

# Standard molar enthalpies of formation of some methylfuran derivatives

Manuel A. V. Ribeiro da Silva ·  
Luísa M. P. F. Amaral

Portuguese Special Chapter

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**Abstract** The standard ( $p^\circ = 0.1$  MPa) molar enthalpies of formation  $\Delta_f H_m^\circ(1)$ , of the liquid 2-methylfuran, 5-methyl-2-acetylfuran and 5-methyl-2-furaldehyde were derived from the standard molar energies of combustion, in oxygen, at  $T = 298.15$  K, measured by static bomb combustion calorimetry. The Calvet high temperature vacuum sublimation technique was used to measure the enthalpies of vaporization of the three compounds. The standard ( $p^\circ = 0.1$  MPa) molar enthalpies of formation of the compounds, in the gaseous phase, at  $T = 298.15$  K have been derived from the corresponding standard molar enthalpies of formation in the liquid phase and the standard molar enthalpies of vaporization. The results obtained were  $-(76.4 \pm 1.2)$ ,  $-(253.9 \pm 1.9)$ , and  $-(196.8 \pm 1.8)$  kJ mol $^{-1}$ , for 2-methylfuran, 5-methyl-2-acetylfuran, and 5-methyl-2-furaldehyde, respectively.

**Keywords** 2-Methylfuran · 5-Methyl-2-acetylfuran · 5-Methyl-2-furaldehyde · Energy of combustion · Enthalpy of vaporization · Standard molar enthalpy of formation · Thermochemistry

## Introduction

Furan compounds have been thoroughly studied because of their industrial importance. Furfural (furan-2-carboxaldehyde)

is cheaply prepared from ubiquitous renewable resources in the form of agricultural and forestry by-products [1]. Its major application is being used as a feedstock for furfuryl alcohol which is used in the production of thermosetting furan resins and furan cement, strong adhesive with high resistance to chemicals.

The chemistry of furan polymers represents another area of interest since both the potential availability of the monomers precursors in many countries and their renewable character represent a counterpart to petroleum-based materials [1].

The presence of furans in processed foods has recently received attention since it is considered “possibly carcinogenic to humans” by the International Agency for Research on Cancer [2]; therefore, some recent studies were made about the formation of furan and 2-methylfuran in processed foods [3–5].

This article is part of a broad study, which is being carried out in our research group, on the thermochemical properties of furan derivatives, for which we have already studied the 2-furancarboxylic acid hydrazide [6], 2-furancarboxynitrile [7], 2-acetylfuran [7], 3-furaldehyde [7], 2-furanacrylic acid [8], 3-furanacrylic acid [8], 3-(2-furyl)-2-propenal [8], and 2-furanacrylonitrile [8].

In this study, we report the standard molar enthalpies of formation of 2-methylfuran, 5-methyl-2-acetylfuran and 5-methyl-2-furaldehyde in the gaseous state, obtained by the experimental determination of the standard molar energies of combustion, measured by static bomb calorimetry, and of the enthalpies of vaporization, measured by Calvet microcalorimetry.

The results are interpreted in terms of the energetic increments for the introduction of the substituents in the furan ring.

M. A. V. Ribeiro da Silva (✉) · L. M. P. F. Amaral  
Department of Chemistry, Faculty of Science, Centro de Investigação em Química, University of Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal  
e-mail: risilva@fc.up.pt

## Experimental

### Materials

#### *Compound and purity control*

The 2-methylfuran [CAS 534-22-5], 5-methyl-2-acetylfuran [CAS 1193-79-9], and 5-methyl-2-furaldehyde [CAS 620-02-0] studied in this work were obtained commercially from Alfa Aesar with mass fractions purities of 0.98. The 2-methylfuran was purified by successive fractional distillations, whereas the 5-methyl-2-acetylfuran and 5-methyl-2-furaldehyde were purified by repeated distillations under reduced pressure. The purity of the compounds was checked by gas–liquid chromatography (GLC, HP-1890A), and from the average ratios of the mass of carbon dioxide recovered from the combustion to that calculated from the mass of sample as: 0.99974 for 2-methylfuran, 0.99966 for 5-methyl-2-acetylfuran, and 0.99964 for 5-methyl-2-furaldehyde. The densities, at  $T = 298.15$  K, were taken for 2-methylfuran as  $0.91 \text{ g cm}^{-3}$  [9], for 5-methyl-2-acetylfuran as  $1.066 \text{ g cm}^{-3}$  [9], and for 5-methyl-2-furaldehyde as  $1.107 \text{ g cm}^{-3}$  [9].

