

# Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K

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Vapor pressures of ethylene glycol, hydroxyacetaldehyde, and hydroxyacetone were measured by using a standard closed system equipped with a vacuum line, built recently in our laboratory. First, our vapor pressures measurements of ethylene glycol and their excellent agreement with the literature in the studied temperature range, that is, (308 to 385) K, permitted us to validate our experimental setup and procedure. The data obtained in the temperature ranges of (296 to 356) K and (273 to 304) K were very satisfactorily (absolute relative deviations (ARD) < 2.5 %) fitted according to the Antoine's equation:  $\log_{10}(P^{\circ}_{\text{hydroxyacetaldehyde}}/\text{Pa}) = 12.96 \pm 0.82 - (3657 \pm 238)/(T/\text{K})$  and  $\log_{10}(P^{\circ}_{\text{hydroxyacetone}}/\text{Pa}) = 10.13 \pm 0.06 - (2201 \pm 153)/(T/\text{K})$ . Then, the resulting vapor pressures of both hydroxyacetaldehyde and hydroxyacetone at 293 K were  $P^{\circ} = (3.0 \pm 0.2)$  Pa and  $P^{\circ} = (415 \pm 20)$  Pa for hydroxyacetaldehyde and hydroxyacetone, respectively. The quoted errors correspond to  $2\sigma$  obtained from the least-squares fit analysis and the estimated systematic relative error of 5 %. Finally, these experimental expressions of temperature dependences of  $P^{\circ}$  then permitted the derivation of the enthalpy of vaporization for both compounds.

## Introduction

Hydroxyacetone ( $\text{HOCH}_2\text{C}(\text{O})\text{CH}_3$ ) and hydroxyacetaldehyde ( $\text{HOCH}_2\text{CHO}$ ) are atmospheric pollutants of particular interest. Hydroxyacetone is produced in the atmosphere mainly from the OH-initiated oxidation of isoprene, the main nonmethane hydrocarbon in the troposphere.<sup>1–3</sup> Hydroxyacetaldehyde, usually named glycolaldehyde, is also formed in situ in the atmosphere from the oxidation of several volatile organic compounds including ethene, 2-methyl-3-buten-2-ol, and isoprene.<sup>4–7</sup> Once produced in the atmosphere, these two hydroxyl carbonyl compounds have a potentially large atmospheric impact, since they lead, in the upper troposphere, to  $\text{HO}_x$  radicals known to increase the oxidizing capacity of the atmosphere, and therefore they can influence the ozone budget.<sup>8</sup>

So far, hydroxyacetaldehyde and hydroxyacetone have not been considered to be significant aerosol constituents, since it is assumed that these compounds have relatively high vapor pressures. However, recent field observations indicate that they are important atmospheric aerosol constituents. For example, Matsunaga et al.<sup>9</sup> provide evidence that hydroxyacetone and hydroxyacetaldehyde (and methylglyoxal) contribute significantly to organic aerosols, (10 to 120) Tg annually. These findings have been confirmed, at least for hydroxyacetaldehyde, by Angove et al.<sup>10</sup> in a smog chamber experiment. Note that, in this work, Angove et al.<sup>10</sup> report an estimated value of 5.3 kPa for the equilibrium vapor pressure  $P^{\circ}$  of hydroxyacetaldehyde at 298 K, while Butler et al.<sup>11</sup> report also an estimated value of 4 Pa at room temperature. These two estimated values differ by more than two orders of magnitude. The situation is even worse for hydroxyacetone, for which, to our knowledge, only an estimated upper limit exists, that is,  $P^{\circ} < 0.5$  kPa at room temperature.<sup>12</sup>

The precise knowledge of the equilibrium vapor pressure of a component is important to predict its partitioning between the gas and particle phases in the atmosphere.<sup>13</sup> In addition, the saturation vapor pressure  $P^{\circ}$  can also be used to estimate Henry's law constant that represents the partitioning between the gas and the aqueous phases at equilibrium. These partitionings are key physical properties to understand and predict the behavior of a component in the environment.<sup>14–16</sup>

The main goal of this work is therefore to provide accurate experimental vapor pressures for both hydroxyacetone and hydroxyacetaldehyde. For this, our experimental setup based on previous static devices<sup>17</sup> was built and validated by vapor pressure measurements of ethylene glycol between (308 and 385) K.

