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Thermochemical study of 1-, 3- and 4-piperidinecarboxamide derivatives

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Abstract

The standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation, at $T = 298.15$ K, in the gaseous phase, of three piperidinecarboxamide derivatives, namely 1-, 3- and 4-piperidinecarboxamide, were determined from their enthalpies of combustion and sublimation, obtained by static bomb calorimetry in oxygen and by Calvet microcaloriments, respectively.

The final results are analysed and discussed in terms of molecular structure.

Keywords: Combustion calorimetry; Calvet microcalorimetry; Enthalpy of combustion; Enthalpy of formation; Enthalpy of sublimation; Piperidinecarboxamide

1. Introduction

Piperidine ring systems are a commonest structural sub-unit in natural compounds and are of great interest in pharmaceutical industry. They exhibit a wide range of biological activities and so, the applicability of piperidine derivatives as raw-material and intermediates for medicines or drugs has been object of great interest. As examples of the applications of piperidinecarboxamides, in medicine, they are referred as inhibitors against aggregation of human platelets [1] and anti-HIV-1 activity [2]. Piperidinecarboxamides are also involved in computational and NMR spectroscopy studies to identify ligand-binding sites of macromolecules, namely proteins [3]. Jurkiewicz-Herbich et al. had studied the adsorption of nipecotamide (3-piperidinecarboxamide) from aqueous solutions in mercury electrodes [4], in order to investigate the factors that govern the adsorption of molecules from aqueous solutions, upon the type of interface and the structure of the solutions, to elucidate the adsorption mechanisms and structure details of the adsorption layer. That molecule has been chosen for this investigation as the model typical nitrogen heterocycle in which all the bonds in the ring are saturated.

As a part of our extensive work on the thermochemistry of nitrogen heterocyclic compounds, we have recently been interested on the derivatives of piperidine [5–9].

The number of compounds with carboxamide substituents for which thermochemical data are available is very scarce, and so, this work is also a contribution for the knowledge of the thermochemical properties of the carboxamide type of compounds.

This paper presents the thermochemical study of 1-, 3-, and 4-piperidinecarboxamide, reporting their standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation in the crystalline state derived from the standard molar enthalpy of combustion determined by static bomb calorimetry and their standard molar enthalpies of sublimation measured by Calvet microcalorimetry. From these two thermochemical parameters, the standard molar enthalpies of formation in the gaseous phase, of the three compounds, at $T = 298.15$ K, have been derived.

2. Experimental

2.1. Compounds

The piperidinecarboxamide derivatives studied, 1-piperidinecarboxamide, [CAS 2158-03-4], 3-piperidinecarboxamide, [CAS 4138-26-5], and 4-piperidinecarboxamide [CAS 39546-32-2] were all supplied by Aldrich Chemical with initial purity of 99%, 95%, and 97%, respectively. These three compounds were purified by repeated vacuum sublimation and the final

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purity of the compounds was determined by the recovering the carbon dioxide produced in the combustion experiments and also checked by d.s.c. and g.l.c. The average ratios of the mass of carbon dioxide recovered after combustion experiments to that calculated from the mass of sample were (values in percentage): for 1-piperidinecarboxamide (100.030 ± 0.016), for 3-piperidinecarboxamide (99.846 ± 0.012) and for 4-piperidinecarboxamide (99.996 ± 0.050). Except for 1-piperidinecarboxamide, the other two compounds were shown to be highly hygroscopic, so it was necessary to handle them under nitrogen atmosphere. Even with careful manipulation under nitrogen atmosphere, and the use of Melinex bags for enclosing the compounds for the combustion experiments, the 3-piperidinecarboxamide absorbed a small amount of water, as shown by the CO_2 average ratio value, lower than 99.9%. The amount of water presented in the samples of 3-piperidinecarboxamide was confirmed by Karl Fischer titration.

2.2. *Combustion calorimetry*

The calorimetric system used to measure the standard molar energies of combustion was an isoperibol calorimeter. A detailed description of the apparatus and the technique may be found in the literature [10,11]. The combustion bomb used was a twin-valve combustion bomb type 1105, Parr instruments Company, made of stainless steel and with an internal volume of $0.340\,\mathrm{cm}^3$.