### Methods

#### *Combustion calorimetry*

The combustion experiments were performed with an isoperibol calorimetric system. The bomb calorimeter, subsidiary apparatus, and technique have been described previously in the literature [10, 11].

Combustion of certificated benzoic acid NBS Standard Reference Material, Sample 39j, was used for calibration of the bomb. Its massic energy of combustion is  $-(26434 \pm 3) \text{ J g}^{-1}$  under certificate conditions [12]. The calibration results were corrected to give the energy equivalent  $\varepsilon$  (calor) corresponding to the average mass of water added to the calorimeter: 3119.6 g. From six calibration experiments,  $\varepsilon$  (calor) =  $(15917.4 \pm 1.4) \text{ J K}^{-1}$ , where the uncertainty quoted is the standard deviation of the mean.

In all the combustion experiments,  $1.00 \text{ cm}^3$  of deionised water was introduced into the bomb, which is a twin-valve static combustion bomb, Type 1105, Parr Instrument Company, made of stainless steel with an internal volume of  $0.340 \text{ cm}^3$ . The bomb was purged twice to remove air, before being charged with oxygen, at  $p = 3.04 \text{ MPa}$ .

For all the experiments, the calorimeter temperatures were measured to  $\pm(1 \times 10^{-4}) \text{ K}$ , at time intervals of 10 s, with a quartz crystal thermometer (Hewlett Packard HP 2804A) interfaced to a PC. At least 100 readings of the temperature were taken before the ignition of the samples which were made at  $T = (298.150 \pm 0.001) \text{ K}$  by the

discharge of a  $1400\text{-}\mu\text{F}$  capacitor through the platinum ignition wire. After ignition, 100 readings were taken for each of the main and the after periods.

The liquid samples of 5-methyl-2-acetylfuran and 5-methyl-2-furaldehyde were contained in sealed polyester bags made of melinex (0.025 mm of thickness) with massic energy of combustion  $\Delta_c u^0 = -(22902 \pm 5) \text{ J g}^{-1}$  [13], a value which was confirmed in our Laboratory. The mass of melinex used in each experiment was corrected for the mass fraction of water ( $w = 0.0032$ ). The 2-methylfuran was burnt enclosed in polyethylene bags for which the energy of combustion was found to be  $\Delta_c u^0 = -(46282.44 \pm 4.77) \text{ J g}^{-1}$ . For the cotton thread fuse of empirical formula  $\text{CH}_{1.686}\text{O}_{0.843}$ , the massic energy of combustion was assigned to  $\Delta_c u^0 = -16240 \text{ J g}^{-1}$  [14], a value previously confirmed in our Laboratory.

The electrical energy for ignition was determined from the change in potential difference across the capacitor when discharged through the platinum ignition wire. The corrections for nitric acid formation were based on  $-59.7 \text{ kJ mol}^{-1}$  [15], for the molar energy of formation of  $0.1 \text{ mol dm}^{-3} \text{ HNO}_3(\text{aq})$  from  $\text{N}_2$ ,  $\text{O}_2$ , and  $\text{H}_2\text{O}(\text{l})$ . All the necessary weighing was made in a Mettler Toledo AT201 microbalance, sensitivity  $\pm(1 \times 10^{-6}) \text{ g}$ , and corrections from apparent mass to true mass were made. An estimated pressure coefficient of specific energy,  $(\partial u/\partial p)_T = -0.2 \text{ J g}^{-1} \text{ MPa}^{-1}$  at  $T = 298.15 \text{ K}$ , a typical value for most organic compounds [16], was assumed. For each compound, the massic energy of combustion,  $\Delta_c u^0$ , was calculated by the procedure given by Hubbard et al. [17]. The amount of compound used in each experiment was determined from the total mass of carbon dioxide [Mettler Toledo AT 201 balance, sensitivity  $\pm(1 \times 10^{-5}) \text{ g}$ ], produced during the experiments, taking into account that formed from the combustion of the cotton thread fuse and from melinex or polyethylene, in the cases they were used.

