low vapor pressure. For calculations involving vapor pressure, an estimate between 10^{-7} and 10^{-9} torr (at 100 °C) is probably reasonable to use until an experimental value is determined.

Table 3. Comparison of predicted vapor pressures at 100 °C for CL-20 using 3 sets of correlation data with values calculated estimate by Boddu et al. (*29*).

Temperature (°C)	**Boddu et al. Estimate log VP (torr)**	**ARL Prediction for CL-20 log VP (torr)**		
–	–	Full	Limited	RDX/HMX
25	–14.1	–12.5	–	–
100	–9.15	–7.2	–7.1	–7.3

The correlation in figure 5a was generated with TGA weight-loss onset data for eight different compounds (the "full set," which includes 2 data points for caffeine). What if those nine compounds were not available, but common materials found in most energetic material labs were available? What if only RDX and HMX were available? Correlations with these limited calibration sets are given in figure 6. The correlation on the left was produced with four common energetic materials, i.e., TNT, PETN, RDX and HMX, which comprise the "limited set," while RDX and HMX comprise the "RDX/HMX set" (figure 6, right). The slope and intercept of the line from the "limited set" is nearly identical to that from the "full set" (figure 5a); the correlation coefficient of the former is better primarily because the discrepant data for caffeine are omitted. The slope of the line from the "RDX/HMX set" data is slightly higher, but as can be seen in table 3, gives nearly the same predicted values for CL-20 vapor pressure at 100 °C. These results suggest that reasonable vapor predictions can be made in any lab with a TGA and a couple of "standard" materials (energetic or not) with reliable, known vapor pressure values.

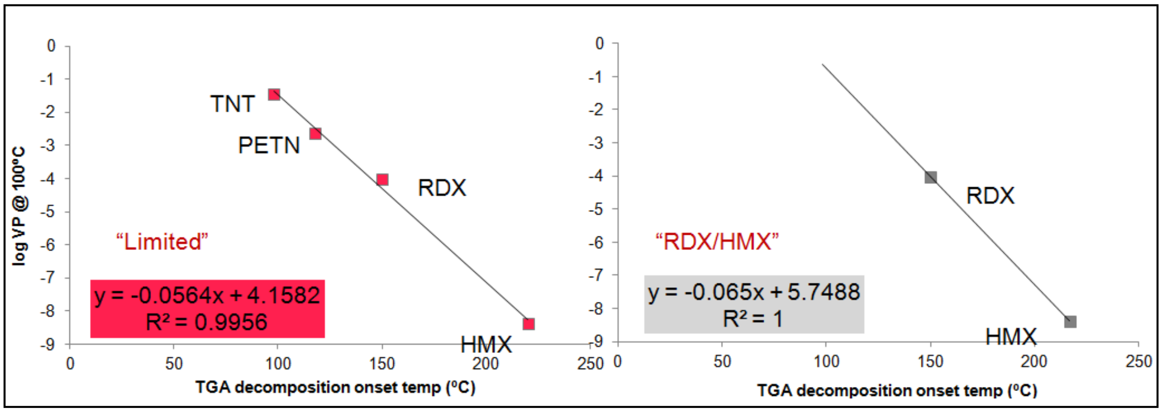

Figure 6. Log vapor pressure at 100 °C vs. TGA weight-loss temperatures "limited" and "RDX/HMX" calibration sets.

Predicted values for the vapor pressure of NTO, DNAN, TATB, and HNS are compared with experimental values from the literature in table 4. Values generally agree to within an order of magnitude (i.e., value agrees within ± 1 log units).

Table 4. Comparison of predicted vapor pressures at 100 °C for several energetics with experimental data from the literature.

