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# Experimental thermochemical study of two polymethylpyrazine $N,N'$-dioxide derivatives

Maria D.M.C. Ribeiro da Silva[a,*], Mónica A.A. Vieira[a], Chelsea Givens[b], Stephanie Keown[b], William E. Acree Jr.[b]

[a] *Centro de Investigação em Química, Departamento de Química, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 687, P-4169-007 Porto, Portugal*
[b] *Department of Chemistry, University of North Texas, Denton, TX 76203-5070, USA*

## Abstract

The standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation of crystalline 2,3,5-trimethylpyrazine-1,4-dioxide and 2,3,5,6-tetramethylpyrazine-1,4-dioxide were measured, at $T = 298.15$ K, by static bomb calorimetry and the standard molar enthalpies of sublimation, at $T = 298.15$ K, were obtained from Calvet microcalorimetric measurements. These values were used to derive the respective standard molar enthalpies of formation in gaseous phase. The mean N–O bond dissociation enthalpy has been calculated for both compounds.

*Keywords:* Polyalkylsubstituted pyrazine *N*,*N*-dioxides; 2,3,5-Trimethylpyrazine-1,4-dioxide; 2,3,5,6-Tetramethylpyrazine-1,4-dioxide; Enthalpy of sublimation; Enthalpy of formation; Mean N–O bond dissociation enthalpy

## 1. Introduction

The pyrazine ring system, one diazine resulting from the formal replacement of a CH unit by a nitrogen atom in position 4 of the pyridine, is a relevant component of aromas of many fruits, vegetables and wines. Many synthetic pyrazine derivatives are important as therapeutic agents, since derivatives of that heterocyclic ring have also a relevant role in several biological processes [1,2]. The pyrazine *N*-oxide derivatives have been also widely investigated due to the interest for their use in synthetic drugs, particularly as antibacterial and hypertensive agents [3].

The thermochemical study of heterocyclic molecules derived from pyridine *N*-oxide [4–7], from quinoxaline $N,N'$-dioxide [8–10] and from a few quinoline *N*-oxides [11] has received a lot of attention from researchers of our Thermochemistry Group, whose main goal is to establish relationships among the energetical, structural and reactivity properties [12], in order to clarify their behaviour. In this context, there is a big interest on the knowledge of the values of the gaseous enthalpy of formation of these compounds and of the parent compounds without the N–O bonds.

Although quinoline *N*-oxide and quinoxaline $N,N'$-dioxide derivatives are bicyclic systems, generated when a benzene ring fuses to the pyridine *N*-oxide or the pyrazine $N,N'$-dioxide, the thermochemical data for the diazine $N,N'$-dioxide systems are scarce [8] and this fact makes difficult the use of such knowledge to establish a scheme to predict parameters for quinoxaline $N,N'$-dioxides.

The present work, reporting the study of two $N,N'$-dioxides: 2,3,5-trimethylpyrazine-1,4-dioxide (TrMePzDO) and 2,3,5,6-tetramethylpyrazine-1,4-dioxide (TeMePzDO), is a contribution to reduce the lack of values of the gaseous standard molar enthalpies of formation of pyrazine *N*-oxide derivatives. The gaseous standard molar enthalpies of formation of these two compounds were derived from the measurements of the standard molar energies of combustion, using a static bomb calorimeter, and from the standard molar enthalpies of sublimation, measured by Calvet microcalorimetry. The results obtained in this study, together with those for the gaseous standard molar enthalpy of formation of the correspondent polyalkylpyrazines, were used to derive the mean dissociation enthalpy of the N–O bonds for both compounds studied.

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* Corresponding author. Tel.: +351 22 6082 838; fax: +351 22 6082 822.
*E-mail address:* mdsilva@fc.up.pt (M.D.M.C. Ribeiro da Silva).