The relative atomic masses used throughout this article were those recommended by the IUPAC Commission in 2005 [18].

#### *High temperature microcalorimetry*

The standard molar enthalpies of vaporization of the three studied compounds were measured with a Calvet High Temperature Microcalorimeter (Setaram, HT 1000D) [19], using for the liquid compounds a similar technique [20] to that described for the sublimation of solids [21]. Samples of about 4–8 mg of liquid compound, contained in a small thin glass capillary tube sealed at one end, and a blank capillary were simultaneously dropped at room temperature into the hot reaction vessels in the Calvet high temperature microcalorimeter held at a predefined convenient temperature,  $T$ , and were removed from the hot zone by

vacuum evaporation. The thermal corrections for the glass capillary tubes were determined in separate experiments, and were minimized, as far as possible, by dropping tubes of nearly equal mass, to within  $\pm 10 \mu\text{g}$ , into each of the twin calorimeter cells.

The observed enthalpies of vaporization  $\Delta_{1,298.15\text{K}}^{g,T} H_m^0$ , were corrected to  $T = 298.15 \text{ K}$  using values of  $\Delta_{298.15\text{K}}^T H_m^0(\text{g})$  estimated by a group additivity method based on data of Stull et al. [22], where  $T$  is the temperature of the hot reaction vessel. The microcalorimeter was calibrated in situ for these measurements using the reported standard molar enthalpy of vaporization of decane [23] in the case of 2-methylfuran and undecane [24] for the other two compounds.

## Results

Detailed results for all the combustion experiments of each compound are given in Tables 1, 2, and 3, where  $\Delta m(\text{H}_2\text{O})$  is the deviation of the mass of water added to the calorimeter from 3116.9 g, the mass assigned to  $\varepsilon(\text{calor})$ , and  $\Delta U_\Sigma$  is the correction to the standard state. The remaining terms have been previously described [17]. The samples were ignited at  $T = (298.150 \pm 0.001) \text{ K}$ , with

$$\Delta U(\text{IPB}) = -\{\varepsilon_{\text{cal}} + \Delta m(\text{H}_2\text{O})c_P(\text{H}_2\text{O}, 1) + \varepsilon_f\}\Delta T_{\text{ad}} + \Delta U(\text{ign}), \quad (1)$$

where  $\Delta U(\text{IPB})$  is the energy associated to the isotherm bomb process,  $\varepsilon_f$  is the energy of the bomb contents after ignition,  $\Delta U(\text{ign})$  is the ignition energy,  $\Delta T_{\text{ad}}$  is the adiabatic temperature rise, and  $\Delta_c u^0$  is the massic energy of combustion which refers to the idealized combustion reaction yielding  $\text{CO}_2(\text{g})$  and  $\text{H}_2\text{O}(\text{l})$ . For each compound, the mean values of the massic energy of combustion  $\langle \Delta_c u^0 \rangle$ , and its standard deviation are given in the respective tables of combustion results.

Table 4 lists the derived standard molar energies and enthalpies of combustion and the standard molar enthalpies of formation for the methylfuran derivatives, in the condensed phase, at  $T = 298.15 \text{ K}$ . In accordance with normal thermochemical practice [25, 26], the uncertainties assigned to the standard molar energies and 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 used. In order to derive  $\Delta_f H_m^0(\text{l})$  from  $\Delta_c H_m^0(\text{l})$ , the standard molar enthalpies of formation of  $\text{CO}_2(\text{g})$  and  $\text{H}_2\text{O}(\text{l})$ , at  $T = 298.15 \text{ K}$ ,  $-(393.51 \pm 0.13) \text{ kJ mol}^{-1}$  [27] and  $-(285.830 \pm 0.040) \text{ kJ mol}^{-1}$  [27], respectively, were

