

Heats of Combustion of Butanal and Some Related Compounds

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Heats of combustion values have been determined and from these, heat of formation data at 25°C calculated in kcal.mole⁻¹ for the following six carbon-hydrogen-oxygen compounds:

2-butenal ($\Delta H_f^\circ = -34.45 \pm 0.09$), butanal ($\Delta H_f^\circ = -57.06 \pm 0.17$), butanol-1 ($\Delta H_f^\circ = -79.55 \pm 0.10$), 2-ethyl-2-hexenal ($\Delta H_f^\circ = -62.46 \pm 0.17$), 2-ethyl-hexenal ($\Delta H_f^\circ = -83.32 \pm 0.18$), 2-ethyl-hexanol-1 ($\Delta H_f^\circ = -103.46 \pm 0.19$).

Precise data on heats of combustion of aliphatic aldehydes are lacking in the literature, and since the appearance of Kharasch's compilation¹ no further determinations have been published. Therefore it was judged of interest to study a number of aliphatic aldehydes, the choice of compounds being mainly governed by an interest in the aldol condensation reaction and associated processes for butanal.

Verkade and Coops² have accurately determined the heats of combustion of the lower 1-alkanols. However, a redetermination for butanol-1 was performed in order to ascertain the internal consistency within this investigation**. No value of the heat of combustion of 2-ethyl-hexanol-1 has been found in the literature.

SAMPLE PURITY

It was found difficult to obtain the aldehydes in a very pure state. Before describing the special problems met with in handling the aldehydes, the general procedure for preparing the samples for combustion will be given.

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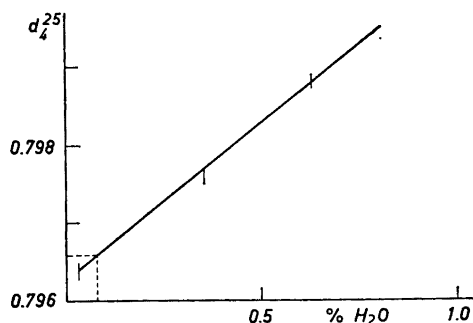
** Verkade and Coops' value recalculated³ to present day units is $\Delta H_c^\circ(\text{butanol-1}) = -638.25 \pm 0.32$ kcal.mole⁻¹, and the value given in this paper is $\Delta H_c^\circ(\text{butanol-1}) = -638.25 \pm 0.10$ kcal.mole⁻¹.

Table 1. Density of butanal *versus* water content.

Water %	d_4^{25} g · ml ⁻¹
x	$0.7966_0 \pm 0.0000_8$
$x + 0.275$	$0.7976_1 \pm 0.0000_8$
$x + 0.551$	$0.7988_3 \pm 0.0000_8$

Procedure. All six substances used in this investigation were prepared and carefully purified by the Research Laboratory, Mo och Domsjö AB, Örnköldsvik, Sweden. After the final distillation in a Podbielniak column with 50–70 theoretical plates, samples of the main fraction were enclosed in sealed Pyrex-glass ampoules in an atmosphere of carbon dioxide or helium. The purity was established using gas-liquid chromatographic technique on the contents of one of these ampoules, and a number of ampoules were sent to our laboratory. Immediately upon arrival (2–3 days later) a distillation was performed at room temperature under reduced pressure. All samples were handled in a nitrogen atmosphere and great care was taken to exclude air. The middle fraction from this distillation (about one third of the total sample) was collected in a receiver where *ca.* 10 combustion ampoules (made from soft glass) had been placed in advance, and then the ampoules were filled ⁴ immediately. At the same time ampoules were filled with samples for gas-liquid chromatographic analysis and for density determination. The combustions were made as soon as possible, and in no case did more than six days elapse between ampoule filling and combustion. In the case of butanal all experiments were carried out within two days. Analysis (by Mo & Domsjö) and density determination were performed so as to coincide in time with the middle experiment in the combustion series.

The gas-liquid chromatographic analysis was done in order to determine the amount of impurities, especially water. For all substances except butanal the area under the water peak of the chromatogram was proportional to the water content of the sample, which was found from calibration experiments with known amounts of water added to the sample. The linearity implies that no reaction leading to the formation of water occurred on the column. In the

Fig. 1. Density of butanal *versus* water content.

case of butanal, however, a reaction took place on the column forming water and organic impurities.