The calorimeter calibration was done by combustion of Thermochemical Standard benzoic acid, sample BAS 693976/01 with massic energy of combustion, under bomb conditions, of $\Delta_c u = -26435.1 \pm 3.5\,\mathrm{J\,g^{-1}}$ [12], and corrected to give the energy equivalent, $\varepsilon_{\mathrm{cal}}$, corresponding to the average mass of water of 3119.6 g added to the calorimeter.

For the combustion experiments with 1- and 4-piperidinecarboxamide, the energy equivalent of the calorimeter was determined as $\varepsilon_{\mathrm{cal}} = 15908.78 \pm 0.77\,\mathrm{J\,K^{-1}}$, and for 3-piperidinecarboxamide as $\varepsilon_{\mathrm{cal}} = 15915.83 \pm 0.76\,\mathrm{J\,K^{-1}}$, as the average, in both cases of six combustion experiments of benzoic acid.

The samples were burnt in pellet form and, because of the hygroscopic nature of the 3- and 4-piperidinecarboxamide, the pellets of these two compounds were sealed in previously weighed polyester bags of Melinex, with 0.025 mm of thickness. The mass of Melinex used in each experiment was corrected for the mass fraction of water, $w = 0.0032$, and the mass of CO_2 resulted from the combustion of Melinex was calculated using a factor previously reported [13]. The value of $\Delta_c u^\circ = 22902 \pm 5\,\mathrm{J\,g^{-1}}$, measured by Skinner and Snelson [13], as the massic energy of combustion of dry Melinex, was used; this value was confirmed in our laboratory.

In all combustion experiments, $1.00\,\mathrm{cm}^3$ of water was introduced into the bomb, which was then closed and purged twice with oxygen, to remove the air, before charged with 3.04 MPa of oxygen. The ignition of the sample was made at $T = 298.150 \pm 0.001\,\mathrm{K}$, by the discharge of a 1400 μF capacitor through a platinum ignition wire, using a cotton thread fuse, with empirical formula $CH_{1.686}O_{0.843}$ and massic energy of combustion of $-\Delta_c u^\circ = 16250\,\mathrm{J\,g^{-1}}$ [14], a value that was checked in our laboratory. The electrical energy of ignition was determined from the change of potential across the capacitor.

For all experiments, the calorimeter temperatures were measured to $\pm 1 \times 10^{-4}\,\mathrm{K}$, at time intervals of 10 s, with a quartz crystal thermometer (Hewlett Packard HP 2804A), interfaced to a PC. At least 100 readings were taken in each period: before the ignition, during the main period after ignition, and in the after period.

At the end of the experiment, the amount of compound used in each experiment was determined from the total mass of carbon dioxide produced during the experiments taking into account that formed from the combustions of the cotton-thread fuse and of the Melinex, and that lost due to eventual carbon formation.

Since the amount of the compound used in each experiment was based on the CO_2 recovered from each combustion, the small amount of water presented in 3-piperidinecarboxamid will not interfere with the final result.

The corrections for nitric acid formation were based on—$59.7\,\mathrm{kJ\,mol^{-1}}$, for the molar energy of formation of $0.1\,\mathrm{mol\,dm^{-3}}$ HNO_3 (aq), from N_2 (g), O_2 (g) and H_2O (l) [15]. For the experiments with a small carbon residue soot formed during the combustion, the necessary energetic correction for its formation was based on $\Delta_c u^\circ = -33\,\mathrm{kJ\,g^{-1}}$ [16]. For each compound, an estimated pressure coefficient of massic energy, $(\partial u/\partial p)_T$, at $T = 298.15\,\mathrm{K}$, was assumed to be $-0.2\,\mathrm{J\,g^{-1}\,MPa^{-1}}$, a typical value for most organic compounds [17].

The relative atomic masses used were those recommended by the IUPAC Commission in 2001 [18] yielding the molar mass of the piperidinecarboxamide isomers as $128.172\,\mathrm{g\,mol^{-1}}$.