**Table 1** Standard massic energy of combustion of 2-methylfuran at  $T = 298.15 \text{ K}$

	1	2	3	4	5	6	7
$m$ (cpd)/g	0.29270	0.40457	0.37637	0.40910	0.51184	0.49878	0.53750
$m'$ (fuse)/g	0.00280	0.00277	0.00265	0.00261	0.00276	0.00264	0.00274
$m''$ (polyethy.)/g	0.17559	0.19098	0.19667	0.21816	0.21598	0.23264	0.19198
$\Delta T_{\text{ad}}/\text{K}$	1.12077	1.39774	1.35555	1.48552	1.69265	1.71432	1.67662
$\varepsilon_f/(\text{J K}^{-1})$	16.29	16.71	16.65	16.81	17.17	17.21	17.11
$\Delta m(\text{H}_2\text{O})/\text{g}$	0.1	0.0	0.0	0.0	0.0	0.0	0.0
$-\Delta U(\text{IBP})^a/\text{J}$	17857.62	22270.99	21598.21	23669.90	26970.94	27316.35	26715.48
$\Delta U$ (polyethy.)/J	8126.73	8839.02	9102.37	10096.98	9996.08	10767.15	8885.30
$\Delta U$ (fuse)/J	45.47	44.98	43.04	42.39	44.82	42.87	44.50
$\Delta U(\text{HNO}_3)/\text{J}$	0.99	0.88	1.65	1.32	0.84	1.34	1.33
$\Delta U(\text{ign})/\text{J}$	0.85	0.75	1.19	0.69	0.71	0.67	0.64
$\Delta U_\Sigma/\text{J}$	7.12	9.51	9.04	10.02	12.06	12.06	12.19
$-\Delta_c u^0/\text{J g}^{-1}$	33062.21	33063.75	33058.19	33046.17	33051.62	33066.54	33064.48
	$\langle \Delta_c u^0 \rangle = -(33059.0 \pm 2.8) \text{ J g}^{-1}$						

<sup>a</sup>  $\Delta U(\text{IBP})$  already includes the  $\Delta U(\text{ign})$

$m(\text{cpd})$  is the mass of compound burnt in each experiment;  $m'$  (fuse) is the mass of the fuse (cotton) used in each experiment;  $m''$  (polyethy.) is the mass of the polyethylene bags;  $m''$  (melinex) is the mass of melinex bags;  $\Delta T_{\text{ad}}$  is the corrected temperature rise;  $\varepsilon_f$  is the energy equivalent of the contents in the final state;  $\Delta m(\text{H}_2\text{O})$  is the deviation of mass of water added to the calorimeter from 3119.6 g;  $\Delta U(\text{IBP})$  is the energy change for the isothermal combustion reaction under actual bomb conditions;  $\Delta U(\text{polyethy.})$  or  $\Delta U(\text{melinex})$  is the energy of combustion of the polyethylene or melinex bags;  $\Delta U(\text{fuse})$  is the energy of combustion of the fuse (cotton);  $\Delta U(\text{HNO}_3)$  is the energy correction for the nitric acid formation;  $\Delta U(\text{ign})$  is the electric energy for the ignition;  $\Delta U_\Sigma$  is the standard state correction; and  $\Delta_c u^0$  is the standard massic energy of combustion