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## 2. Experimental

### 2.1. Synthesis of compounds and purity control

2,3,5,6-Tetramethylpyrazine-1,4-dioxide (TeMePzDO) and 2,3,5-trimethylpyrazine-1,4-dioxide (TrMePzDO) were prepared by hydrogen peroxide oxidation of 2,3,5,6-tetramethylpyrazine and 2,3,5-trimethylpyrazine according to Klein and Berkowitz [13]. The crude product was extracted from the sodium hydroxide neutralized reaction mixture by using chloroform. The resulting chloroform solution was concentrated under reduced pressure to about one-third of its original volume and then diluted with an equal volume of cold 2,2,4-trimethylpentane. The solid product formed was collected by vacuum filtration and further purified by vacuum sublimation. Elemental analyses were in excellent agreement with calculated values: mass fractions for TeMePzDO: $C_8H_{12}N_2O_2$: found: C, 0.5707; H, 0.0730; N, 0.1655; calculated: C, 0.5713; H, 0.0719; N, 0.1666 and for TrMePzDO: $C_7H_{10}N_2O_2$: found: C, 0.5460; H, 0.0644; N, 0.1807; calculated: C, 0.5453; H, 0.0654; N, 0.1817. The melting points measured in a melting point apparatus, Stuart Scientific SMP2, were: TeMePzDO, 496 K; TrMePzDO, 406 K.

The average ratios of the mass of carbon dioxide recovered to that calculated from the mass of sample, together with the standard deviation of the mean, were: TrMePzDO, $(1.0000 \pm 0.0004)$; TeMePzDO, $(1.0001 \pm 0.0002)$. The density of the crystalline samples was estimated to be $\rho = 1.00\ \mathrm{g\,cm^{-3}}$ for both compounds.

### 2.2. Combustion calorimetry

The energies of combustion of the two compounds were performed using an isoperibol static bomb calorimeter, with a twin valve bomb of internal volume $0.290\ \mathrm{dm^3}$. The apparatus and the technique have been previously described [14,15,11]. The energy equivalent of the calorimeter was determined using the combustion of benzoic acid NBS, SRM 39j, with the massic energy of combustion of $\Delta_c u = -(26434 \pm 3)\ \mathrm{J\,g^{-1}}$ (value under certificate conditions). The calibration results were corrected to give the energy equivalent, $\varepsilon_{\mathrm{cal}}$, corresponding to the average mass of water added to the calorimeter, 2900.0 g. One set of 12 calibration experiments was made in oxygen at $p = 3.04$ MPa, with $1.00\ \mathrm{cm^3}$ of water added to the bomb, leading to $\varepsilon_{\mathrm{cal}} = (15546.5 \pm 1.1)\ \mathrm{J\,K^{-1}}$, where the uncertainty quoted is the standard deviation of the mean. Combustion experiments were made in the crystalline compounds in pellet form. For all experiments, ignition was made at $T = (298.150 \pm 0.001)$ K. The electrical energy for ignition $\Delta U(\mathrm{ign.})$ was determined from the change in potential difference across a capacitor when discharged through the platinum ignition wire. For the cotton thread fuse of empirical formula $CH_{1.686}O_{0.843}$, the specific energy of combustion is $\Delta_c u^\circ = -16250\ \mathrm{J\,g^{-1}}$ [16]. The corrections for nitric acid formation, $\Delta U(HNO_3)$, were based on $-59.7\ \mathrm{kJ\,mol^{-1}}$ [17], for the molar energy of formation of $0.1\ \mathrm{mol\,dm^{-3}}$ $HNO_3(aq)$ from $N_2$, $O_2$, and $H_2O(l)$. Corrections for carbon soot formation were based on the massic energy of combustion of carbon $\Delta_c u^\circ = -33\ \mathrm{kJ\,g^{-1}}$ [16]. The mass of compound, $m$(compound), used in each experiment was determined from the total mass of carbon dioxide, $m(CO_2$, total), produced after allowance for that formed from the cotton thread fuse. An estimated pressure coefficient of specific energy: $(\partial u/\partial p)T = -0.2\ \mathrm{J\,g^{-1}\,MPa^{-1}}$ at $T = 298.15$ K, a typical value for most organic compounds [18], was assumed. For each compound, the standard massic energy of combustion, $\Delta_c u^\circ$, was calculated by the procedure given by Hubbard et al. [19].