## Experimental Section

**Chemicals.** Ethylene glycol (> 99.5 %) and solid hydroxyacetaldehyde dimer (> 99 %) were purchased from Merck and Aldrich, respectively. Hydroxyacetone (> 95 %) was provided by Alfa Aesar. Before use, hydroxyacetaldehyde dimer was melted at temperatures ranging between (80 and 90) °C for more than 2 h to obtain the hydroxyacetaldehyde monomer.<sup>18</sup> The hydroxyacetaldehyde monomer was then kept as limpid liquid even when temperature decreased typically down to 293 K.

To eliminate the effect of gaseous impurities, all of the compounds were further purified by freeze–pump–thaw cycles using liquid nitrogen/ethanol baths at different temperatures and a vacuum pump (< 0.02 Pa).

**Apparatus and Procedure.** The experimental setup, shown schematically in Figure 1, is a static vapor–liquid equilibrium apparatus. It consists of a Pyrex flask containing the solid or liquid sample, connected to the vacuum line with a glass/metal connection (Caburn MDC). It includes also a thermostatic bath, temperature and pressure measurement devices, and a vacuum system.

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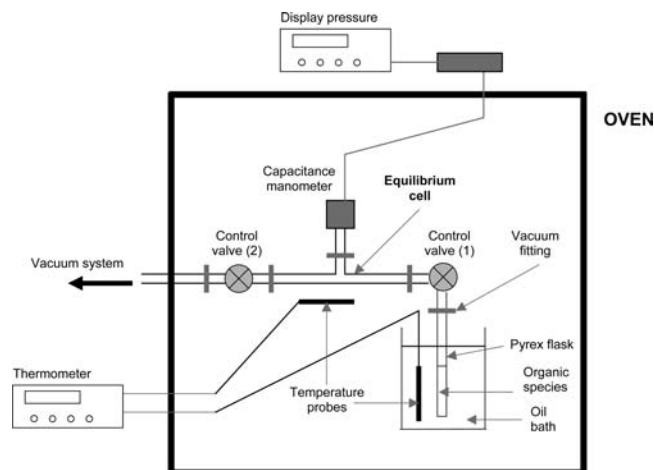


Figure 1. Schematic diagram of the vapor pressure apparatus.

The pressure was measured in the equilibrium cell by a capacitance manometer (Edwards, 622 barocel, ranges from (0 to 1000) Pa and (0 to 10000) Pa) coupled to a digital indicator (BOC Edwards) giving uncertainties of  $(0.1 + 0.15 P/P^*)$  Pa and  $(1 + 0.15 P/P^*)$  Pa, where  $P^* = 100$  Pa, for (0 to 1000) Pa and (0 to 10000) Pa ranges, respectively.

Except for the vacuum system, the entire device was placed in an oven maintained at a temperature slightly higher than that of the oil bath in which the Pyrex flask was immersed, to avoid any vapor condensation on the tube walls. Both bath and oven temperatures were measured with thermocouples K coupled to a laboratory thermometer (Allcat Instruments) having an accuracy of  $\pm 0.25\%$  of the reading values in degrees Celsius. In addition, the thermocouples were calibrated by the manufacturer a few months before the measurements and were checked by dipping them into an ice bath maintained to 273.15 K.

The vacuum system (not shown) is composed of a combination of a turbo-molecular/vacuum pump (Edwards high vacuum, type EXC120/type RV8) and a liquid nitrogen trap. Two control valves allow either isolating the sample from the vacuum system (control valve 1) or isolating the equilibrium cell from the vacuum system, leading to the establishment of an equilibrium between the liquid and the gas phases (control valve 2).

