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Di-hydroxybenzenes: Catechol, resorcinol, and hydroquinone Enthalpies of phase transitions revisited

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ABSTRACT

Molar enthalpies of sublimation of 1,2-di-hydroxybenzene, 1,3-di-hydroxybenzene, and 1,4-di-hydroxybenzene were obtained from the temperature dependence of the vapor pressure measured by the transpiration method. The molar enthalpies of fusion of 1,2- and 1,4-isomers were measured by differential scanning calorimetry (DSC). A large number of the primary experimental results on the temperature dependences of vapor pressure and phase transitions have been collected from the literature and have been treated in a uniform manner in order to derive sublimation, vaporization and fusion enthalpies of di-hydroxybenzenes at the reference temperature 298.15 K. The data sets on phase transitions were checked for internal consistency. This collection together with the new experimental results reported here has helped to resolve contradictions in the available thermochemical data and to recommend consistent and reliable sublimation, vaporization and fusion enthalpies for all three isomers under study.

1. Introduction

The importance of hydrogen bonding extends throughout biological and chemical systems [1]. Although *ortho*-substituted benzenes are probably the most commonly cited examples of intra-molecular hydrogen bonding, there are still not enough reliable thermodynamic data available to enable the formulation of a general rule regarding the quantitative values for its strength [2]. We have commenced studies on the thermochemical properties of *ortho*-substituted benzenes [2–4] with the aim to enlarge insight into the energetics of intra-molecular hydrogen bonds. In this work we have revisited enthalpies of sublimation of three isomeric di-hydroxybenzenes (Fig. 1), which are important as a part of the gaseous enthalpies of formation.

Vapor pressures, enthalpies of vaporization, and enthalpies of sublimation of di-hydroxybenzenes have been measured since 1927 [5] using diverse methods. We have carefully collected the primary experimental results on the temperature dependence of vapor pressure and phase transitions available in the literatures [6–23] (see Tables 1 and 2). The thermochemical database on di-hydroxybenzenes has grown considerably in the last three decades [6,7,9,10,15]. However, inspection of the sublimation enthalpies (Table 1) reveals embarrassingly, that disagreements within the data sets collected for each isomer are considerably large—about 10–15 kJ mol^{-1}. Especially disappointing is that the most recent data [6], as well as direct calorimetric studies of di-hydroxybenzenes [7] do not help to resolve contradictions within available experimental results (see Table 1). At the same time, reliable experimental data on sublimation enthalpies are required for the calculation of energetics of intra-molecular hydrogen bonding [3,24].

For the validation of the available experimental data on phase transitions of the di-hydroxybenzenes, new additional measurements have been performed using the transpiration method and differential scanning calorimetry (DSC).

2. Experimental

2.1. Materials

Samples of di-hydroxybenzenes: 1,2-di-hydroxybenzene (catechol, CAS-number 120-80-9), 1,3-di-hydroxybenzene (resorcinol, CAS-number 108-46-3) and 1,4-di-hydroxybenzene (hydroquinone, CAS-number 123-31-9) were of commercial origin (Aldrich) with a mass-fraction purity of about 0.99. They were purified by repeated fractional sublimation at reduced pressure and in darkness. Examination of the samples using GC showed no discernible amounts (greater than 0.02 mass percent) of impurities. The samples were analyzed using a Hewlett Packard gas chromatograph 5890 Series II equipped with a flame ionization detector

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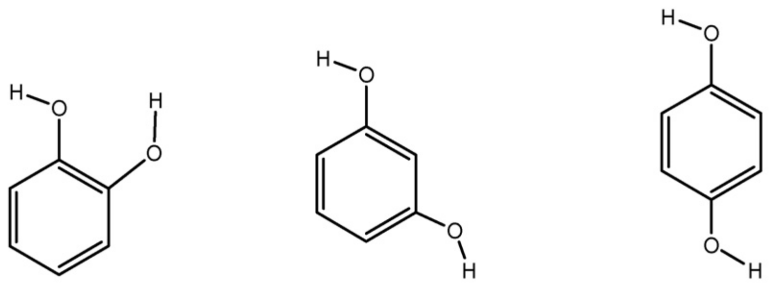

1.2-dihydroxybenzene 1.3-dihydroxybenzene 1.4-dihydroxybenzene

Fig. 1. Structure of di-hydroxybenzenes studied in this work.

and Hewlett Packard 3390A integrator. The carrier gas (nitrogen) flow was 12.1 cm^3 s^{-1}. A capillary column HP-5 (stationary phase crosslinked 5% PH ME silicone) of column length 25 m, inside diameter 0.32 mm, and film thickness 0.25 μm has been used. The standard temperature program of the GC was T = 323 K, followed by a heating rate of 0.167 K s^{-1} to T = 523 K.

2.2. Vapour pressure measurements on di-hydroxybenzenes

Vapor pressures and enthalpies of sublimation of di-hydroxybenzenes were determined using the transpiration method in a saturated N$_2$-stream and applying the Clausius–Clapeyron equation [25,26]. About 0.5 g of the sample was mixed with glass beads and placed in a thermostated U-shaped tube having a length of 20 cm and a diameter of 0.5 cm. Glass beads with diameter of 1 mm provide a surface which is sufficient enough for vapor–liquid equilibration. At constant temperature (±0.1 K), a nitrogen stream was passed through the U-tube and the transported amount of material was collected in a cooling trap. The flow rate of the nitrogen stream was measured using a soap bubble flow meter and optimized in order to reach the saturation equilibrium of the transporting gas at each temperature under study. The amount of condensed substance was determined by GC analysis using an external standard (hydrocarbon n-C$_n$H$_{2n+2}$) or by direct weighing of sample in the cold trap. The saturated vapor pressure p_i^{sat} at each temperature T_i was calculated from the amount of product collected within a definite period of time. Assuming that Dalton's law of partial pressures applied to the nitrogen stream saturated with the substance i of interest is valid, values of p_i^{sat} were calculated according to the following equation:

$$p_i^{\mathrm{sat}} = \frac{m_i R T_{\mathrm{a}}}{V M_i}; \qquad V = V_{\mathrm{N_2}} + V_i \quad (V_{\mathrm{N_2}} \gg V_i), \tag{1}$$

where R = 8.314472 J K^{-1} mol^{-1}; m_i is the mass of transported compound, M_i is the molar mass of the compound, and V_i is volume contribution of the substance i to the gaseous phase. $V_{\mathrm{N_2}}$ is the volume of transporting gas and T_{a} is the temperature of the soap bubble meter. $V_{\mathrm{N_2}}$ was determined from flow rate and time measurements.