The water content of the butanal sample was evaluated using the observation that the density of a sample of this compound was found to vary linearly with the water content, at least within a small interval. A sample of butanal was prepared exactly as the material for combustion. This sample was divided into three parts and water was added to two of them, increasing the amount of water by 0.275 resp. 0.551 %. The densities of the three parts were determined, Table 1. The slope of the line, density *versus* per cent water, was calculated, and the line was drawn (Fig. 1) using the value of Smith and Bronner⁵: $d_4^{25} = 0.7964$ at 0.03 % water. As indicated by dotted lines in the diagram the density 0.7966 then corresponds to a water content of 0.08 ± 0.02 %.

Special problems. The unsaturated aldehydes studied were found to be stable during storage in Pyrex-glass ampoules for two weeks. However, distillation at temperatures higher than *ca.* 50°C caused rapid decomposition. These compounds were found to be very sensitive to oxidation; and it was therefore necessary to exclude all traces of air in handling them.

Butanal was found to be unstable even when every precaution was taken in storing the samples. The decomposition was followed by measuring the density, and an increase in d_4^{25} of 0.00003 per day was observed. Distillation of butanal above room temperature caused an increase in water content and in amounts of other impurities. When distillation was performed at room temperature with the receiver kept at -40 to -80°C , the distillate showed a marked tendency to polymerize to solid products. A few successful distillations were performed with the receiver kept at -20°C and the distilling flask at 35°C (pressure 40–50 mm Hg).

In a number of cases condensation of butanal took place within the sealed combustion ampoule, which then invariably burst*. This was shown by the following series of experiments. Twelve ampoules (of the combustion type) were filled with butanal and left to stand for some days. During this time several ampoules burst and now and then one of the intact ampoules was opened. The refractive index** of the content was immediately determined for both cases and was found unchanged for all intact ampoules, but altered for every broken ampoule, usually about 0.002 units.

The handling of 2-ethyl-hexanal offered the same kind of difficulties as did butanal but to a much smaller extent. Distillation could be performed at 85°C and 35 mm Hg, and gas-liquid chromatography was successfully run at 150°C . With the alcohols of this investigation no special problems were met, and the analyses showed that perfect purity was obtained in both cases.

Results of purity determinations. In Table 2 values of densities and amounts of impurities have been summarized. As a comparison, density values found in the literature have also been given.

* In a few cases the ampoule burst in the bomb during filling with oxygen. The butanal then exploded, and in a separate experiment it was found that oxygen caused the butanal to explode at a pressure of 12 atm.

** The small amount of substance in an ampoule made a density determination impossible, and therefore refractive indices were chosen as an aid to follow the purity.

Table 2. Sample purity.

Substance	d_4^{20} g · ml ⁻¹	d_4^{25} g · ml ⁻¹	H ₂ O %	Org.matter %	Literature
2-Butenal	0.8526	0.8475	0.02	0.05	$d_4^{17,8} = 0.8557$ ⁶
Butanal	—	0.7966	0.08	—	$d_4^{25} = 0.7964/0.03$ % H ₂ O ⁵
Butanol-1	0.8099	0.8059	0	0	$d_4^{25} = 0.8057$ ⁷
2-Ethyl-2-hexenal	0.8522	0.8461	0.014	0.4	$d_4^{25} = 0.8528$ ⁸
2-Ethyl-hexanal	0.8201	0.8156	0.03	0.7	$d_4^{18} = 0.8231$ ⁹
2-Ethyl-hexanol-1	0.8332	0.8291	0	0	$d_4^{20} = 0.8328$ ¹⁰

The organic impurity of 2-butenal was small enough to be neglected, but this was not the case with 2-ethyl-2-hexenal. Three organic impurities gave traces on the chromatogram, but one of them made up for 75 % of the total amount. This one was isolated with the aid of a preparative column and examined by infrared spectroscopy. The spectrogram was compared with that of 2-ethyl-2-hexenal and differences were found on three frequencies, namely 979 cm⁻¹ had changed to 969 cm⁻¹; 1 202 cm⁻¹ to 1 180 cm⁻¹ and at 1 730 cm⁻¹ a new absorption peak appeared. The impurity was most certainly 2-ethyl-3-hexenal, and its presence would not affect the heat of combustion value to a noticeable extent. The organic impurity found in 2-ethyl-hexenal was thought to be formed during analysis. The peak on the chromatogram corresponding to this impurity was always found when analysing samples from different steps of the purification process and was always of the same relative size, while all other impurity-peaks gradually disappeared. As the purification involved distillations at different pressures, the presence of an azeotropic mixture was not likely.