## Results and Discussion

**Ethylene Glycol.** The vapor pressure of ethylene glycol was measured in the temperature range of (308 to 385) K to validate the experimental setup.

After degassing of ethylene glycol in situ in the pyrex flask, the measurements of the saturation vapor pressure were performed by first establishing a highly stable vacuum in the equilibrium cell. The control valve (2) was then rapidly closed, allowing the establishment of equilibrium between the liquid phase and the gas phase, while the pressure values in the equilibrium cell were monitored on a computer. Figure 2 illustrates a typical data plot obtained for a given temperature (here at 326.1 K).

As shown in Figure 2 (see solid line), the pressure increased quickly at the beginning of the experiment, and after a time scale of about 15 min, it leveled off, meaning that the liquid phase reached equilibrium with the gas phase. Nevertheless, when this equilibrium was reached, the pressure continued to slowly increase linearly with time because of the presence of leaks (see dash-dot-dot line in Figure 2). This leak is specific to equipment used in our system, that is, vacuum fittings with

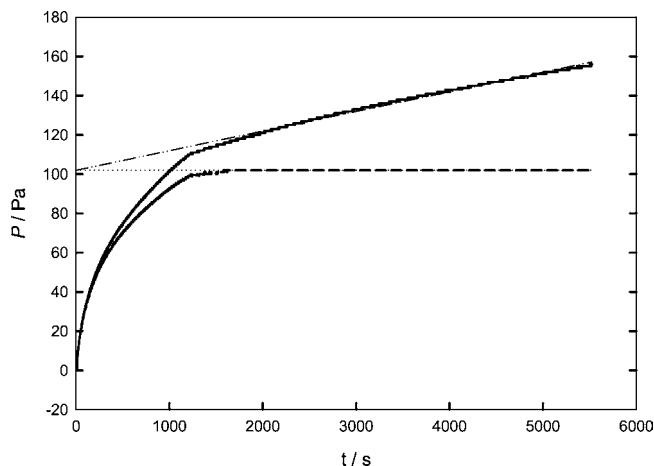


Figure 2. Plot of both  $P$  (solid line) and  $P_{\text{corrected}}$  (short dash line) recorded as a function of time during an experiment performed on ethylene glycol at 326.1 K. The leak rate is determined from the slope of the linear asymptote (dash-dot-dot line).

Table 1. Experimental Vapor Pressures of Ethylene Glycol Measured in This Work and Comparison with the Literature<sup>a</sup>

$T$ K	$P_{\text{lit}}^b$ Pa	$P^c$ Pa	$100 \cdot \Delta P^d / P^d$
307.7 ( $\pm 0.1$ )	26 ( $\pm 1$ )	28 ( $\pm 1$ )	0.81
312.6 ( $\pm 0.1$ )	39 ( $\pm 2$ )	41 ( $\pm 2$ )	1.30
316.5 ( $\pm 0.1$ )	52 ( $\pm 3$ )	55 ( $\pm 3$ )	2.52
318.8 ( $\pm 0.1$ )	62 ( $\pm 3$ )	61 ( $\pm 3$ )	5.12
322.1 ( $\pm 0.1$ )	79 ( $\pm 4$ )	77 ( $\pm 4$ )	5.38
326.1 ( $\pm 0.1$ )	124 ( $\pm 6$ )	124 ( $\pm 6$ )	0
328.2 ( $\pm 0.1$ )	128 ( $\pm 6$ )	137 ( $\pm 23$ )	0.74
334.5 ( $\pm 0.2$ )	192 ( $\pm 10$ )	196 ( $\pm 13$ )	2.11
335.2 ( $\pm 0.2$ )	201 ( $\pm 10$ )	201 ( $\pm 14$ )	0.11
340.2 ( $\pm 0.2$ )	282 ( $\pm 14$ )	278 ( $\pm 19$ )	0.37
347.9 ( $\pm 0.2$ )	464 ( $\pm 23$ )	454 ( $\pm 32$ )	0.03
359.2 ( $\pm 0.2$ )	923 ( $\pm 46$ )	900 ( $\pm 58$ )	1.32
367.9 ( $\pm 0.2$ )	1528 ( $\pm 76$ )	1483 ( $\pm 91$ )	1.98
373.4 ( $\pm 0.2$ )	2086 ( $\pm 104$ )	1950 ( $\pm 131$ )	1.02
384.5 ( $\pm 0.2$ )	3772 ( $\pm 189$ )	3467 ( $\pm 236$ )	1.29