2.3. Phase transitions in the solid state. DSC measurements

The thermal behaviour of substituted benzenes including melting temperatures and enthalpies of fusion were determined with a computer-controlled PerkinElmer DSC-2C. For all measurements, an empty pan was used as reference. The fusion temperatures and enthalpies were determined as the peak onset temperature and by using a straight baseline for integration, respectively. The temperature and heat flow rate scale of the DSC was calibrated by measuring high-purity indium (T_0 = 429.8 K and ΔH_{ref} = 28.5 J g^{-1}). The thermal behaviour of each specimen was investigated during heating the sample at a cooling rate of 10 K min^{-1}. The uncertainty for temperature is ±0.5 K and for enthalpy of fusion ±1 J g^{-1}. The DSC measurements on each sample of di-hydroxybenzenes were repeated twice and values agreed within the experimental uncertainties ±0.2 kJ mol^{-1} for the enthalpy of fusion and ±0.5 K for the melting temperature.

3. Results and discussion

3.1. Enthalpies of fusion of 1,2- and 1,4-di-hydroxybenzenes

Many hydroxy-substituted benzenes undergo phase transitions in the crystalline state. For example, 1,3-di-hydroxybenzene exhibits a α-, β-phase transition at 369 K [23]. Information about the possible phase transitions in the sample under study is indispensable for the sublimation enthalpy measurements using the transpiration method. Such knowledge helps choosing of the temperature range for investigation and allows vapor pressure measurements within the range where the compound of interest exists in only a certain crystalline modification. That is why prior to the transpiration experiments, the samples of 1,2-di-hydroxybenzenes and 1,4-di-hydroxybenzenes were carefully studied by DSC. No phase transitions other than melting of both of these compounds have been detected. Experimental values for melting temperatures and enthalpies of fusion are presented in Table 2. Our new results are in close agreement with other available data [19–23], except for those from Ref. [7].

3.2. Vapour pressure measurements on di-hydroxybenzenes

Vapor pressures of di-hydroxybenzenes obtained by the transpiration method were fitted using the following equation [25]:

$$R \ln p_i^{\mathrm{sat}} = a + \frac{b}{T} + \Delta_{\mathrm{cr}}^{\mathrm{g}} C_{\mathrm{p}} \ln\left(\frac{T}{T_0}\right) \tag{2}$$

where a and b are adjustable parameters. T_0 appearing in Eq. (2) is an arbitrarily chosen reference temperature, which has been chosen to be 298.15 K. Consequently, the expression for the sublimation enthalpy at temperature T is derived:

$$\Delta_{\mathrm{cr}}^{\mathrm{g}} H_{\mathrm{m}} T = -b + \Delta_{\mathrm{cr}}^{\mathrm{g}} C_{\mathrm{p}} T \tag{3}$$

Values of $\Delta_{\mathrm{cr}}^{\mathrm{g}} C_{\mathrm{p}}$, required for the correction of the sublimation enthalpies, have been derived according to a procedure developed by Chickos and Acree [27] using the isobaric molar heat capacities of the solid di-hydroxybenzenes $C_{\mathrm{p}}^{\mathrm{cr}}$ [28]. When the vapor pressures of liquid samples of di-hydroxybenzenes have been treated, Eqs. (2) and (3) give the expression for the vaporization enthalpy $\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$ at temperature T. Values of the isobaric molar heat capacities of liquid di-hydroxybenzenes $C_{\mathrm{p}}^{\mathrm{l}}$ and $\Delta_{\mathrm{l}}^{\mathrm{g}} C_{\mathrm{p}}$ required for the data treatment

Table 1
Compilation of data on enthalpies of sublimation $\Delta_{cr}^{g}H_m$ (298.15 K) of di-hydroxybenzenes

Technique[a]	T-range (K)	$\Delta_{cr}^{g}H_m$ (T) (kJ mol^{-1})	$\Delta_{cr}^{g}H_m$ (298 K) (kJ mol^{-1})[b]	Reference
1,2-Di-hydroxybenzene (cr)				
K	295.3–309.8	80.0 ± 0.5	80.1 ± 0.5[d]	[6]
TE	304–314	80.8 ± 1.7	81.0 ± 1.7[d]	[8]
DMC	380		86.6 ± 1.6	[9]
C	298.15		87.5 ± 0.3	[7]
T	298–353	88.7 ± 0.2	89.3 ± 0.2	[10]
T(GC)	303.2–361.5	89.6 ± 0.3	90.3 ± 0.3	This work
T(W)	317.0–377.0	88.7 ± 0.5	89.7 ± 0.5	This work
T	303.2–377.0	88.8 ± 0.3	89.7 ± 0.3[d]	This work
			88.7 ± 0.7	Average
1,2-Di-hydroxybenzene (l)[c]				
E	391.7–518.7	57.9 ± 0.2	68.7 ± 0.2	[11]
E	378.2–439.2	59.9 ± 0.3	67.3 ± 0.3	[12]
DBT	378.2–439.2	59.9 ± 0.4	70.5 ± 0.4	[13]
T	378.2–389.2	66.1 ± 0.8	71.9 ± 0.8	This work
			69.6 ± 1.0	Average
			70.0 ± 0.7[e]	This work
1,3-Di-hydroxybenzene (cr) (α-phase)				
C	334.6	85.3 ± 0.5	86.1 ± 0.5[d]	[7]
K	283–323	93.3	93.4[d]	[14]
T	328.5–368.8	93.0 ± 1.5	94.2 ± 1.5	[15]
TE	324–335	95.4 ± 1.7	96.1 ± 1.7	[8]
T	298–343	94.7 ± 0.2	95.1 ± 0.2	[10]
T	323.1–364.3	96.0 ± 0.2	96.8 ± 0.2	This work
			95.6 ± 0.6	Average
1,3-Di-hydroxybenzene (l)[c]				
DBT	419.4–527.9	70.04 ± 0.61	81.8 ± 0.6	[13]
E	392.2–463.2	71.3 ± 0.5	80.0 ± 0.5	[12]
E	424.7–549.7	67.6 ± 0.3	80.7 ± 0.3	[11]
			80.8 ± 0.5	Average
			78.4 ± 1.3[e]	This work
1,4-Di-hydroxybenzene (cr)				
K	322.8–339.4	100.6 ± 1.2	101.3 ± 1.2[d]	[6]
QFM	325.9–345.4	110.0 ± 7.0[f]	110.8 ± 7.0[d]	[5]
QFM	329.6–345.4	100.3 ± 0.7[g]	101.3 ± 0.7[d]	[5]
TE	345–358	99.2 ± 1.7	100.3 ± 1.7[d]	[8]
N/A	298.15		90.1 ± 0.9[d]	[16]
C	334.6	93.7 ± 0.5	94.5 ± 0.5[d]	[7]
S	298		103.8 ± 5.0	[17]
T	341.0–399.6	101.6 ± 0.6	103.1 ± 0.6	[15]
TE	329.8–351.2	103.9 ± 1.0	104.8 ± 1.0	[18]
T	298–353	103.9 ± 0.5	104.5 ± 0.5	[10]
T(GC)	318.4–382.4	103.5 ± 0.6	104.6 ± 0.6	This work
T(W)	343.8–381.2	103.4 ± 0.5	104.7 ± 0.5	This work
T	318.4–382.4	104.0 ± 0.3	104.9 ± 0.3[d]	This work
			104.3 ± 0.3	Average
1,4-Di-hydroxybenzene (l)[c]				
E	432.3–559.2	69.2 ± 0.3	82.8 ± 0.3	[11]
			84.4 ± 0.4[e]	This work

[a] *Techniques*: E = Ebulliometry; S = static manometer; TE = torsion effusion method; T = transpiration; W, weighing of the condensate; GC, gas-chromatographic determination of the mass of the condensate; K = Knudsen effusion method; DBT = dynamical boiling tube; DMC = "vacuum-sublimation" drop microcalorimeter; QFM = quartz fiber manometer.