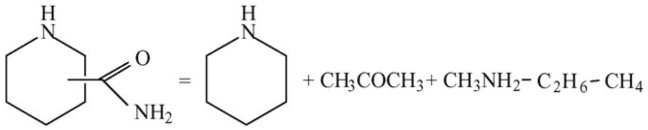
All the weighing necessary for the combustion experiments, namely, the weighing of the platinum crucible where the pallet to hold the pellet during the experiment, the pellet itself, the cotton thread fuse and the Melinex bags, when they were necessary, were made in a Mettler Toledo 240 balance, sensitivity $\pm 1 \times 10^{-5}$ g. The water added to the calorimeter was weighing with a Mettler PC 8000 balance, sensitivity ±0.1 g and the CO_2 recovering tubes were weighing with a Mettler Toledo AT 201 balance, sensitivity $\pm 1 \times 10^{-4}$ g.

2.3. *Calvet microcalorimetry*

The standard molar enthalpies of sublimation of the compounds were determined using a Calvet High Temperature Microcalorimeter (Setaram, HT 1000D) by the "vacuum-sublimation drop-microcalorimetric method", of Skinner et al. [19]. Apparatus and technique is already described in the literature [20].

Samples of about 3–4 mg of each compound, contained in a thin glass capillary tube sealed at one end, were dropped from room temperature into the hot zone of the calorimeter, held at a predefined convenient temperature, T, and then removed from the hot zone by vacuum sublimation.

The experimental temperature for the different compounds were: for 1 and 3-piperidinecarboxamide, $T = 386.0\,\mathrm{K}$, and for 4-piperidinecarboxamide, $T = 426.8.0\,\mathrm{K}$. The thermal corrections for the glass capillaries were made by dropping tubes of nearly equal mass into each of the twin cells. The observed standard molar enthalpies of sublimation, $\Delta_{\mathrm{cr},298.15\ \mathrm{K}}^{\mathrm{g},T} H_{\mathrm{m}}^{\circ}$, were corrected to $T = 298.15\ \mathrm{K}$ using $\Delta_{298.15\ \mathrm{K}}^{T} H_{\mathrm{m}}^{\circ}(\mathrm{g})$ estimated by a group method based on the values of Messerly et al. [21] and Stull et al. [22]. The scheme applied for all piperidinecarboxamide isomers was the one represented by Eq. (1):



(1)

which gives for 1- and 3-piperidinecarboxamide, at $T = 386.0\ \mathrm{K}$, $\Delta_{298.15\ \mathrm{K}}^{386.0\ \mathrm{K}} H_{\mathrm{m}}^{\circ}(\mathrm{g}) = 13.96\ \mathrm{kJ\ mol^{-1}}$; for 4-piperidinecarboxamide, at $T = 426.8\ \mathrm{K}$, $\Delta_{298.15\ \mathrm{K}}^{426.8\ \mathrm{K}} H_{\mathrm{m}}^{\circ}(\mathrm{g}) = 21.55\ \mathrm{kJ\ mol^{-1}}$.

The calorimeter was calibrated *in situ* by the sublimation of naphthalene, using the same experimental procedure as for the samples, and using the value of $\Delta_{\mathrm{cr}}^{\mathrm{g}} H_{\mathrm{m}}^{\circ} = 72.60 \pm 0.60\ \mathrm{kJ\ mol^{-1}}$ [23] for the standard molar enthalpy of sublimation of the naphthalene, at $T = 298.15\ \mathrm{K}$. The calibration constants of the calorimeter, k_{cal}, were obtained, at each temperature, as the average of five independent experiments: at $T = 386\ \mathrm{K}$, $k_{\mathrm{cal}} = 1.0104 \pm 0.0038$; at $T = 427\ \mathrm{K}$, $k_{\mathrm{cal}} = 0.9846 \pm 0.0033$.