<sup>a</sup>  $100 \cdot \Delta P^d / P^d$  corresponds to the percentage deviation between experimental and literature values. <sup>b</sup> The quoted uncertainties correspond to the  $2\sigma$  level + 5% where  $\sigma$  is the standard deviation of the linear fit of the plot of  $\log_{10} P_{\text{lit}}$  versus  $1/T$ .<sup>19</sup> <sup>c</sup> The quoted uncertainties correspond to the  $2\sigma$  level + 5%. <sup>d</sup> The deviation between the experimental and the literature values is defined as follows:  $\Delta P^d / P^d = (P^o - P_{\text{lit}}^o) / P^o$ .

Viton seals (NW references, Edwards). The pressure reading at a given experimental time was then corrected by subtracting the leak contribution as follows:

$$P_{\text{corrected}} = P - vt \quad (1)$$

where  $P$  is the reading pressure,  $v$  is the leak rate, and  $t$  is the time from the beginning of experiment.

The leak rate  $v$  was obtained from the slope of the linear part of the plot of  $P$  versus  $t$  (see dash-dot-dot line in Figure 2). The plot of the resulting corrected pressures (see solid line in Figure 2) reaches now a horizontal plateau that corresponds to the saturation vapor  $P^o$  at a given temperature.

Similar experiments were repeated for temperatures ranging between (308 and 385) K (see Table 1). The relative errors on the vapor pressure measurements correspond to  $2\sigma + 5\%$ , where  $\sigma$  is obtained from the least-squares linear fit analysis and 5% is the estimated systematic relative error. The resulting relative errors varied between (5 and 7) %.

Since the plot of  $\log_{10} P^o$  versus  $1/T$  showed a linear behavior (see Figure 3), the results were fitted according to a simplified Antoine's equation:

$$\log_{10}(P^\circ/\text{Pa}) = (12.02 \pm 0.72) - \frac{3257 \pm 204}{(T/\text{K})}$$

where the quoted errors correspond to  $2\sigma$  obtained from the least-squares linear fit analysis and the estimated systematic relative error of 5 %.

The absolute relative deviation (ARD) was defined as follows:

$$\text{ARD} = \frac{1}{n} \sum_{i=0}^n \left[ \frac{|P^\circ - P^\circ_{\text{calc}}|}{P^\circ} \right]_i \quad (2)$$

where  $n$  is the total number of experimental data points and  $P^\circ_{\text{calc}}$  is the calculated vapor pressure.

According to eq 2, the ARD value is less than 2 %. It appears therefore that our data can be conveniently fitted according to the simplified Antoine's equation.

The vapor pressure of ethylene glycol derived from the experimental simplified Antoine's equation is  $P^\circ = (8.02 \pm 0.41)$  Pa at 293 K.

The enthalpy of vaporization  $\Delta_{\text{vap}}H$  is constant for the investigated temperature range. This, later, derived from the slope of  $\log_{10} P^\circ$  versus  $1/T$ , is then found to be  $(62.4 \pm 4.0)$   $\text{kJ}\cdot\text{mol}^{-1}$ .