[b] Original vapor pressure available in the literature were treated using Eqs. (2) and (3) in order to evaluate enthalpy of sublimation at 298.15 K in the same way as our own results in Table 3.

[c] Enthalpy of vaporization, $\Delta_{l}^{g}H_m$.

[d] Value was not taken into account for calculation of the average.

[e] Obtained as the difference of the averaged $\Delta_{l}^{g}H_m$ (this table) and the averaged $\Delta_{cr}^{l}H_m$ (from Table 2).

[f] Treatment of all four experimental points available in the Ref. [5].

[g] Treatment of three experimental points available in the Ref. [5] (the first point was rejected).

in this case have been derived according to a procedure developed by Chickos and Acree [29]. We have checked our procedure by using measurements of vapor pressures of n-alcohols [25] and substituted naphthalenes [30]. It turned out, that vapor pressures derived from the transpiration method were reliable within 1–3%. In order to assess the uncertainty of the vaporization enthalpy, the experimental data were approximated with the linear equation $\ln(p_i^{sat}) = f(T^{-1})$ using the method of least squares. The uncertainty in the enthalpy of vaporization was derived from the uncertainty in the slope of the linear correlation. Experimental results and parameters a and b according to Eq. (2) are listed in Tables 1 and 3 .

The reliability of the experimental results obtained by the transpiration method is crucially dependent on two factors: the proper flow rate of the transporting gas and the accuracy of the mass, m_i, determination in Eq. (1).

The flow rate of the nitrogen stream in the saturation tube should be not too slow in order to avoid the transport of material from the U-tube due to diffusion, and not too fast in order to reach

Table 2
Compilation of data on heat capacities and enthalpies of fusion of the di-hydroxybenzenes

Compound	C_p^{cr} ($\Delta_{cr}^{g}C_p$) (J mol^{-1} K^{-1})[a]	C_p^{l} ($\Delta_{l}^{g}C_p$) (J mol^{-1} K^{-1})[b]	$\Delta_{cr}^{l}H_m/T_{fus}$ (K) (kJ mol^{-1})	$\Delta_{cr}^{l}H_m$/298 K (kJ mol^{-1})[c]
1,2-Di-hydroxybenzene	137.4 (21.36) [28]	224.0 (68.8)	22.76/377.5 [19]	
			22.00/376.85 [20]	
			15.00/377.80[d] [7]	
			22.54/377.7 [21]	
			22.87/377.6 (this work)[e]	
			22.5 ± 0.2 (average)	18.7 ± 0.2
1,3-Di-hydroxybenzene (α-phase)	139.7 (21.71) [28]	224.0 (68.8)	21.30/382.8[d] [19]	
			20.50/381.0[d] [22]	
			15.25/383.5[d] [7]	18.3[f] [23]
			20.89/382.7 [23]	16.1[h] [20]
			18.90/382.6 [20]	
				17.2 ± 1.1[g]
1,4-Di-hydroxybenzene	136.8 (21.27) [28]	224.0 (68.8)	21.09/445.98[d] [7]	
			27.11/445.5 [19]	
			26.50/445.0 [20]	
			27.23/445.1 (this work)[e]	
			26.9 ± 0.2 (average)	19.9 ± 0.2

[a] C_p^{cr} is the molar heat capacity of crystals at constant pressure; $\Delta_{cr}^{g}C_p$ is the difference of the molar heat capacities at constant pressure for the gaseous and crystal phase, respectively.

[b] C_p^{l} is the molar heat capacity of liquid at constant pressure; $\Delta_{l}^{g}C_p$ is the difference of the molar heat capacities at constant pressure for the gaseous and liquid phase, respectively. Both values were calculated according to procedure developed by Chickos and Acree [29].

[c] The enthalpy of fusion $\Delta_{cr}^{l}H_m$ was adjusted to the reference temperature (see text).

[d] This value was not taken into account for calculation of the average.

[e] The enthalpy of fusion measured in this work using a DSC-2C, PerkinElmer (reproducibility: ±0.21 kJ mol^{-1}).

[f] A phase transition at 369.0 K with ΔH_{tr} = 1.37 kJ mol^{-1} [23]was taken into account.

[g] Average value from Refs. [20,23].

[h] A phase transition at 366.8 K with ΔH_{tr} = 1.20 kJ mol^{-1} [20]was taken into account.

the saturation of the nitrogen stream. Our apparatus was tested at different flow rates of the carrier gas in order to check the lower boundary of the flow below which the contribution of the vapor condensed in the trap by diffusion becomes comparable to the transpired one. In our apparatus the contribution due to diffusion was negligible at a flow rate up to 0.45 dm^3 h^{-1}. The upper limit for our apparatus where the speed of nitrogen could already disturb the equilibration was at a flow rate of 9.0 dm^3 h^{-1}. Thus, we performed the experiments in the flow rate interval of 1.0–5.6 dm^3 h^{-1}, which ensured that the transporting gas was in saturated equilibrium with the coexisting liquid phase in the saturation tube.

In order to check any inconsistency of the results due to the flow rate, we have studied each isomer at several gas flow rates. For instance, vapor pressures of 1,3-di-hydroxybenzene were measured at flows 1.5, 2.5, and 5.1 dm^3 h^{-1}, but the resulting vapor pressures were indistinguishable.

In order to check any inconsistency of the results due to GC determination of the mass m_i, using an external standard (hydrocarbon n-C_nH_{2n+2}), we have checked at least two different hydrocarbon standards during investigation of each isomer (see Table 3). For example, vapor pressures of 1,3-di-hydroxybenzene were studied with n-dodecane (peak of the standard eluated before main peak) as well as with n-pentadecane (peak of the standard eluated after main peak). No influence on the results was observed.

In order to check the validity of the GC determination of the mass m_i, we have performed independent experiments for 1,2- and 1,4-di-hydroxybenzene, where the transported material was collected in a special trap and amount of condensed product was determined by weighing (±0.0001 g). The results from both analytical procedures (see Tables 1 and 3) have been indistinguishable within experimental uncertainties of 1–3%.

Thus, careful studies of the two most important factors influencing the results obtained by the transpiration method have been shown not to be influencing the reproducibility and reliability of the vapor pressures.