3. Experimental results

Table 1 lists detailed results for a typical combustion experiment of each compound, where $\Delta m(\mathrm{H_2O})$ is the deviation of the mass of water added to the calorimeter from 3119.6 g and $\Delta U(\mathrm{IBP})$ is the energy change for the isothermal combustion reaction under bomb conditions, with

$$\Delta U(\mathrm{IBP}) = -\{\varepsilon_{\mathrm{cal}} + \Delta m(\mathrm{H_2O})c_{\mathrm{p}}(\mathrm{H_2O, l}) + \varepsilon_{\mathrm{f}}\}\Delta T_{\mathrm{ad}} + \Delta U(\mathrm{ign}), \qquad (2)$$

and the remaining quantities are as previously defined [24], the corrections to the standard state, ΔU_{Σ}, and the massic energies of combustion, $\Delta_{\mathrm{c}} u^{\circ}$, were calculated by the procedure of Hubbard et al. [24]. Table 2 presents the results of the individual massic energies of combustion together with the mean values and their standard deviation.

Table 3 lists the piperidinecarboxamide isomers studied, the derived standard molar values for the energies, $\Delta_{\mathrm{c}} U_{\mathrm{m}}^{\circ}$, and enthalpies, $\Delta_{\mathrm{c}} H_{\mathrm{m}}^{\circ}$, of the combustion the reactions described by Eq. (3), and the standard molar enthalpies of formation, $\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\circ}$, in the crystalline phases.

$$\mathrm{C_6H_{12}N_2O(cr)} + 17/2\,\mathrm{O_2(g)} \rightarrow 6\mathrm{CO_2(g)} + \mathrm{N_2(g)} + 6\mathrm{H_2O(l)} \qquad (3)$$

The uncertainties assigned to the standard molar enthalpies of combustion, in accordance with the normal thermochemical practice are, in each case, twice the overall standard deviation of the mean and include the uncertainties in calibration [25,26] and in the values of auxiliary quantities. The values of the standard molar enthalpies of formation in the crystalline phase, $\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\circ}(\mathrm{cr})$, were derived from $\Delta_{\mathrm{c}} H_{\mathrm{m}}^{\circ}$, using the values, at $T = 298.15\ \mathrm{K}$, of the standard molar enthalpies of formation of liquid water and gaseous carbon dioxide, respectively, as $\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\circ}$ $(\mathrm{H_2O,\ l}) = -285.830 \pm 0.042\ \mathrm{kJ\ mol^{-1}}$ [16] and $\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\circ}$ $(\mathrm{CO_2,\ g}) = -393.51 \pm 0.13\ \mathrm{kJ\ mol^{-1}}$ [16].

Results of the microcalorimetric determination of the enthalpies of sublimation are given in Table 4, with uncertain-

Table 1
Results of a typical combustion experiment, at $T = 298.15\ \mathrm{K}$

Experiment	1-Piperidinecarboxamide	3-Piperidinecarboxamide	4-Piperidinecarboxamide
$m(\mathrm{CO_2}$, total) (g)	1.62575	2.06419	1.72904
m(cpd) (g)	0.78732	0.95136	0.77837
m(Melinex) (g)	–	0.04273	0.05290
m(fuse) (g)	0.00437	0.00394	0.00365
ΔT_{ad} (K)	1.43945	1.81202	1.50670
ε_{f} ($\mathrm{J\ K^{-1}}$)	16.89	17.48	16.97
$\Delta m(\mathrm{H_2O})$ (g)	0	0	+0.1
$-\Delta U(\mathrm{IBP})^{\mathrm{a}}$ (J)	22923.07	28870.45	23994.79
ΔU(Melinex) (J)	–	978.67	1211.46
ΔU(fuse) (J)	70.97	63.99	59.28
$\Delta U(\mathrm{HNO_3})$ (J)	59.70	72.95	58.80
ΔU(ign) (J)	1.16	0.97	1.20
$-\Delta U$(carbon) (J)	30.03	0	14.19
ΔU_{Σ} (J)	12.31	16.16	13.28
$-\Delta_{\mathrm{c}} u^{\circ}$ ($\mathrm{J\ g^{-1}}$)	28971.85	29156.87	29120.03