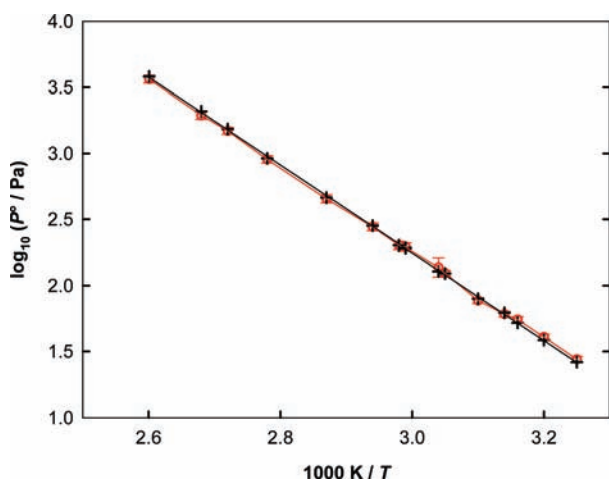
**Comparison with the Literature.** The equation derived from the literature<sup>19</sup> in the same temperature range is:

$$\log_{10}(P^\circ_{\text{lit}}/\text{Pa}) = (12.22 \pm 0.69) - \frac{3325 \pm 193}{(T/\text{K})}$$

The calculated literature values<sup>19</sup> are summarized in Table 1 together with our experimental values ( $P^\circ$ ). Our extrapolated experimental value at 293 K ( $P^\circ = 8.02 \pm 0.41$  Pa) is in good agreement with that of Stull ( $P^\circ_{\text{lit}} = 7.45 \pm 0.38$  Pa) at the same temperature. In the temperature range of (308 to 385) K, the differences between the two sets of data are at most 5 %, indicating that our experimental setup is suitable to measure equilibrium vapor pressure with good accuracy.

Similarly, our vaporization enthalpy of  $(62.4 \pm 4.0)$   $\text{kJ}\cdot\text{mol}^{-1}$  is consistent with the literature values of  $65.6 \pm 0.3$   $\text{kJ}\cdot\text{mol}^{-1}$ ,<sup>20</sup>  $67.6$   $\text{kJ}\cdot\text{mol}^{-1}$ ,<sup>21</sup> and  $61.9$   $\text{kJ}\cdot\text{mol}^{-1}$ .<sup>22</sup>

**Hydroxyacetone and Hydroxyacetaldehyde.** Once the setup was validated, saturation vapor pressures of hydroxyacetaldehyde and hydroxyacetone were measured in the temperature ranges of (296 to 356) K and (273 to 304) K, respectively. The



**Figure 3.** Comparison for vapor pressures of ethylene glycol measured from this study (red circles) and those from literature<sup>19</sup> (black cross) and the resulting fits using the simplified Antoine's equation (see solid lines). The quoted uncertainties on experimental data correspond to  $2\sigma$  level + 5 % (see text).

**Table 2.** Experimental Vapor Pressures of Both Hydroxyacetaldehyde and Hydroxyacetone Measured in This Work<sup>a</sup>