3.3. Enthalpies of sublimation of di-hydroxybenzenes

Temperature dependencies of vapor pressures of di-hydroxybenzenes have been reported numerous times (see Table 3). However in most cases, the authors did not calculate enthalpies of sublimation from their results. That is why the original experimental results available in the literature have been treated using Eqs. (2) and (3). Sublimation enthalpies, $\Delta_{cr}^{g}H_m$ (298.15 K), have been calculated (see Table 1) for the sake of comparison with results from this work.

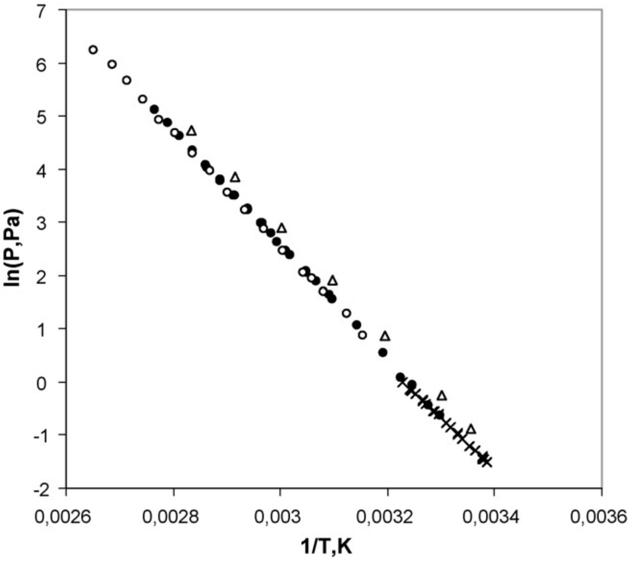

Fig. 2. Experimental data of the vapor pressures of the solid 1,2-di-hydroxybenzene. ○: this work (weighing); ●: this work (GC); △: [10]; ×: [6].

Table 3

Results for the vapor pressures p and $\Delta_{cr}^{g}H_m$ obtained by the transpiration method

T (K)[a]	m (mg)[b]	V_{N_2} (dm^3)[c]	p (Pa)[d]	$\Delta_{cr}^{g}H_m$ ($kJ\,mol^{-1}$)
1,2-Di-hydroxybenzene (cr) $\Delta_{cr}^{g}H_m$ (298.15 K) = 89.65 ± 0.28 kJ mol^{-1}				
$\ln(p\,(Pa)) = \frac{311.85}{R} - \frac{96019.16}{RT\,(K)} - \frac{21.36}{R}\ln\left(\frac{T\,(K)}{298.15}\right)$				
N_2 gas flow: 5.1 $dm^3\,h^{-1}$, external standard *n*-pentadecane				
303.2	1.42	62.00	0.53	90.19
305.3	1.33	47.04	0.65	90.14
308.0	0.79	19.21	0.95	90.08
313.2	1.12	15.08	1.72	89.97
318.2	1.26	10.00	2.90	89.87
323.5	2.93	13.17	5.10	89.75
328.1	1.35	3.87	8.00	89.66
331.3	1.51	3.25	10.63	89.59
334.1	3.10	5.08	13.94	89.53
335.3	1.89	2.67	16.19	89.50
337.2	2.52	2.92	19.74	89.46
340.2	2.83	2.54	25.47	89.40
343.3	3.00	2.08	32.88	89.33
346.3	3.15	1.67	43.27	89.27
349.5	4.87	1.87	59.37	89.20
352.6	5.04	1.50	76.87	89.13
355.6	5.58	1.25	102.0	89.07
358.6	5.46	0.958	130.2	89.01
361.6	4.24	0.583	166.2	88.94
N_2 gas flow: 2.2 $dm^3\,h^{-1}$, external standard *n*-undecane				
310.0	4.99	102.3	1.09	90.04
318.3	5.09	38.86	2.93	89.87
322.9	7.79	36.89	4.72	89.77
326.0	9.12	31.27	6.52	89.70
328.1	10.36	29.75	7.78	89.66
332.3	13.12	25.24	11.61	89.57
334.0	10.83	17.45	13.87	89.53
337.3	10.83	12.48	19.40	89.46
340.3	11.21	9.61	26.06	89.40
343.2	10.83	7.33	33.04	89.33
346.2	10.26	5.13	44.71	89.27
349.2	12.16	4.86	55.90	89.21
N_2 gas flow: 3.3–5.5 $dm^3\,h^{-1}$, weighing of condensate				
316.2	8.20	81.21	2.41	89.31
320.1	9.70	61.83	3.65	89.24
324.6	7.60	32.02	5.45	89.15
326.6	8.90	29.05	6.97	89.10
328.6	9.70	28.31	7.76	89.06
332.8	7.90	15.04	11.83	88.97
336.8	8.20	10.52	17.42	88.89
340.8	8.00	7.06	25.38	88.80
344.7	7.60	4.86	34.97	88.72
348.7	7.90	3.39	52.05	88.63
352.7	7.80	2.39	72.78	88.55
356.8	9.20	1.92	107.0	88.46
360.7	7.70	1.25	137.6	88.38
364.5	9.00	1.01	199.8	88.29
368.5	11.10	0.858	288.2	88.21
372.3	14.00	0.815	383.5	88.13
377.0	18.20	0.798	507.5	88.03
1,2-Di-hydroxybenzene (liq) $\Delta_{l}^{g}H_m$ (298.15 K) = 71.92 ± 0.79 kJ mol^{-1}				
$\ln(p\,(Pa)) = \frac{314.02}{R} - \frac{92433.21}{RT\,(K)} - \frac{68.8}{R}\ln\left(\frac{T\,(K)}{298.15}\right)$				
N_2 gas flow: 1.0 $dm^3\,h^{-1}$, external standard *n*-undecane				
378.2	23.75	0.878	604.6	66.42
378.7	10.38	0.373	621.2	66.38
379.3	16.08	0.560	641.5	66.34
380.3	11.26	0.373	673.7	66.27
381.3	9.50	0.299	710.9	66.20
382.2	8.85	0.261	756.2	66.14
383.3	7.42	0.205	807.4	66.07
384.3	5.56	0.149	831.4	66.00
385.3	6.00	0.149	897.0	65.93
386.3	5.51	0.131	942.7	65.86
387.3	4.97	0.112	990.5	65.79
389.2	3.63	0.075	1085.6	65.66

Table 3 (*Continued*)