**Table 2** Standard massic energy of combustion of 5-methyl-2-acetylfuran, at  $T = 298.15$  K

	1	2	3	4	5	6	7
$m$ (cpd)/g	0.65565	0.62776	0.68487	0.69297	0.66990	0.68290	0.66017
$m'$ (fuse)/g	0.00301	0.00227	0.00252	0.00269	0.00285	0.00251	0.00283
$m''$ (melinex)/g	0.06375	0.05915	0.06112	0.05772	0.05582	0.05716	0.05206
$\Delta T_{ad}/K$	1.28438	1.22677	1.33322	1.34293	1.29886	1.32366	1.27575
$\varepsilon_p/(J K^{-1})$	16.42	16.33	16.48	16.51	16.44	16.48	16.40
$\Delta m(H_2O)/g$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$-\Delta U$ (IBP) <sup>a</sup> /J	20464.42	19546.39	21242.75	21397.55	20695.16	21090.39	20326.89
$\Delta U$ (melinex)/J	1460.01	1354.69	1399.70	1321.80	1278.39	1309.00	1192.27
$\Delta U$ (fuse)/J	48.88	36.86	40.92	43.69	46.28	40.76	45.96
$\Delta U$ (HNO <sub>3</sub> )/J	1.00	1.43	2.24	1.10	0.96	1.10	1.33
$\Delta U$ (ign)/J	0.66	0.63	0.62	0.58	0.67	0.65	0.66
$\Delta U_{\Sigma}/J$	12.70	12.05	13.21	13.30	12.81	13.08	12.54
$-\Delta_c u^0/J g^{-1}$	28890.15	28898.56	28891.15	28886.76	28894.94	28886.30	28893.75
	$\langle \Delta_c u^0 \rangle = -(28891.7 \pm 1.7) J g^{-1}$						

<sup>a</sup>  $\Delta U$  (IBP) already includes the  $\Delta U$  (ign)

**Table 3** Standard massic energy of combustion of 2-methyl-5-furaldehyde at  $T = 298.15$  K

	1	2	3	4	5	6
$m$ (cpd)/g	0.62213	0.61671	0.68220	0.58984	0.62690	0.57683
$m'$ (fuse)/g	0.00328	0.00268	0.00254	0.00270	0.00230	0.00300
$m''$ (melinex)/g	0.05142	0.04946	0.05026	0.04900	0.05007	0.05079
$\Delta T_{ad}/K$	1.12955	1.11675	1.22900	1.07044	1.13472	1.05155
$\varepsilon_p/(J K^{-1})$	16.10	16.08	16.24	16.01	16.11	15.99
$\Delta m(H_2O)/g$	0.0	0.0	0.0	0.0	0.0	0.0
$-\Delta U$ (IBP) <sup>a</sup> /J	17996.77	17793.13	19581.77	17055.11	18079.42	16754.12
$\Delta U$ (melinex)/J	1177.65	1132.64	1151.15	1122.13	1146.81	1163.25
$\Delta U$ (fuse)/J	53.27	43.52	41.25	43.85	37.35	48.72
$\Delta U$ (HNO <sub>3</sub> )/J	1.28	1.86	1.44	1.91	0.76	1.47
$\Delta U$ (ign)/J	0.91	0.58	0.67	0.65	0.65	0.64
$\Delta U_{\Sigma}/J$	12.11	11.96	13.26	11.42	12.16	11.20
$-\Delta_c u^0/J g^{-1}$	26927.59	26922.14	26934.43	26915.43	26929.88	26922.11
	$\langle \Delta_c u^0 \rangle = -(26925.3 \pm 2.8) J g^{-1}$					

<sup>a</sup>  $\Delta U$  (IBP) already includes the  $\Delta U$  (ign)

**Table 4** Derived standard ( $p^0 = 0.1$  MPa) molar energies,  $\Delta_c U_m^0$ ; standard molar enthalpies of combustion,  $\Delta_c H_m^0$ ; and standard molar enthalpies of formation,  $\Delta_f H_m^0$  for the compounds at  $T = 298.15$  K

	$-\Delta_c U_m^0/$ kJ mol <sup>-1</sup>	$-\Delta_c H_m^0/$ kJ mol <sup>-1</sup>	$\Delta_f H_m^0(1)/$ kJ mol <sup>-1</sup>
2-Methylfuran	$2714.2 \pm 0.9$	$2716.7 \pm 0.9$	$-108.3 \pm 1.1$
5-Methyl-2-acetylfuran	$3586.6 \pm 1.1$	$3589.1 \pm 1.1$	$-311.3 \pm 1.4$
5-Methyl-2-furaldehyde	$2964.8 \pm 1.1$	$2966.0 \pm 1.1$	$-252.6 \pm 1.4$

used. Measurements of the standard molar enthalpies of vaporization are given in Table 5.