hydroxyacetaldehyde			hydroxyacetone		
$T$	$P^\circ$	$100 \cdot \Delta P^\circ / P^\circ$ <sup>b</sup>	$T$	$P^\circ$	$100 \cdot \Delta P^\circ / P^\circ$ <sup>b</sup>
K	Pa		K	Pa	
295.85	3.7 ( $\pm 0.2$ )	0.44	273.22	127 ( $\pm 9$ )	3.26
305.10	9.0 ( $\pm 0.5$ )	5.24	275.48	136 ( $\pm 9$ )	4.73
305.51	9.6 ( $\pm 1.2$ )	2.26	277.78	162 ( $\pm 11$ )	2.59
319.50	33 ( $\pm 3$ )	2.72	278.55	167 ( $\pm 11$ )	4.44
319.84	33 ( $\pm 3$ )	0.00	278.55	172 ( $\pm 11$ )	1.55
322.38	37 ( $\pm 3$ )	6.37	280.90	201 ( $\pm 42$ )	0.48
323.64	46 ( $\pm 3$ )	2.06	281.69	205 ( $\pm 13$ )	3.52
327.73	62 ( $\pm 5$ )	1.38	281.69	210 ( $\pm 13$ )	1.47
333.04	98 ( $\pm 10$ )	4.01	289.86	356 ( $\pm 21$ )	1.74
339.32	154 ( $\pm 9$ )	2.14	290.70	360 ( $\pm 21$ )	2.25
340.91	170 ( $\pm 10$ )	0.74	290.70	363 ( $\pm 21$ )	1.23
341.95	182 ( $\pm 12$ )	0.15	290.70	360 ( $\pm 21$ )	2.25
342.82	198 ( $\pm 15$ )	2.57	293.26	431 ( $\pm 25$ )	0.84
346.83	253 ( $\pm 18$ )	1.33	295.86	516 ( $\pm 30$ )	3.83
355.98	486 ( $\pm 26$ )	2.00	295.86	495 ( $\pm 29$ )	0.10
			296.74	531 ( $\pm 31$ )	1.90
			300.30	617 ( $\pm 35$ )	3.04
			301.20	642 ( $\pm 36$ )	4.05
			302.11	717 ( $\pm 40$ )	2.03
			303.03	746 ( $\pm 42$ )	1.06
			303.95	817 ( $\pm 46$ )	4.96

<sup>a</sup> The quoted uncertainties correspond to the 2s level + 5 %. <sup>b</sup> The individual deviation  $\Delta P^\circ / P^\circ$  is calculated as follows:  $\Delta P^\circ / P^\circ = ((P^\circ - P^\circ_{\text{Antoine}}) / P^\circ)$  where  $P^\circ_{\text{Antoine}}$  is calculated from the simplified Antoine's equation and  $P^\circ$  is the experimental value.

results are listed in Table 2. The relative uncertainties on the measurements varied between (5 and 13) % for hydroxyacetaldehyde and (5 and 7) % for hydroxyacetone.

The vapor pressures were fitted according to the Antoine's equation:

$$\log_{10}(P^\circ(\text{hydroxyacetaldehyde})/\text{Pa}) = (12.97 \pm 1.70) - \frac{3668 \pm 1101}{(T/\text{K}) + (0.45 \pm 48)}$$

$$\log_{10}(P^\circ(\text{hydroxyacetone})/\text{Pa}) = (10.12 \pm 2.88) - \frac{2193 \pm 1657}{(T/\text{K}) - (0.46 \pm 10)}$$

where the quoted uncertainties correspond to  $1\sigma$  obtained from the least-squares fit analysis.

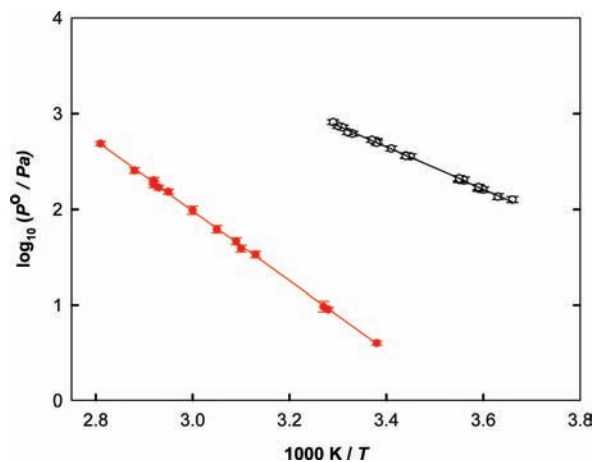
Similarly to ethylene glycol, the data of  $\log_{10} P^\circ$  versus  $1/T$  can conveniently be fitted, as shown in Figure 4, with a two-parameter Antoine's equation:

$$\log_{10}(P^\circ(\text{hydroxyacetaldehyde})/\text{Pa}) = (12.96 \pm 0.82) - \frac{3657 \pm 238}{(T/\text{K})}$$

$$\log_{10}(P^\circ(\text{hydroxyacetone})/\text{Pa}) = (10.13 \pm 0.06) - \frac{2201 \pm 153}{(T/\text{K})}$$

where the quoted errors correspond to  $2\sigma$  obtained from the least-squares fit analysis and include a estimated systematic relative error of 5 %.