T (K)[a]	m (mg)[b]	V_{N_2} (dm^3)[c]	p (Pa)[d]	$\Delta_{cr}^{g}H_m$ (kJ mol^{-1})
1,3-Di-hydroxybenzene (α-phase) $\Delta_{cr}^{g}H_m$ (298.15 K) = 96.75 ± 0.24 kJ mol^{-1}				
$\ln(p\,(\mathrm{Pa})) = \frac{313.82}{R} - \frac{103219.53}{RT\,(\mathrm{K})} - \frac{21.71}{R}\ln\left(\frac{T\,(\mathrm{K})}{298.15}\right)$				
N_2 gas flow: 1.5 dm^3 h^{-1}, external standard *n*-dodecane				
323.1	1.00	55.81	0.400	96.21
326.1	1.48	60.32	0.548	96.14
329.1	1.84	53.12	0.774	96.08
332.1	1.64	34.67	1.06	96.01
335.2	2.40	36.41	1.47	95.95
339.3	3.44	34.37	2.23	95.86
344.3	3.99	25.23	3.54	95.75
349.3	2.08	8.16	5.69	95.64
352.2	2.39	6.93	7.731	95.58
355.2	3.44	7.39	10.38	95.51
358.2	3.48	5.71	13.62	95.45
361.3	3.39	4.36	17.41	95.38
N_2 gas flow: 2.5 dm^3 h^{-1}, external standard *n*-dodecane				
330.1	1.19	30.30	0.881	96.06
333.3	1.77	31.97	1.24	95.99
341.2	4.20	34.621	2.72	95.82
343.5	1.16	7.62	3.41	95.77
346.2	1.52	7.41	4.58	95.71
348.3	1.48	6.01	5.53	95.66
350.3	2.03	7.08	6.43	95.62
353.3	2.03	5.23	8.71	95.55
356.3	2.03	3.99	11.41	95.49
358.6	1.55	2.47	14.04	95.44
360.2	3.85	5.35	16.10	95.40
364.3	3.30	3.17	23.30	95.32
N_2 gas flow: 5.1 dm^3 h^{-1}, external standard *n*-pentadecane				
326.7	0.41	15.38	0.617	96.13
331.2	0.28	6.75	0.966	96.03
334.2	0.39	6.62	1.34	95.97
337.1	0.43	5.29	1.86	95.91
340.3	0.41	3.67	2.54	95.84
341.3	0.49	4.16	2.71	95.81
343.3	0.50	3.37	3.40	95.77
344.4	0.55	3.46	3.67	95.75
346.4	0.62	3.04	4.68	95.70
348.4	0.66	2.75	5.56	95.66
350.2	0.71	2.51	6.49	95.62
351.3	0.76	2.37	7.32	95.60
354.3	1.14	2.67	9.84	95.53
357.4	1.52	2.79	12.58	95.47
360.4	1.02	1.46	16.07	95.40
1,4-Di-hydroxybenzene (cr) $\Delta_{cr}^{g}H_m$ (298.15 K) = 104.97 ± 0.32 kJ mol^{-1}				
$\ln(p\,(\mathrm{Pa})) = \frac{323.02}{R} - \frac{111312.58}{RT\,(\mathrm{K})} - \frac{21.27}{R}\ln\left(\frac{T\,(\mathrm{K})}{298.15}\right)$				
N_2 gas flow: 2.5 dm^3 h^{-1}, external standard *n*-dodecane				
333.2	0.81	95.03	0.191	103.83
338.2	0.81	55.60	0.326	103.73
343.2	1.15	45.06	0.569	103.62
347.2	1.38	35.96	0.856	103.54
350.2	1.88	34.77	1.21	103.47
353.3	1.44	19.77	1.63	103.41
356.2	1.29	13.64	2.12	103.34
359.3	1.77	13.27	2.99	103.28
362.2	1.88	10.12	4.15	103.22
365.2	1.96	8.16	5.38	103.15
368.2	2.26	7.19	7.01	103.09
371.2	2.30	6.08	8.45	103.02
374.2	2.40	4.89	10.99	102.96
377.2	2.09	3.22	14.48	102.90
N_2 gas flow: 5.1 dm^3 h^{-1}, external standard *n*-pentadecane				
318.4	0.16	104.3	0.035	104.15
323.2	0.15	54.47	0.062	104.05
327.3	0.25	55.71	0.103	103.96
328.2	0.22	42.67	0.116	103.94
331.1	0.42	63.55	0.153	103.88
333.3	0.22	24.51	0.202	103.83
336.2	0.32	25.10	0.293	103.77
338.2	0.31	20.60	0.344	103.73
340.4	0.20	10.88	0.425	103.68
343.3	0.26	10.52	0.575	103.62
343.5	0.26	9.79	0.616	103.61

Table 3 (*Continued*)

T (K)[a]	m (mg)[b]	V_{N_2} (dm^3)[c]	p (Pa)[d]	$\Delta_{cr}^{g}H_m$ (kJ mol^{-1})
346.3	0.22	6.65	0.774	103.55
348.5	0.28	6.57	0.989	103.51
349.5	0.24	5.23	1.070	103.49
352.5	0.28	4.18	1.518	103.42
353.3	0.31	4.12	1.702	103.41
355.5	0.39	4.22	2.119	103.36
358.5	0.34	2.75	2.848	103.29
358.6	0.63	4.77	3.050	103.29
362.7	0.83	4.31	4.414	103.21
363.3	0.35	1.80	4.504	103.19
364.7	0.53	2.51	4.846	103.16
367.7	0.72	2.47	6.734	103.10
368.3	0.44	1.37	7.308	103.09
370.8	0.62	1.63	8.768	103.03
373.3	0.59	1.30	10.501	102.98
376.3	0.78	1.26	14.263	102.92
378.4	0.53	0.687	17.624	102.87
379.4	1.02	1.26	18.591	102.85
382.4	1.09	1.05	23.837	102.79
N_2 gas flow: 3.4–5.6 dm^3 h^{-1}, weighing of condensate				
343.8	7.30	240.2	0.680	103.77
347.7	8.80	200.9	0.971	103.68
351.1	13.70	213.8	1.42	103.61
351.6	8.70	132.5	1.45	103.60
353.7	8.60	108.2	1.76	103.56
354.6	10.10	108.6	2.06	103.54
357.6	5.80	50.99	2.52	103.47
359.5	8.60	60.15	3.18	103.43
363.5	8.30	39.54	4.66	103.35
366.5	10.70	39.09	6.04	103.28
369.2	8.40	23.83	7.80	103.22
372.1	13.60	28.80	10.53	103.16
373.3	9.50	18.45	11.47	103.14
375.1	7.70	12.73	13.46	103.10
376.3	8.30	12.65	14.49	103.07
378.0	9.60	12.19	17.51	103.04
379.2	6.40	7.52	18.92	103.01
381.1	8.00	7.77	22.87	102.97
381.2	11.40	10.99	23.06	102.97

[a] Temperature of saturation. N_2 gas flow: 1.0–5.6 dm^3 h^{-1}.

[b] Mass of transferred sample condensed at T = 243 K (for GC analysis) or at T = 284 K (by weighing of condensate).

[c] Volume of nitrogen used to transfer mass m of sample.

[d] Vapor pressure at temperature T calculated from m and the residual vapor pressure at the temperature of the cold trap.