$m(\mathrm{CO_2}$, total) is the total mass of carbon dioxide recovered in the combustion; m(cpd) is the mass of compound burnt in each experiment; m(Melinex) is the mass of Melinex used to enclose the 3- and 4-piperidinecarboxamide; m(fuse) is the mass of the cotton thread fuse; ΔT_{ad} is the adiabatic temperature rise; ε_{f} is the energy equivalent of the calorimeter including the contents of the bomb in the final state; $\Delta m(\mathrm{H_2O})$ is the deviation of the mass of water added to the calorimeter from 3119.6 g; $\Delta U(\mathrm{IBP})$ is the energy change for isothermal combustion reaction under actual bomb conditions; ΔU(Melinex) is the energy of combustion of the Melinex used in each experiment; ΔU(fuse) is the energy of combustion of the fuse (cotton); $\Delta U(\mathrm{HNO_3})$ is the energy correction for the nitric acid formation; ΔU(ign) is the electrical energy supplied for ignition, ΔU(carbon) is the energy correction for the carbon residue soot formation; ΔU_{Σ} is the standard state correction; $\Delta_{\mathrm{c}} u^{\circ}$ is the massic energy of combustion of the compound.

[a] $\Delta U(\mathrm{IBP})$ already includes ΔU(ign).

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

1-Piperidinecarboxamide	3-Piperidinecarboxamide	4-Piperidinecarboxamide
$-\Delta_c u^\circ$ (J g^{-1})		
28962.90	29156.87	29113.36
28958.04	29153.59	29135.80
28965.28	29153.98	29120.03
28952.32	29173.87	29122.62
28959.49	29174.19	29124.12
28971.85	29159.21	29129.32
$-\langle \Delta_c u^\circ \rangle$ (J g^{-1})		
28961.6 ± 2.7	29162.0 ± 3.9	29124.2 ± 3.2

Table 3
Derived standard ($p^\circ = 0.1$ MPa) molar energies of combustion, $\Delta_c U_m^\circ$, standard molar enthalpies of combustion, $\Delta_c H_m^\circ$, and the standard molar enthalpies of formation for the compounds in the crystalline phase, $\Delta_f H_m^\circ$(cr), at $T = 298.15$ K

Compound	$-\Delta_c U_m^\circ$(cr) (kJ mol^{-1})	$-\Delta_c H_m^\circ$(cr) (kJ mol^{-1})	$-\Delta_f H_m^\circ$(cr) (kJ mol^{-1})
1-Piperidinecarboxamide	3712.08 ± 0.92	3715.08 ± 0.92	360.2 ± 1.2
3-Piperidinecarboxamide	3737.8 ± 1.4	3741.5 ± 1.4	334.5 ± 1.7
4-Piperidinecarboxamide	3732.9 ± 1.3	3736.6 ± 1.3	339.4 ± 1.6

ties, as twice the standard deviation of the mean. The standard molar enthalpies of formation, $\Delta_f H_m^\circ$, both in condensed and gaseous phases, and the standard molar enthalpies of sublimation, $\Delta_{cr}^{g} H_m^\circ$, of the three piperidinecarboxamide isomers studied, are presented in Table 5.

4. Discussion

The number of compounds with carboxamide substituents for which thermochemical data is available is too scarce to allow a long discussion about the effect of the carboxamide group into the piperidine ring, and so, in the present state of knowledge only a limited discussion is possible.

Taking into account the value of the standard molar enthalpy of formation of gaseous piperidine, measured by Good [27], $\Delta_f H_m^\circ$ (piperidine, g) $= -47.15 \pm 0.63$ kJ mol^{-1}, the enthalpic increments for the introduction of the –CONH$_2$ group in the different positions of the piperidine ring are shown in Scheme 1.

As it can be seen the greatest stabilization due to CONH$_2$ group introduction is verified for 1-piperidinecarboxamide, which is the opposite effect to the one verified for methylpiperidines, where this position was the less favourable due to interaction of the methyl group with the lone pair of electrons of the piperidine nitrogen [8]. In the present case, the extra stabilization can be explained by some electronic delocalization between the lone pairs of the oxygen and of the piperidine nitrogen atoms.

The introduction of the –CONH$_2$ group in the position 3 of the ring provides a slightly more stabilization than similar introduction in the position 4, as the introduction of the –CONH$_2$ group in position 3 could be followed by the formation of an intramolecular hydrogen bond as shown in Scheme 2, as had been verified for other compounds like 1-methyl-3-piperinol [28].