Again, the values of ARD, determined according to eq 2 and found to be equal to 2.0 % and 2.5 % for hydroxyacetone and hydroxyacetaldehyde, respectively, confirm that the experimental values can be conveniently fitted according to the simplified Antoine's equation. These equations then permit the derivation of the vapor pressures of both hydroxyacetaldehyde and hydroxyacetone at 293 K, which were  $P^\circ = (3.0 \pm 0.2)$  Pa and  $P^\circ = (415 \pm 20)$  Pa for hydroxyacetaldehyde and hydroxyacetone, respectively.



**Figure 4.** Plot of  $\log_{10}(P^\circ/\text{Pa})$  as a function of  $1000/T$  for: ● (solid red circle), hydroxyacetaldehyde; ○, hydroxyacetone. The solid lines correspond to the fit using the simplified Antoine's equation. The quoted uncertainties on experimental data correspond to the  $2\sigma$  level + 5 % (see text).

Similarly to ethylene glycol, the enthalpies of vaporization of both compounds were derived from the Clausius–Clapeyron's equation:  $\Delta_{\text{vap}}H(\text{hydroxyacetaldehyde}) = (70 \pm 5) \text{ kJ}\cdot\text{mol}^{-1}$  and  $\Delta_{\text{vap}}H(\text{hydroxyacetone}) = (42 \pm 3) \text{ kJ}\cdot\text{mol}^{-1}$ .

**Comparison with the Literature.** As noted in the introduction, the literature data concerning the vapor pressures of hydroxyacetaldehyde and hydroxyacetone are rather limited. For the determination of the millimeter- and submillimeter-wave spectrum of hydroxyacetaldehyde, Butler et al. estimated that the vapor pressure at room temperature was roughly  $4 \text{ Pa}^{11}$  which is in good agreement with our determination of  $(3 \pm 1) \text{ Pa}$  at  $293 \text{ K}$ . On the contrary, Angove et al. reported an estimated value of about  $5300 \text{ Pa}$  at  $298 \text{ K}$ , a value three orders of magnitude higher than our determination,  $(4.9 \pm 0.3) \text{ Pa}$  at  $298 \text{ K}$ . Besides, in measurements of UV absorption cross section, Magneron et al. used partial pressures as high as  $66 \text{ Pa}$  at  $298 \text{ K}$  and  $2100 \text{ Pa}$  at  $333 \text{ K}$ .<sup>23</sup> If this value obtained at  $333 \text{ K}$  is roughly consistent with the vapor pressure of  $980 \text{ Pa}$  found in this work, their value reported at  $298 \text{ K}$  is approximately 20 times higher than our absolute determination. These discrepancies might be due to the presence of volatile impurities in hydroxyacetaldehyde in their study, while they were removed, in the current work, after obtaining of hydroxyacetaldehyde monomers, by freeze–pump–thaw cycles.

Similarly, in experiments dedicated to Raman spectroscopy, the vapor pressure of hydroxyacetone was estimated to be less than  $500 \text{ Pa}$  at room temperature.<sup>12</sup> This reported upper limit is consistent with our determination of  $(415 \pm 20) \text{ Pa}$  at  $293 \text{ K}$ .

## Conclusion

Our static device was tested to measure the vapor pressure of ethylene glycol, and the obtained data show an excellent agreement with those reported in the literature.

We have then measured the vapor pressures of hydroxyacetone and hydroxyacetaldehyde as a function of temperature. These data are the first direct measurements for these two compounds. They will be particularly valuable in laboratory studies where they are often necessary.

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