3.3.1. *Catechol (1,2-di-hydroxybenzene)*

The set of available sublimation enthalpies of catechol shows a large spread in values from 80 to 90 kJ mol^{-1} (see Table 1). Temperature dependencies of vapor pressures for the solid 1,2-di-hydroxybenzene are presented in Fig. 2. As can be seen, our vapor pressures are in acceptable agreement with the latest data measured by the effusion method [6]. Surprisingly, these data from Ref. [6] provides a sublimation enthalpy which is about 10 kJ mol^{-1} lower in comparison with ours. The vapor pressures reported by Smirnov et al. [10] are systematically higher. This data were also measured by the transpiration method, but the mass of transported compound was determined using IR-spectroscopy. One of the possible reasons for disagreement could be due to calibration of the IR method. However, in spite of a systematic deviation, the slope of the data by Smirnov et al. [10] provides a sublimation enthalpy which is in close agreement with our result (see Table 1). There are two direct calorimetric measurements of sublimation enthalpy of catechol [7,9]. Both results are slightly lower than our value (Table 1), but the difference is still acceptable within the boundaries of the experimental uncertainties. Thus, we have used results from Refs. [7,9,10] together with own new results in order to calculate the average enthalpy of sublimation $\Delta_{cr}^{g}H_m = 88.7 \pm 0.7$ kJ mol^{-1} of 1,2-di-hydroxybenzene (see Table 1).

3.3.2. *Resorcinol (1,3-di-hydroxybenzene)*

Resorcinol is a solid at room temperature with the α-crystal structure [23]. At 369 K, resorcinol transforms into a crystalline β-phase, which melts at 382.7 K [23]. In this work we have performed extended vapor pressure measurements of resorcinol on the α-phase and its appropriate enthalpy of sublimation has been obtained (see Tables 1 and 3). In contrast to our work, this phase transition was not taken into account in the very accurate work by Bender et al. [15]. For this reason we have treated their results only for the α-phase (328.5–365.8) K and rejected their two experimental points (373.2 and 379.1 K), which belongs to the β-phase. After such a correction, the sublimation enthalpy of resorcinol from Ref. [15] is now in close agreement with results from Refs. [8,10,15] as well as with our new value (see Table 1). Surprisingly, the direct calorimetric value of sublimation enthalpy published by Sabbah and Buluku [7] is about 10 kJ mol^{-1} lower (see Table 1) and we do not have any reasonable explanation for this fact. However, it should be mentioned, that disagreements of available results with those reported by Sabbah and Buluku [7] have been often found in the literatures [31,32]. Literature values for the temperature dependence of vapor pressure for solid 1,3-di-hydroxybenzene are presented in Fig. 3. As can be seen, all available vapor pressures, including our own, are in acceptable agreement. Thus, we have used results from

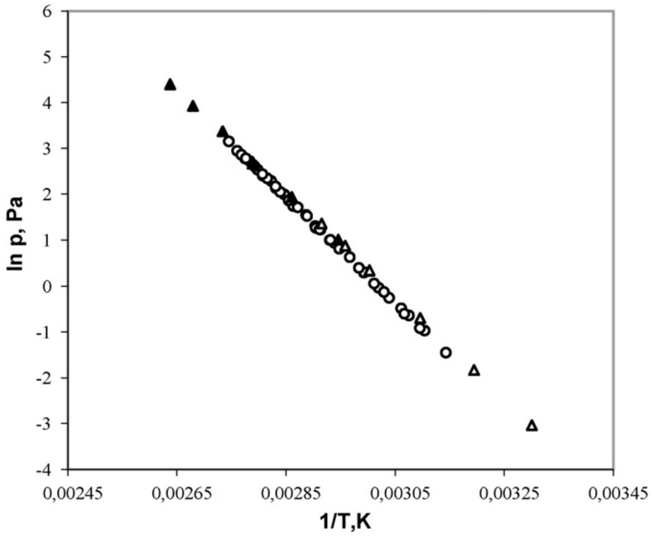

Fig. 3. Experimental data of the vapor pressures of the solid 1,3-di-hydroxybenzene. ○: this work; △: [10]; ▲: [15].

Refs. [8,10,15] together with own new results in order to calculate the average enthalpy of sublimation $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}} = 95.6 \pm 0.6\,\mathrm{kJ\,mol^{-1}}$ of 1,3-di-hydroxybenzene (see Table 1).

3.3.3. Hydroquinone (1,4-di-hydroxybenzene)

The spread of the sublimation enthalpies of 1,4-di-hydroxybenzene 90–105 kJ mol^{-1} available from the literature is confusing. Temperature dependences of vapor pressures for the solid 1,4-di-hydroxybenzene are presented in Fig. 4. As can be seen, the available vapor pressures are in acceptable agreement except for the data set from torsion–effusion [18]. Unfortunately, only smoothed data were presented in [18], and the correct comparison is not possible. However, in spite of a systematic deviation, the slope of the data from Ref. [18] provides a sublimation enthalpy which is in close agreement with our result as well as with those from Refs. [10,15,17,18] (see Table 1). The most recent vapor pressures from Knudsen effusion method [6] are also consistent with other available results. The direct calorimetric value of sublimation enthalpy published by Sabbah and Buluku [7] is again about 10 kJ mol^{-1} lower than our result (see Table 1). Thus, we have used results from Refs. [10,15,17,18] together with own new results in order to calculate the average enthalpy of sublimation $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}} = 104.3 \pm 0.3\,\mathrm{kJ\,mol^{-1}}$ of 1,3-di-hydroxybenzene (see Table 1).

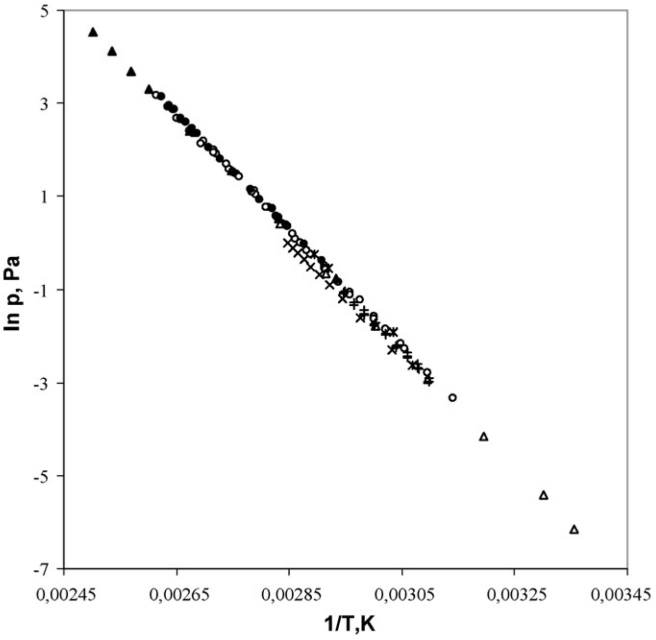

Fig. 4. Experimental data of the vapor pressures of the 1,4-di-hydroxybenzene. ○: this work (GC); ●: this work (weighing); △: [10]; ▲: [15]; +: [6]; ×: [5].