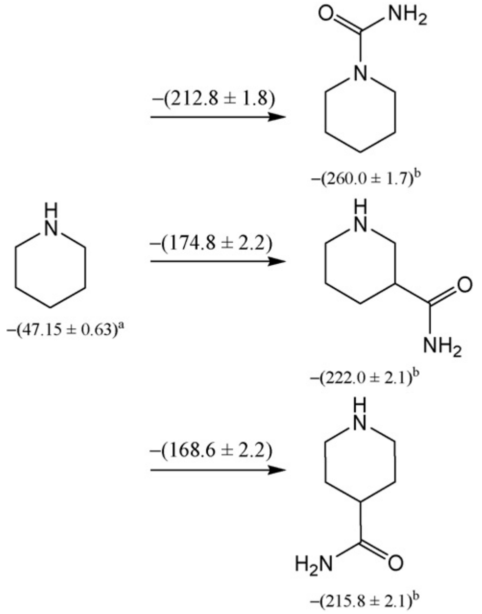
When the introduction of the –CONH$_2$ group takes place in position 4, due to the distance between the substituting group and the nitrogen lone pair, the piperidine ring has to adopt a boat

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

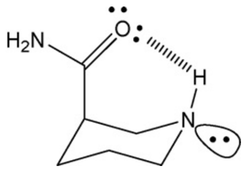
Compound	Number of experiments	T (K)	$\Delta_{\mathrm{cr},298\ \mathrm{K}}^{\mathrm{g},T} H_m^\circ$ (kJ mol^{-1})	$\Delta_{298.15\ \mathrm{K}}^{T} H_m^\circ$(g) (kJ mol^{-1})	$\Delta_{cr}^{g} H_m^\circ$ (T = 298.15 K) (kJ mol^{-1})
1-Piperidinecarboxamide	5	386.0	114.12 ± 0.57	13.96	100.2 ± 1.2
3-Piperidinecarboxamide	5	386.0	126.47 ± 0.59	13.96	112.5 ± 1.3
4-Piperidinecarboxamide	5	426.8	145.15 ± 0.55	21.55	123.6 ± 1.3

Table 5
Derived standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation, $\Delta_f H_m^\circ$, and of sublimation, $\Delta_{cr}^{g} H_m^\circ$, at $T = 298.15$ K

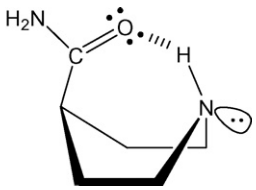
Compound	$-\Delta_f H_m^\circ$(cr) (kJ mol^{-1})	$\Delta_{cr}^{g} H_m^\circ$ (kJ mol^{-1})	$-\Delta_f H_m^\circ$(g) (kJ mol^{-1})
1-Piperidinecarboxamide	360.2 ± 1.2	100.2 ± 1.2	260.0 ± 1.7
3-Piperidinecarboxamide	334.5 ± 1.7	112.5 ± 1.3	222.0 ± 2.1
4-Piperidinecarboxamide	339.4 ± 1.6	123.6 ± 1.3	215.8 ± 2.1



Scheme 1. Changes in the enthalpy of formation of piperidine due to the insertion of the carboxamide group in different positions. ^{a}Ref. [27]; ^{b}This work.



Scheme 2. Source of stabilization in 3-piperidinecarboxamide.



Scheme 3. Source of stabilization in 4-piperidinecarboxamide.

conformation, as shown in Scheme 3, which is less stable than the chair conformation.