### 2.3. Calvet microcalorimetry

The standard molar enthalpies of sublimation were measured using the *vacuum sublimation* drop microcalorimetric method [20]. Samples, about 3–5 mg of the crystalline compounds, contained in a thin glass capillary tube sealed at one end, were dropped, at room temperature, into the hot reaction vessel, in a high temperature Calvet microcalorimeter (SETARAM HT 1000) held at a convenient temperature, $T$, and then removed from the hot zone by vacuum evaporation. Simultaneously, an empty capillary of the same mass is dropped in the reference cell of the Calvet microcalorimeter, thus compensating the heat uptaken for heating the glass of the capillary. The observed enthalpies of sublimation were corrected to $T = 298.15$ K, by means of $\Delta_{298.15\,\mathrm{K}}^{T} H_{\mathrm{m}}^{\circ}(\mathrm{g})$ estimated by a group method based on values of Stull et al. [21], using the following equations:

TrMePzDO

$$= (\text{3-methylpyridine}) + 2 \times (\text{2-methylpyridine}) - \text{pyridine} - \text{benzene} + 2 \times \text{NO} \quad (1)$$

TeMePzDO

$$= (\text{3-methylpyridine}) + 3 \times (\text{2-methylpyridine}) - 2 \times \text{pyridine} - \text{benzene} + 2 \times \text{NO} \quad (2)$$

The microcalorimeter was calibrated *in situ* for these measurements using the reported standard molar enthalpies of sublimation of naphthalene [22].

The molar masses used for the elements were those recommended by the IUPAC Commission [23].

## 3. Experimental results

Results for a typical combustion experiment of each compound are given in Table 1. As samples were ignited at $T = 298.15$ K, the energy associated to the isothermal bomb process is:

$$\Delta U(\mathrm{IBP}) = -\{\varepsilon_{\mathrm{cal}} + \Delta m(H_2O)c_p(H_2O,l) + \varepsilon_f\}\Delta T_{\mathrm{ad}} + \Delta U(\mathrm{ign.}) \quad (3)$$

where $\Delta m(H_2O)$ is the deviation of the mass of water added to the calorimeter from the average mass (2900.0 g) assigned to $\varepsilon_{\mathrm{cal}}$, $c_p(H_2O,\ l)$ is the heat capacity of liquid water, $\varepsilon_f$ is the energy of the bomb contents after ignition, $\Delta T_{\mathrm{ad}}$ is

Table 1
Typical combustion experiments at $T = 298.15$ K

| | TrMePzDO | TeMePzDO |
|---|---|---|
| $m(CO_2$, total) (g) | 1.51861 | 1.43940 |
| $m$(compound) (g) | 0.75777 | 0.68540 |
| $m$(fuse) (g) | 0.00232 | 0.00289 |
| $\Delta T_{ad}$ (K) | 1.30587 | 1.25328 |
| $\varepsilon_f$ (J K$^{-1}$) | 14.73 | 14.60 |
| $\Delta m(H_2O)$ (g) | −1.1 | −3.5 |
| $-\Delta U(\mathrm{IBP})$[a] (J) | 20313.75 | 19482.88 |
| $-\Delta U$(fuse) (J) | 37.68 | 46.93 |
| $-\Delta U(HNO_3)$ (J) | 48.43 | 53.94 |
| $\Delta U$(ign.) (J) | 1.18 | 1.18 |
| $-\Delta U_\Sigma$ (J) | 13.38 | 11.64 |
| $-\Delta_c u^\circ$ (J g$^{-1}$) | 26675.99 | 28261.41 |

$m(CO_2$, total) is the total mass of $CO_2$ formed in the experiment; $m$(compound) is the mass of compound burnt in the experiment; $m$(fuse) is the mass of fuse (cotton) used in the experiment; $\Delta T_{ad}$ is the corrected temperature rise; $\varepsilon_f$ is the energy equivalent of contents in the final state; $\Delta m(H_2O)$ is the deviation of the mass of water added to the calorimeter from 2900.0 g; $\Delta U$(IBP) is the energy change for the isothermal combustion reaction under actual bomb conditions; $\Delta U$(fuse) is the energy of combustion of the fuse (cotton); $\Delta U(HNO_3)$ is the energy correction for the nitric acid formation; $\Delta U$(ign.) is the energy of combustion of the fuse; $\Delta U_\Sigma$ is the energy correction to the standard state; $\Delta_c u^\circ$ is the standard massic energy of combustion.

[a] $\Delta U$(IBP) includes $\Delta U$(ign.).