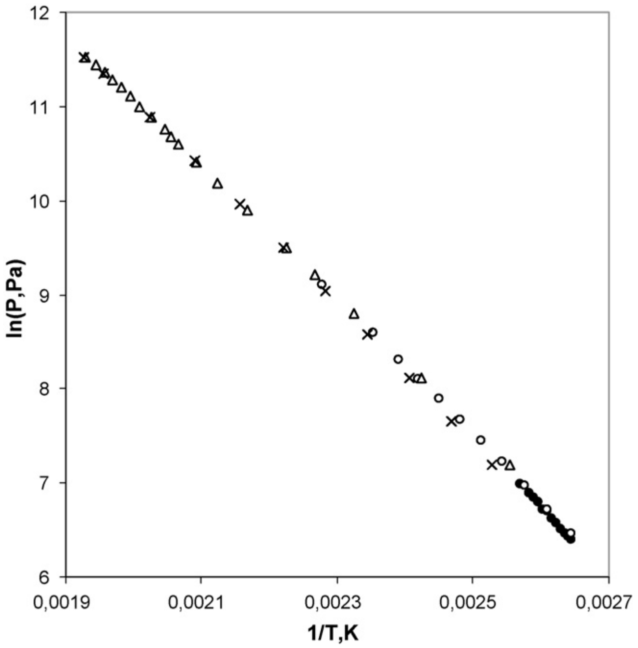

Fig. 5. Experimental data of the vapor pressures of the liquid 1,2-di-hydroxybenzene. ●: this work; ○: [12]; △: [11]; ×: [13].

3.4. Enthalpies of vaporization of di-hydroxybenzenes

The embarrassing scatters of the experimental results for $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}$ available from the literature has prompted a careful testing of our results for internal consistency. Ebulliometric vapor pressure measurements over liquid di-hydroxybenzenes could provide very important additional information to this striking situation. Because the di-hydroxybenzenes are compounds with relatively high-melting points, the measurements of vapor pressures over the liquid phase have been restricted [11–13]. The original experimental results available in the literature have been treated using Eqs. (2) and (3), and $\Delta_{\mathrm{l}}^{\mathrm{g}}H_{\mathrm{m}}$ (298.15 K) has been calculated (see Table 1) for the sake of comparison with the results from this work. We have measured vapor pressures over liquid catechol and the results are presented in Tables 1 and 3 and in Fig. 5. In contrast to the experiments in Refs. [11–13] our measurements have been performed in the temperature range close to the melting point, but they are in agreement with vapor pressures derived from other dynamic methods [11–13]. Thus, we have used results from Refs. [11–13] and the own new results and have calculated the average enthalpy of vaporization $\Delta_{\mathrm{l}}^{\mathrm{g}}H_{\mathrm{m}} = 69.6 \pm 1.0\,\mathrm{kJ\,mol^{-1}}$ (see Table 1). The available vapor pressures over the liquid 1,3-di-hydroxybenzene [11–13] are compared in Fig. 6. These data are remarkably consistent and an average enthalpy of vaporization, $\Delta_{\mathrm{l}}^{\mathrm{g}}H_{\mathrm{m}}$ (298.15 K) = 80.8 ± 0.5 kJ mol^{-1}, has been calculated (see Table 1). Only one data set of vapor pressure data over the liquid 1,4-di-hydroxybenzene was available [11]. Taking into account that the results from those [11] work were in agree-

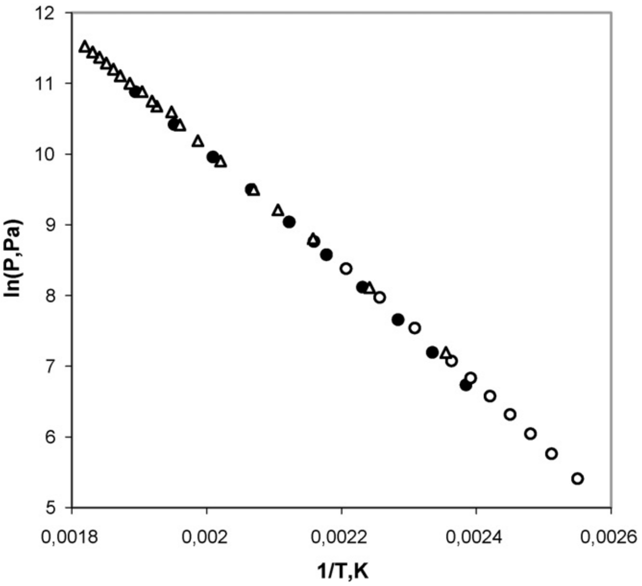

Fig. 6. Experimental data of the vapor pressures of the liquid 1,3-di-hydroxybenzene. ○: [12]; ●: [13]; △: [11].

ment for 1,2- and 1,3-isomer, the vaporization enthalpy, $\Delta_l^g H_m$ (298.15 K) = 82.8 ± 0.3 kJ mol^{-1}, calculated from the temperature dependence of vapor pressures seems to be reliable.

3.5. *Consistency tests of the experimental results*

Since a significant discrepancy in the available experimental results collected for sublimation enthalpies in Table 1 have been found, additional arguments to support the reliability of our new measurements as well as of the data sets selected for calculation of the average values, are required.

3.5.1. *Internal consistency of the vaporization, sublimation and fusion enthalpies*

A valuable test of the internal consistency of the experimental data on sublimation enthalpies, $\Delta_{cr}^g H_m$, and fusion enthalpies, $\Delta_{cr}^l H_m$, measured in this work (see Tables 1 and 2) is the comparison with the enthalpy of vaporization of di-hydroxybenzenes obtained by ebulliometry [11–13] (see Table 1) according to the general equation:

$$\Delta_l^g H_m = \Delta_{cr}^g H_m - \Delta_{cr}^l H_m \qquad (4)$$

As a rule, for comparison, all three thermodynamic quantities should be referred to the same temperature, often T = 298.15 K. But experimental enthalpies of fusion of di-hydroxybenzenes measured by DSC (see Table 2) are measured at the melting temperature T_{fus}. Because of the differences in the reference temperatures, the experimental enthalpies of fusion were adjusted to T = 298.15 K. The adjustment was calculated from the equation [33]:

$$\begin{aligned}&\{\Delta_{cr}^l H_m(T_{fus}\,(\mathrm{K})) - \Delta_{cr}^l H_m(298.15\,\mathrm{K})\}\,(\mathrm{J\,mol^{-1}})\\ &= \{(0.75 + 0.15 C_p^{cr})[T_{fus}\,(\mathrm{K}) - 298.15]\}\\ &\quad - \{(10.58 + 0.26 C_p^l)[T_{fus}\,(\mathrm{K}) - 298.15]\} \qquad (5)\end{aligned}$$

With this adjustment (the uncertainty of the correlation was not taken into account), the standard enthalpy of fusion, $\Delta_{cr}^l H_m$ (298.15 K), was calculated from the average values of the data available in Table 2. Substituting these values into Eq. (4), the vaporization enthalpies, $\Delta_l^g H_m$, can be derived independently from the difference $\Delta_{cr}^g H_m - \Delta_{cr}^l H_m$ (see Table 1, footnote d). It should be mentioned, that the values of sublimation and fusion enthalpies taken into the comparison for each isomer were those averaged in this work. As can be seen in Table 1, enthalpies of vaporization calculated according to Eq. (4) are in close agreement (within the boundaries of the experimental uncertainties) with those experimental values derived from ebulliometry. Thus, our selected results for sublimation, fusion, and vaporization enthalpies of di-hydroxybenzenes have been proven to be internally consistent.