COMBUSTION CALORIMETRY

All calorimetric quantities are expressed in terms of the defined calorie which is equal to 4.1840 absolute joules. All weighings have been reduced to mass. The molecular weight for each compound has been given in the Tables and is based upon the 1954 International Atomic Weights.

In this work the symbols introduced by Hubbard, Scott and Waddington ¹¹ have been used.

Apparatus and method. The calorimetric system of Bjellerup ¹² was used with the difference that his rotating bomb was replaced by a static one of the same construction. The aldehydes showed a marked tendency for splashing upon ignition, and therefore a platinum baffle was used together with a platinum shield ⁴. Paraffin oil of known heat of combustion ¹³ was used as an ignition aid. The amount of HNO₃ formed was determined by titration with NaOH.

In each experiment the calorimeter vessel was filled with water until a fixed total weight of calorimeter with mounted bomb was reached, and the energy equivalent of the system was calculated using the following principles ¹². The result of the calibration (see below) is reported as ϵ° which is the theoretical energy equivalent (in cal.deg⁻¹) of the calorimeter with mounted, empty,

Table 3. Calibration.

$t_h = 25.0^\circ\text{C}$, $t_l = 24.1^\circ\text{C}$, $P^i(\text{Gas}) = 30.0 \text{ atm}$, $V(\text{Bomb}) = 0.2751 \text{ l}$, $V^i(\text{water}) = 0.000820 \text{ l}$, $\Delta E_c/M$ (Benzoic acid) = $-6\,317.83 \pm 0.62 \text{ cal} \cdot \text{g}^{-1}$, $m(\text{Pt}) = 29.790 \text{ g}$, $\Delta E_c^o/M$ (Fuse) = $3\,971 \pm 4 \text{ cal} \cdot \text{g}^{-1}$

m' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$\varepsilon^o(\text{calor})$ cal · deg ⁻¹
0.824826	0.005553	42.23	0.88885	1.13	5 927.08
0.826326	0.005858	42.20	0.89059	0.78	5 927.16
0.826176	0.005785	42.20	0.89034	1.39	5 928.10
0.825124	0.005468	42.20	0.88899	1.44	5 928.21
0.825990	0.005809	42.20	0.88996	0.40	5 928.29
0.824832	0.005695	42.20	0.88894	0.72	5 926.67
0.825694	0.005692	42.20	0.88979	1.40	5 927.91

$\varepsilon^o(\text{calor}) = 5\,927.63 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$ Mean 5 927.63
 Stand. dev. of mean 0.24

bomb and filled with water until the fixed total weight. In an actual experiment $m^i(\text{Cont})$ grams (total substance, oxygen, ampoule, water and loose platinum parts) are introduced into the bomb, and the amount of calorimeter water must be reduced accordingly in order to maintain the fixed total weight. The energy equivalent of the system is thus diminished by $C_p(\text{H}_2\text{O}) \cdot m^i(\text{Cont}) \text{ cal} \cdot \text{deg}^{-1}$, and at the same time the energy equivalent $\varepsilon^i(\text{Cont})$ of the added bomb content must be taken into account. The total energy equivalent of the calorimetric system will therefore be:

$$\varepsilon^o(\text{calor}) - C_p(\text{H}_2\text{O}) \cdot m^i(\text{Cont}) + \varepsilon^i(\text{Cont}) \text{ cal} \cdot \text{deg}^{-1}$$

Calibration. The calorimetric system was calibrated by burning benzoic acid (National Bureau of Standards Standard Sample 39 g) under specified conditions¹⁴, and the calibration combustions are reported in Table 3.