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References

[1] Z. Guoa, X. Zhenga, W. Thompsona, M. Dugdaleb, R. Gollamudi, Bioorg. Med. Chem. 8 (2000) 1041–1058.
[2] S. Imamura, T. Ichikawa, Y. Nishikawa, N. Kanzaki, K. Takashima, S. Niwa, Y. Iizawa, M. Baba, Y. Sugihara, J. Med. Chem. 49 (2006) 2784–2793.
[3] F. Sirockin, C. Sich, S. Improta, M. Schaefer, V. Saudek, N. Froloff, M. Karplus, A. Dejaegere, J. Am. Chem. Soc. 124 (2002) 11073–11084.
[4] M. Jurkiewicz-Herbich, A. Muszalska, Colloid Surf. A: Physicochem. Eng. Aspects 106 (1996) 49–57.
[5] M.A.V. Ribeiro da Silva, J.I.T.A. Cabral, J. Chem. Thermodyn. 38 (2006) 1008–1012.
[6] M.A.V. Ribeiro da Silva, J.I.T.A. Cabral, J.R.B. Gomes, J. Chem. Thermodyn. 38 (2006) 1072–1078.
[7] M.A.V. Ribeiro da Silva, J.I.T.A. Cabral, J. Chem. Eng. Data 51 (2006) 171–767.
[8] M.A.V. Ribeiro da Silva, J.I.T.A. Cabral, P. Gomes, J.R. Gomes, J. Org. Chem. 71 (2006) 3677–3685.
[9] M.A.V. Ribeiro da Silva, J.I.T.A. Cabral, J. Chem. Thermodyn. 38 (2006) 1461–1466.
[10] M.A.V. Ribeiro da Silva, M.D.M.C. Ribeiro da Silva, G. Pilcher, Rev. Por. Quím. 26 (1984) 163–172.
[11] M.A.V. Ribeiro da Silva, M.D.M.C. Ribeiro da Silva, G. Pilcher, J. Chem. Thermodyn. 16 (1984) 1149–1155.
[12] G. Pilcher, Personal communication, University of Manchester, 1995.
[13] H.A. Skinner, A. Snelson, Trans. Faraday Soc. 56 (1960) 1776–1783.
[14] J. Copps, R.S. Jessup, K. Van Nes, in: F.D. Rossini (Ed.), Experimental Thermochemistry, vol. 1, Interscience, New York, 1956 (Chapter 3).
[15] D.D. Wagman, W.H. Evans, V.B. Parker, R.H. Shum, F. Halow, S.M. Bailey, K.L. Churney, R.L. Nuttall, J. Phys. Chem. Ref. Data 11 (Suppl. 2) (1982).
[16] J.D. Cox, D.D. Wagman, V.A. Medvedev, CODATA Key Values for Thermodynamics, Hemisphere, New York, 1989.
[17] E.N. Washburn, J. Res. Nalt. Bur. Stand. (U.S.) 10 (1933) 525–558.
[18] R.D. Loss, Pure Appl. Chem. 35 (2003) 1107–1122.
[19] F.A. Adedeji, D.L.S. Brown, J.A. Connor, M. Leung, M.I. Paz-Andrade, H.A. Skinner, J. Organomet. Chem. 97 (1975) 221–228.
[20] L.M.N.B.F. Santos, S. Schröder, O.O.P. Fernandes, M.A.V. Ribeiro da Silva, Thermochim. Acta 415 (2004) 15–20.
[21] J.F. Messerly, S.S. Todd, H.L. Fink, W.D. Good, B.E. Gammon, J. Chem. Thermodyn. 20 (1988) 209–224.
[22] R.D. Stull, E.F. Westrum, G.C. Sinke, The Chemical Thermodynamics of Organic Compounds, Wiley, New York, 1969.
[23] R. Sabbah, A. Xu-wu, J.D. Chickos, M.L. Planas Leitão, M.V. Roux, L.A. Torres, Thermochim. Acta 331 (1999) 93–204.
[24] W.N. Hubbard, D.W. Scott, G. Waddington, in: F.D. Rossini (Ed.), Experimental Thermochemistry, vol. 1, Interscience, New York, 1956 (Chapter 5).
[25] F.D. Rossini, in: F.D. Rossini (Ed.), Experimental Thermochemistry, vol. 1, Interscience, New York, 1956 (Chapter 14).
[26] G. Olofson, in: S. Sunner, M. Månsson (Eds.), Combustion Calorimetry, Pergamon, Oxford, 1979 (Chapter 6).
[27] W. Good, J. Chem. Eng. Data 17 (1972) 28–31.
[28] A. Goldblum, O. Deeb, G.H. Loew, J. Mol. Struct. Theochem. 207 (1990) 1–14.