Table 4
Comparison of vaporization enthalpies $\Delta_l^g H_m$ (298.15 K) of mono- and di-substituted benzenes in kJ mol^{-1}

	Hydroxybenzenes	Nitro-phenols
Mono-	57.7 ± 0.6 (phenol) [3]	56.1 ± 0.4 (nitrobenzene) [36]
1,4-Isomer	84.4 ± 0.7	85.4 ± 0.5 [2]
1,3-Isomer	78.4 ± 1.3	80.1 ± 0.5 [2]
1,2-Isomer	70.0 ± 0.7	58.4 ± 0.5 [2]

3.5.2. *Analysis of the vaporization enthalpies of di-hydroxybenzenes*

Comparison of enthalpies of vaporization of the *ortho*-, *meta*-, and *para*-isomers of di-hydroxybenzenes shows that the $\Delta_l^g H_m$ values of *ortho*-substituted isomer is about 8–15 kJ mol^{-1} lower (see Table 1) than those of *meta*- and *para*-isomers. Such a decrease is typical for substituted benzenes [32]. It is also obvious from Table 1, that the vaporization enthalpies of *meta*- and *para*-isomers differ by ca. 5 kJ mol^{-1}. Such behaviour is typical for the most of *meta*- and *para*-substituted benzenes [34]. This is quite understandable due to the higher symmetry of the 1,4-di-substituted benzenes, which causes a more structured liquid phase. As a consequence, somewhat more energy is required to transfer molecules in the gaseous phase in comparison with the less symmetrical 1,3-di-substituted benzene. Thus, a set of the apparently reliable experimental vaporization enthalpies is derived.

3.5.3. *Comparison of vaporization enthalpies of substituted benzenes*

Another valuable check for the validity of our selection of enthalpies of phase transitions for the di-hydroxybenzenes could be obtained by comparison of the vaporization enthalpies of di-hydroxybenzenes with those of nitro-phenols (see Table 4). Indeed, phenol and nitrobenzene have very similar enthalpies of vaporization. Hence, except for the 1,2-disubstituted benzenes (with intra-molecular hydrogen bonding), enthalpies of vaporization of 1,3- and 1,4-isomers are expected to be similar as well. As can be seen from Table 4, this expectation comes completely true – when enthalpies of vaporization of *meta*- and *para*-di-substituted benzenes are really indistinguishable, but at the same time they follow the same pattern – enthalpies of vaporization of the *meta*-isomers are slightly lower than those of the *para*-isomers. Enthalpies of vaporization of the 1,2-di-substituted benzenes are profoundly lower in comparison to 1,3- and 1,4-isomers due to intra-molecular hydrogen bonding. It is well established, that the strength of the intra-molecular hydrogen bonding in the *ortho*-nitrophenols is substantially large in comparison to *ortho*-di-hydroxybenzene. Accordingly, the vaporization enthalpies of the *ortho*-isomers follow the same logic—enthalpy of vaporization of the *ortho*-nitrophenol is substantially lower than those of the 1,2-di-hydroxybenzene (see Table 4). Thus, consistency of the set of the vaporization enthalpies selected in this work has been proven again successfully.

3.5.4. Analysis of strength of the inter-molecular hydrogen bonding in hydroxybenzenes

An additional possibility to test the consistency of the selected data is the comparison of enthalpies of vaporization of di-hydroxybenzenes (Table 1) and those of their homomorph methyl-benzenes. Such a test could be performed in the manner we suggested recently [3] for comparison of the enthalpies of vaporization of the di-hydroxybenzenes. Indeed, for methyl-benzenes only non-associating inter-molecular van der Waals' interactions determine the values of their enthalpies of vaporization. Enthalpies of vaporization of methyl-benzenes which are obtained by subsequently replacing the OH-group by a CH_3-group will essentially represent the non-associative contribution of the arenol to its enthalpy of vaporization. The difference of the enthalpies of vaporization between di-hydroxybenzene, and its homomorph, di-methylbenzene, presents a crude measure of the contribution to the enthalpy of vaporization of the self-association of alcohols and arenols [3,25].

Following this pattern, experimental data on the enthalpies of vaporization of di-hydroxybenzenes at 298.15 K (Table 1) are compared with those $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}$ (298.15 K) of their homomorphs (di-methylbenzenes), available from the literature [35]: 1,3-di-methylbenzene 42.7 kJ mol^{-1}, 1,4-di-methylbenzene 42.4 kJ mol^{-1}, and methyl-benzene 38.1 kJ mol^{-1}. For the 1,3-di-hydroxybenzene and 1,4-di-hydroxybenzene, these differences could be interpreted as the contribution to the enthalpy of vaporization of self-association. In other words these differences are a rough measure for the strength of the inter-molecular hydrogen bonding in these species. It is obvious, that 1,3-di-hydroxybenzene and 1,4-di-hydroxybenzene possess two inter-molecular hydrogen bonds. Thus, enthalpic differences for these molecules, divided with the number of bonds (for 1,3-di-hydroxybenzene $(42.7 - 78.4)/2 = -17.9$ kJ mol^{-1}; for 1,4-di-hydroxybenzene $(42.4 - 84.4)/2 = -20.8$ kJ mol^{-1}), provide an averaged value of -19.9 kJ mol^{-1} as an assessment of the strength of the inter-molecular hydrogen bond in di-hydroxybenzenes. This value is constant with the strength of the inter-molecular hydrogen bond ($38.1 - 57.7 = -19.7$ kJ mol^{-1}) obtained in a similar way for the mono-hydroxybenzene (phenol).

4. Conclusion

This investigation was undertaken to establish a consistent set of vapor pressures, sublimation, vaporization, and fusion enthalpies of di-hydroxybenzenes. We collected from the literature a large number of the primary experimental results and treated them uniformly in order to derive the appropriate enthalpies at the reference temperature 298.15 K. This collection, together with our new own results have been used to select reliable values for the enthalpies of the phase transition of the di-hydroxybenzenes. This data will be useful for evaluation of the gaseous enthalpies of formation of di-hydroxybenzenes and for quantification of the intra-molecular hydrogen bonding in the forthcoming work.

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