Heats of combustion and formation. The six combustion series are reported Tables 4 to 9. The found heat of combustion value for a sample containing x % water was called $\Delta E_c^o/M$ (in $\text{cal} \cdot \text{g}^{-1}$) and the heat of combustion of the pure compound has been calculated thus:

$$\Delta E_c^o/M = \frac{100}{100 - x} \cdot \Delta E_c^o/M \text{ cal} \cdot \text{g}^{-1}$$

Washburn corrections were applied as described by Hubbard, Scott and Waddington¹¹. No accurate information concerning the heat capacities of the substances was available. For butanol-1 the value $0.7 \text{ cal} \cdot \text{g}^{-1} \cdot \text{deg}^{-1}$ was used and for the other five compounds $0.5 \text{ cal} \cdot \text{g}^{-1} \cdot \text{deg}^{-1}$. Anticipating an error in these values of $0.2 \text{ cal} \cdot \text{g}^{-1} \cdot \text{deg}^{-1}$ a value of the uncertainty introduced into the heat of combustion determinations was found to be 0.05 cal per combustion, *i.e.* $0.1 \text{ cal} \cdot \text{g}^{-1}$ in the $\Delta E_c^o/M$ values. This uncertainty could therefore be neglected in the calculations.

Table 4. 2-Butenal (containing 0.02 % water).

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P^i(\text{Gas}) = 28.5 \text{ atm}$, $V(\text{Bomb}) = 0.2751 \text{ l}$, $V^i(\text{water}) = 0.000820 \text{ l}$, $\epsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.762 \text{ g}$, $\Delta E_c^\circ/M (\text{Oil}) = -1\,0979.6 \pm 0.9 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E^\circ/M (\text{Fuse}) = -3\,971 \pm 4 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 2.18 \text{ cal}$, $M' = 70.092 \text{ g} \cdot \text{mole}^{-1}$.

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c'/M$ cal · g ⁻¹
0.420223	0.175318	0.005772	41.73	0.88735	2.79	7 790.10
0.416744	0.179539	0.005815	41.66	0.89040	2.21	7 788.19
0.408634	0.178871	0.005343	41.62	0.87792	0.76	7 789.02
0.415021	0.176115	0.005425	41.65	0.88137	1.06	7 789.46
0.441231	0.159940	0.005605	41.65	0.88633	2.17	7 791.34
0.435677	0.157640	0.005594	41.69	0.87459	1.65	7 791.14

Mean 7 789.88
Stand. dev. of mean 0.50

$$\Delta E_c'/M = -7\,789.9 \text{ cal} \cdot \text{g}^{-1}$$

$$\Delta E_c^\circ/M = -7\,791.4 \text{ cal} \cdot \text{g}^{-1}$$

Table 5. Butanal (containing 0.08 % water).

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P^i(\text{Gas}) = 30.0 \text{ atm}$, $V(\text{Bomb}) = 0.2751 \text{ l}$, $V^i(\text{water}) = 0.000820 \text{ l}$, $\epsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.692 \text{ g}$, $\Delta E_c^\circ/M (\text{Oil}) = -1\,0979.6 \pm 0.9 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_c^\circ/M (\text{Fuse}) = -3\,971 \pm 4 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 1.72 \text{ cal}$, $M' = 72.108 \text{ g} \cdot \text{mole}^{-1}$.

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c'/M$ cal · g ⁻¹
0.417289	0.163881	0.004594	42.11	0.88990	1.36	8 196.91
0.407458	0.171305	0.004868	42.12	0.89038	1.51	8 198.56
0.372048	0.193951	0.004177	42.11	0.88255	1.14	8 194.94

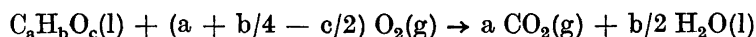
Mean 8 196.80
Stand. dev. of mean 1.13 *

$$\Delta E_c'/M = -8\,196.8 \text{ cal} \cdot \text{g}^{-1}$$

$$\Delta E_c^\circ/M = -8\,203.4 \text{ cal} \cdot \text{g}^{-1}$$

* Another series using less pure substance gave the same precision, so it was felt permissible to use only three values for obtaining the standard deviation.

ΔH_c° values were computed from the ΔE_c° values. If the combustion reaction is:



this relation holds:

$$-\Delta H_c^\circ = -\Delta E_c^\circ - (\text{b}/4 - \text{c}/2) \cdot 0.592 \text{ kcal} \cdot \text{mole}^{-1}$$

Table 6. Butanol-1.