Sample	Experimental log VP (torr)	Predicted Values (from 3 Correlation Sets) log VP (torr)		
		Full	Limited	RDX/HMX
NTO	–4.6 (*30*)	–4.9	–5.2	–5.0
DNAN	–1.5 (*30*)	–1.5	–1.8	–1.0
TATB	–8.8 (*20*)	–	–7.4	–7.6
HNS	–11.0 (*20*)	–	–11.4	–12.1

Table 5 gives predicted vapor pressures for 29 high-nitrogen energetic materials using both the “full” and “RDX/HMX” correlation data sets. Most of the high-nitrogen samples were synthesized by Klapötke’s group at the Ludwig-Maximilian University of Munich and stored at ARL since 2007. Each was analyzed as received. There are some obvious questions about the data. For example, why do samples 2 and 3, 1-methyl-5-aminotetrazolium nitrate and 1,4-dimethyl-5-aminotetrazolium nitrate, which differ by just a methyl group, have predicted vapor pressures that vary by four orders of magnitude? The difference may be real, or may be due to sample impurities. It is beyond the scope of the current work to resolve such differences. The predicted values listed in table 5 will be further investigated based on mission needs.

Table 5. Predicted vapor pressures at 100 °C for 29 high-nitrogen energetic materials.

Control Number	Nomenclature	TGA Wt-loss Onset (ºC)	Predicted log VP at 100 °C (torr) (Full Cal)	Predicted log VP at 100 °C (torr) (RDX/HMX Cal)
1	**HAT NO3** 5-Aminotetrazolium nitrate	102	–1.5	–0.9
2	1-Methyl-5-aminotetrazolium nitrate	91	–0.8	–0.2
3	1,4-Dimethyl-5-aminotetrazolium nitrate	160	–4.8	–4.7
6	1,4-Dimethyl-5-aminotetrazolium dinitramide	150	–4.3	–4.0
7	Guanidinium-5-nitrotetrazolate	152	–4.4	–4.1
8	Aminoguanidinium-5-nitrotetrazole	82	–0.3	0.4
9	1,4-dimethyl-5-aminotetrazolium-5,5’-azotetrazolate	105	–1.6	–1.1
10	**H2BTA** Biz(tetrazolyl)amine; (N,N-bis (1(2)H-tetrazol-5-yl)amine	233	–9.1	–9.4
14	**GNT** Guanazinium nitrotetrazolate	149	–4.2	–3.9
16	**NTNAP,** 1-nitrotetrazolato-2-nitro-2-aza-propane	130	–3.1	–2.7
17	**TNMM-oxamide** N,N'- Bis-(tris-(nitratomethyl)-methyl)-oxamide;	152	–4.4	–4.1
21	Ammonium-1-methyl-5-nitriminotetrazolate	125	–2.8	–2.4

Table 5. Predicted vapor pressures at 100 °C for 29 high-nitrogen energetic materials (continued).

Control Number	Nomenclature	TGA Wt-loss Onset (°C)	Predicted log VP at 100 °C (torr) (Full Cal)	Predicted log VP at 100 °C (torr) (RDX/HMX Cal)
22	Diammonium-5,5'-azotetrazolate	140	–3.7	–3.4
24	**DMATNT** 1,4-Dimethyl-5-aminotetrazolium 5-nitrotetrazolate	160	–4.8	–4.7
26	Triaminoguanidinium-1-methyl-5-nitriminotetrazolate	171	–5.5	–5.4
27	Hydrazinebistetrazole	206	–7.5	–7.6
29	**TAGDN** (Triaminoguanidinium-5-dinitrate)	81	–0.2	0.5
----	**Fox-7** (1,1-Diamino-2,2-dinitroethene)	159	–4.8	–4.6
----	**Fox-12** (N-guanylurea-dinitramide)	198	–7.0	–7.1
----	**TAGZT** (triaminoguanidinium azotetrazolate)	170	–5.4	–5.3
----	**BTAT** bis(2,2,2-trinitroethyl)-3,6- diaminotetrazine	143	–3.8	–3.5
----	**DAUHAT NG** Diaminouronium 5-Nitriminotetrazolate	174	–5.6	–5.6
----	**NGA2** 1-Nitramino-2,3-dinitroxypropane	98	–1.2	–0.6
----	**ANG** 1-amino-3-nitroguanidine	165	–5.1	–5.0
----	**AMBTT** ammonium bis (1-methyl tetrazolyl) triazenate	175	–5.7	–5.6
----	**1-NAP-5-AT** 1-(2-Nitro-2-aza-propyl)-5-aminotetrazole	104	–1.6	–1.0
----	**HAO-TAF** 4-(1-hydroxylammoniumoxy)tetrazolyl-3-amino furazan	126	–2.9	–2.4
----	**ABTOX** Bis(1-ammoniumoxy)tetrazolate	140	–3.7	–3.4
----	**TKX-50** Bis(1-hydroxylammo-niumoxy)tetrazolate	147	–4.1	–3.8