Table 2
Individual values of the massic energy of combustion, $\Delta_c u^\circ$, at $T = 298.15$ K

| TrMePzDO | TeMePzDO |
|---|---|
| 26675.43 | 28289.69 |
| 26675.99 | 28235.32 |
| 26675.62 | 28261.41 |
| 26663.87 | 28277.51 |
| 26663.41 | 28279.89 |
| 26676.74 | 28253.92 |
| $-\langle \Delta_c u^\circ \rangle$ (J g$^{-1}$) | |
| 26671.8 ± 2.6 | 28266.3 ± 8.2 |

Table 3
Derived standard ($p^\circ = 0.1$ MPa) molar values in the condensed phase, at $T = 298.15$ K (kJ mol$^{-1}$)

| Compound | $\Delta_c U_m^\circ$ (cr) | $\Delta_c H_m^\circ$ (cr) | $\Delta_f H_m^\circ$ (cr) |
|---|---|---|---|
| TrMePzDO | −4112.0 ± 1.1 | −4113.2 ± 1.1 | −(70.5 ± 1.4) |
| TeMePzDO | −4754.1 ± 2.8 | −4756.6 ± 2.8 | −(106.5 ± 3.0) |

Table 5
Derived standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation, at $T = 298.15$ K (kJ mol$^{-1}$)

| Compound | $\Delta_f H_m^\circ$ (cr) | $\Delta_{cr}^{g} H_m^\circ$ | $\Delta_f H_m^\circ$ (g) |
|---|---|---|---|
| TrMePzDO | −(70.5 ± 1.4) | 116.2 ± 2.9 | 45.7 ± 3.2 |
| TeMePzDO | −(106.5 ± 3.0) | 107.5 ± 1.6 | 1.0 ± 3.4 |

the adiabatic temperature raise and $\Delta U$(ign.) is the energy of ignition. The individual results of all combustion experiments, together with the mean value and its standard deviation, are given, for each compound, in Table 2. Table 3 lists the derived standard molar energies and enthalpies of combustion, $\Delta_c U_m^\circ$ (cr) and $\Delta_c H_m^\circ$ (cr), and the standard molar enthalpies of formation for the compounds in the condensed phase $\Delta_f H_m^\circ$ (cr) at $T = 298.15$ K. In accordance with normal thermochemical practice [24], the uncertainties assigned to the standard molar enthalpies of combustion are, in each case, twice the overall standard deviation of the mean and include the uncertainties in calibration and in the values of auxiliary quantities. To derive $\Delta_f H_m^\circ$ (cr) from $\Delta_c H_m^\circ$ (cr) the standard molar enthalpies of formation of $H_2O$(l) and $CO_2$(g), at $T = 298.15$ K, −(285.830 ± 0.042) kJ mol$^{-1}$ [25] and −(393.51 ± 0.13) kJ mol$^{-1}$ [25], respectively, were used.

Measurements yielding the standard molar enthalpies of sublimation $\Delta_{cr}^{g} H_m^\circ$, at $T = 298.15$ K, are given in Table 4 with uncertainties of twice the standard deviation of the mean. The derived standard molar enthalpies of formation, in both the condensed and gaseous phases, for both compounds are summarized in Table 5.

## 4. Discussion

The first thermochemical data found in the literature for derivatives of pyrazine *N,N′*-dioxide is for the pyrazine 1,4-dioxide (PzDO) itself [8], and so the experimental results reported in the present work are a new contribution enlarging the knowledge about the properties and chemical behaviour of these heterocyclic nitrogen compounds. In the literature, there are studies reporting data for several pyrazine (Pz) derivatives, particularly for the polymethylpyrazines 2,3,5-trimethylpyrazine (TrMePz) and 2,3,5,6-tetramethylpyrazine (TeMePz) [26]. All these values are summarized in Table 6 and based on these values we can discuss two aspects: the effect of the substitution of hydrogen atoms by methyl groups in the molecule of pyrazine 1,4-dioxide comparatively with the effect caused in pyrazine, and the values of the mean dissociation enthalpy of the N–O bonds for the two pyrazine 1,4-dioxide derivatives. Table 6 reports also the enthalpic increments for the substitution, $Z$, of three or four methyl groups, Me, into the pyrazine ring (Pz) and in the pyrazine 1,4-dioxide (PzDO) ring, calculated as the difference between the standard molar enthalpies of formation, in the gaseous state, of substituted pyrazines or pyrazine 1,4-dioxides and of the pyrazine or pyrazine 1,4-dioxide itself, as it