The values of the enthalpies of vaporization of each compound, at the experimental temperature  $T$ , correspond

**Table 5** Microcalorimetric standard ( $p^0 = 0.1$  MPa) molar enthalpies of vaporization at  $T = 298.15$  K

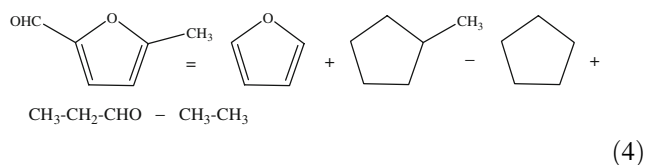
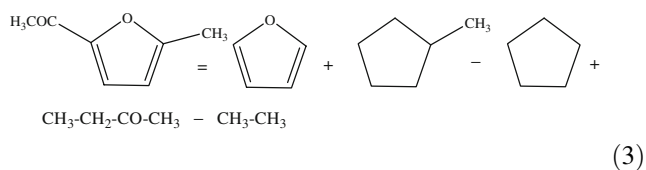
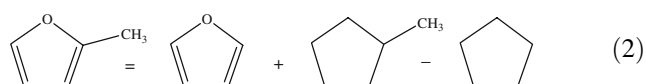
	Number of expts	$T/K$	$\Delta_1^{g,T} H_m^0(T)/$ kJ mol <sup>-1</sup>	$\Delta_{298.15K}^T H_m^0(g)/$ kJ mol <sup>-1</sup>	$\Delta_1^g H_m^0(298.15 K)/$ kJ mol <sup>-1</sup>
2-Methylfuran	6	315	$33.5 \pm 0.2$	1.62	$31.9 \pm 0.5$
5-Methyl-2-acetylfuran	6	325	$61.7 \pm 0.2$	4.26	$57.4 \pm 1.3$
5-Methyl-2-furaldehyde	6	325	$59.4 \pm 0.2$	3.58	$55.8 \pm 1.2$

to the mean values of six independent experiments, with the uncertainties given by their standard deviations of the mean. The group schemes applied for calculating the

**Table 6** Derived standard ( $p^\circ = 0.1$  MPa) molar enthalpies of formation  $\Delta_f H_m^\circ$  (g) at  $T = 298.15$  K

	$\Delta_f H_m^\circ(1)/$ $\text{kJ mol}^{-1}$	$\Delta_f^\circ H_m^\circ(298.15\text{ K})/$ $\text{kJ mol}^{-1}$	$\Delta_f H_m^\circ(\text{g})/$ $\text{kJ mol}^{-1}$
2-Methylfuran	$-108.3 \pm 1.1$	$31.9 \pm 0.5$	$-76.4 \pm 1.2$
5-Methyl-2-acetylfuran	$-311.3 \pm 1.4$	$57.4 \pm 1.3$	$-253.9 \pm 1.9$
5-Methyl-2-furaldehyde	$-252.6 \pm 1.4$	$55.8 \pm 1.2$	$-196.8 \pm 1.8$

corrections of the observed enthalpies of sublimation at the experimental temperature  $T$ , to the reference temperature of 298.15 K,  $\Delta_{\text{cr}, 298.15\text{ K}}^{\text{g}, T} H_m$ , were the ones indicated by Eqs. 2, 3, and 4, respectively, for 2-methylfuran 5-methyl-2-acetylfuran and 5-methyl-2-furaldehyde:

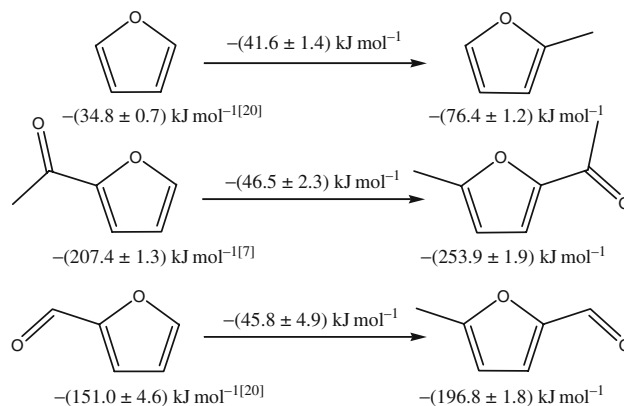
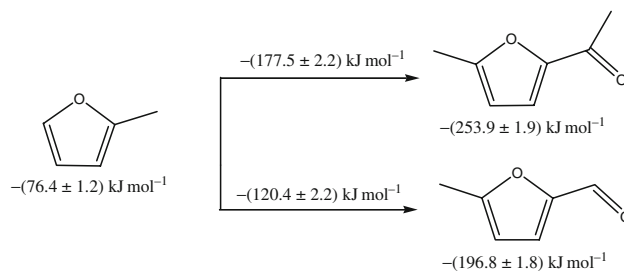


The uncertainties associated to the standard molar enthalpies of vaporization, at  $T = 298.15$  K, are twice the standard deviation of the mean and include the uncertainties associated with the calibration process.

The derived standard molar enthalpies of formation in the condensed phase, and the standard molar enthalpies of the phase transition, yield the standard molar enthalpies of formation in the gaseous phase of the three compounds, which are summarized in Table 6. The standard molar enthalpy of formation in the gaseous phase of 2-methylfuran determined in this study,  $\Delta_f H_m^\circ(\text{g}) = -(76.4 \pm 1.2)$   $\text{kJ mol}^{-1}$ , is, within the associated uncertainties, identical to that obtained from G3-calculations  $\Delta_f H_m^\circ(\text{g}) = -78$   $\text{kJ mol}^{-1}$  [28].

## Discussion

From the experimental results obtained for the standard molar enthalpies of formation of gaseous 2-methylfuran,

**Scheme 1** Enthalpic increments of the introduction of a methyl group into the *ortho* position of furan, acetylfuran, and furaldehyde**Scheme 2** Enthalpic increments of the introduction of a  $-\text{COCH}_3$  or  $-\text{CHO}$  group into the *ortho* position of methylfuran

5-methyl-2-acetylfuran, and 5-methyl-2-furaldehyde, presented in Table 6, and the literature values for furan,  $\Delta_f H_m^\circ(\text{g}) = -(34.8 \pm 0.7)$   $\text{kJ mol}^{-1}$  [23], 2-acetylfuran,  $\Delta_f H_m^\circ(\text{g}) = -(207.4 \pm 1.3)$   $\text{kJ mol}^{-1}$  [7] and 2-furaldehyde,  $\Delta_f H_m^\circ(\text{g}) = -(151.0 \pm 4.6)$   $\text{kJ mol}^{-1}$  [23], the enthalpic effects of the introduction of a methyl group in furan, 2-acetylfuran and 2-furaldehyde, are calculated and shown in Scheme 1.

The enthalpic increments found for the introduction of a methyl group are analogous within the experimental uncertainties associated.

In a similar way, using the values of standard molar enthalpies of formation determined in this study, we can calculate the enthalpic effect of the introduction of a  $-\text{COCH}_3$  or  $-\text{CHO}$  group into the *ortho* position of methylfuran as shown in Scheme 2.

Comparing the enthalpic increments obtained,  $-(177.5 \pm 2.2)$   $\text{kJ mol}^{-1}$  for the  $-\text{COCH}_3$  substitution and  $-(120.4 \pm 2.2)$   $\text{kJ mol}^{-1}$  for the  $-\text{CHO}$ , with the values for the introduction of the same groups in furan,  $-(172.6 \pm 1.5)$   $\text{kJ mol}^{-1}$  [7] and  $-(116.2 \pm 4.6)$   $\text{kJ mol}^{-1}$  [7] for the  $-\text{COCH}_3$  and the  $-\text{CHO}$ , respectively, it can be seen that the introduction of a  $-\text{COCH}_3$  or a  $-\text{CHO}$  group into the furan or methylfuran

rings are similar, within the experimental uncertainties associated, showing that the results are very consistent giving us confidence in the experimental results presented in this article.

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