4. Conclusions

We drew the following conclusions from this work:

- A new micro-method for predicting vapor pressure has been developed.
- The method requires a TGA and several energetic and/or inert materials with reliable experimentally determined vapor pressures at the temperatures of interest.

- The new method gives predicted vapor pressures that seem to be within about an order of magnitude of experimentally determined vapor pressures (i.e., value agrees within ± 1 log units).
- It appears that the method can give reasonable values by calibrating with as few as two standards (RDX and HMX).
- The method has been used to predict the vapor pressures of approximately 30 energetic materials whose vapor pressures have not previously been determined.
- Predicted values are expected to be close enough to true values to be useful for processing, use, and fate and transport calculations.
- The new micro-method does not replace more rigorous methods of vapor pressure determination.

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List of Symbols, Abbreviations, and Acronyms

1-NAP-5-AT	1-(2-nitro-2-aza-propyl)-5-aminotetrazole
ABTOX	bis(1-ammoniumoxy)tetrazolate
AMBTT	ammonium bis (1-methyl tetrazolyl) triazenate
ANG	1-amino-3-nitroguanidine
ARDEC	U.S. Army Armaments Research and Development Engineering Center
ARL	U.S. Army Research Laboratory
BTAT	bis(2,2,2-trinitroethyl)-3,6- diaminotetrazine
DAUHAT NG	diaminouronium 5 nitriminotetrazolate
DMATNT	1,4-Dimethyl-5-aminotetrazolium 5-nitrotetrazolate
DNAN	2,4-dinitroanisole
DSC	differential scanning calorimetry
EQT-OEP	Environment Quality Technology-Ordnance Environmental Program
Fox-12	N-guanylurea-dinitramide
Fox-7	1,1-diamino-2,2-dinitroethene
GC	gas chromatography
GNT	guanazinium nitrotetrazolate
H2BTA	biz(tetrazolyl)amine (N,N-bis (1(2)H-tetrazol-5-yl)amine
HAO-TAF	4-(1-hydroxylammoniumoxy)tetrazolyl-3-amino furazan
HAT NO	3 5-Aminotetrazolium nitrate
HMX	cyclotetramethylenetetranitramine
HNS	hexanitrostilbene
NGA2	1-nitramino-2,3-dinitroxypropane
NSWC-IHD	Naval Surface Warfare Center, Indian Head Division

NTNAP	1-nitrotetrazolato-2-nitro-2-aza-propane
NTO	nitrotriazolone
ONR	Office of Naval Research
PETN	pentaerythrite tetranitrate
RDX	cyclotrimethylenetrinitramine
TAGDN	triaminoguanidinium-5-dinitrate
TAGZT	triaminoguanidinium azotetrazolate
TATB	triaminotrinitrobenzene
TGA	thermogravimetric analysis
TKX-50	bis(1-hydroxylammo-niumoxy)tetrazolate
TNMM-oxamide	N,N'- bis-(tris-(nitratomethyl)-methyl)-oxamide
TNT	2,4,6-trinitrotoluene

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