Table 4
Standard ($p^\circ = 0.1$ MPa) molar enthalpies of sublimation, at $T = 298.15$ K

| Compound | No. of experiments | $T$ (K) | $\Delta_{cr,298.15\,K}^{g,T} H_m^\circ$ (kJ mol$^{-1}$) | $\Delta_{298.15\,K}^{T} H_m^\circ$ (g) (kJ mol$^{-1}$) | $\Delta_{cr}^{g} H_m^\circ$ (298.15 K) (kJ mol$^{-1}$) |
|---|---|---|---|---|---|
| TrMePzDO | 6 | 389 | 133.4 ± 2.9 | 17.24 | 116.2 ± 2.9 |
| TeMePzDO | 6 | 425 | 135.9 ± 1.6 | 28.41 | 107.5 ± 1.6 |

Table 6
Comparison of values of enthalpy of formation, in the gaseous state, at $T = 298$ K, measured in this work with literature values

| Z–Pz/Z–PzDO | $\Delta_f H_m^\circ$ (g) (kJ mol$^{-1}$) | Z-increment (kJ mol$^{-1}$) |
|---|---|---|
| Pz | 196.1 ± 1.3 [27] | – |
| TrMePz | 74.3 ± 2.7 [26] | −(121.8 ± 3.0) |
| TeMePz | 54.7 ± 4.5 [26] | −(141.4 ± 4.7) |
| PzDO | 186.5 ± 1.9 [8] | – |
| TrMePzDO | 45.7 ± 3.2[a] | −(140.8 ± 3.7) |
| TeMePzDO | 1.0 ± 3.4[a] | −(185.5 ± 3.9) |

[a] This work.

is represented in Eqs. (4) and (5), respectively:

$$Z\text{-increment} = \Delta_f H_m^\circ(Z - \text{Pz,g}) - \Delta_f H_m^\circ(\text{Pz,g}) \quad (4)$$

$$Z\text{-increment} = \Delta_f H_m^\circ(Z - \text{PzDO,g}) - \Delta_f H_m^\circ(\text{PzDO,g}) \quad (5)$$

The tendency on the relative variations of the standard molar enthalpies of formation by three or four methyl groups is consistent for the heteroaromatic rings, Pz or PzDO, although the increments for pyrazine-1,4-dioxide point for a higher stabilization in comparison with identical substitution on the pyrazine ring. This aspect is consistent with the fact that the electron donating character of the substituents should increase the electron density of the aromatic rings turning more stable the ring with the two N–O covalent dative bonds.

The mean dissociation enthalpy of the N–O bonds, $\langle DH_m^\circ(\text{N–O})\rangle$, for a polymethylpyrazine *N*,*N*-dioxide, $Z-$PzDO, can be derived as one half of the enthalpy of the gaseous reaction (4), and for the calculation of this value, $\Delta_f H_m^\circ(\text{O, g}) = (249.18 \pm 0.10)$ kJ mol$^{-1}$ [28] is required:

$$(Z - \text{PzDO, g}) \rightarrow (Z - \text{Pz, g}) + 2\text{O(g)} \quad (6)$$

Using the results reported in this work, $\Delta_f H_m^\circ(\text{TrMePzDO}) = (45.7 \pm 3.2)$ kJ mol$^{-1}$ and $\Delta_f H_m^\circ(\text{TeMePzDO}) = (1.0 \pm 3.4)$ kJ mol$^{-1}$, as well as the literature values $\Delta_f H_m^\circ(\text{TrMePz}) = (74.3 \pm 2.7)$ kJ mol$^{-1}$ [26] and $\Delta_f H_m^\circ(\text{TeMePz}) = (54.7 \pm 4.5)$ kJ mol$^{-1}$ [26], the $\langle \text{DH}_m^\circ(\text{N–O})\rangle$ for TrMePzDO and TeMePzDO are $(263.5 \pm 3.4)$ and $(276.0 \pm 5.5)$ kJ mol$^{-1}$, respectively. These results and the previous data obtained for pyrazine 1,4-dioxide, $\langle \text{DH}_m^\circ(\text{N–O})\rangle = (254.0 \pm 2.3)$ kJ mol$^{-1}$ [8], confirm that the propensity of the pyrazine *N*,*N*-dioxide derivatives for promoting oxidation is decreasing with an increase on the number of electron donating groups present in the molecule, as it should be expected by considering the inductive effect of the methyl groups.

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