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P_i(\text{Gas}) = 30.0\text{ atm}$, $V(\text{Bomb}) = 0.2751\text{ l}$, $V^i(\text{water}) = 0.000820\text{ l}$, $\epsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24\text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.762\text{ g}$, $\Delta E_c^\circ/M$ (Oil) = $-1\,0979.6 \pm 0.9\text{ cal} \cdot \text{g}^{-1}$, $\Delta E_c^\circ/M$ (Fuse) = $-3\,971 \pm 4\text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 1.49\text{ cal}$, $M' = 74.124\text{ g} \cdot \text{mole}^{-1}$

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c/M$ cal · g ⁻¹
0.385950	0.168523	0.005271	42.21	0.88161	2.96	8 593.34
0.365678	0.181195	0.005454	42.16	0.87557	1.01	8 595.43
0.390181	0.166171	0.005834	42.18	0.88379	2.39	8 595.06

$\Delta E_c^\circ/M = -8\,594.6\text{ cal} \cdot \text{g}^{-1}$	Mean Stand. dev. of mean	8 594.61 0.64
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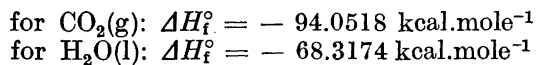
Table 7. 2-Ethyl-2-hexenal (containing 0.014 % water).

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P_i(\text{Gas}) = 30.0\text{ atm}$, $V(\text{Bomb}) = 0.2751\text{ l}$, $V^i(\text{water}) = 0.000820\text{ l}$, $\epsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24\text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.764\text{ g}$, $\Delta E_c^\circ/M$ (Oil) = $-1\,0979.6 \pm 0.9\text{ cal} \cdot \text{g}^{-1}$, $\Delta E_c^\circ/M$ (Fuse) = $-3\,971 \pm 4\text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 1.88\text{ cal}$, $M' = 126.200\text{ g} \cdot \text{mole}^{-1}$

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c/M$ cal · g ⁻¹
0.454216	0.088487	0.005031	42.16	0.88147	1.87	9 238.25
0.489861	0.063730	0.005127	42.18	0.89155	1.10	9 242.87
0.469287	0.078639	0.005934	42.17	0.88752	1.26	9 240.40
0.459681	0.087428	0.005704	42.18	0.88864	1.24	9 241.10
0.467358	0.082095	0.005348	42.17	0.89054	1.14	9 241.78
0.457202	0.089691	0.005328	42.18	0.88879	1.14	9 242.28

$\Delta E_c^\circ/M = -9\,241.1\text{ cal} \cdot \text{g}^{-1}$	Mean Stand. dev. of mean	9 241.11 0.67
$\Delta E_c^\circ/M = -9\,242.4\text{ cal} \cdot \text{g}^{-1}$		

Heats of formation were calculated using the heat of formation values at 25°C^{15} :



Final overall standard deviations were computed by the method of Bjelle-rup¹⁶ and include the errors of (i) the heat of combustion value for benzoic acid, (ii) the calibration experiments, (iii) the paraffin oil combustions, (iv) the determination of mass including water analysis and finally (v) the standard deviation of the actual combustion series.

Table 8. 2-Ethyl-hexanal (containing 0.03 % water).

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P(\text{Gas}) = 30.0 \text{ atm}$, $V(\text{Bomb}) = 0.2751 \text{ l}$, $V(\text{water}) = 0.000820 \text{ l}$, $\varepsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$ in all experiments except the fourth where $\varepsilon^\circ(\text{calor}) = 5\,935.48 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.516 \text{ g}$, $\Delta E_c^\circ/M$ (Oil) = $-1\,0979.6 \pm 0.9 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_c^\circ/M$ (Fuse) = $-3\,971 \pm 4 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 1.70 \text{ cal}$, $M' = 128.216 \text{ g} \cdot \text{mole}^{-1}$

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c^\circ/M$ cal · g ⁻¹
0.409769	0.113481	0.004335	41.87	0.87338	1.18	9 463.74
0.435605	0.093896	0.004083	41.87	0.87808	1.27	9 461.74
0.446309	0.085515	0.004645	41.90	0.88011	1.21	9 462.86
0.422621	0.107697	0.004037	41.87	0.88172	1.38	9 461.17
0.433487	0.094669	0.004231	41.90	0.87634	1.82	9 462.06
0.443856	0.090238	0.004371	41.87	0.88488	1.55	9 463.36
0.413009	0.115624	0.004799	41.86	0.88260	1.58	9 458.61
0.439658	0.108168	0.004788	41.89	0.91189	2.55	9 461.79
0.439684	0.089070	0.004654	41.87	0.87641	2.48	9 464.18

Mean 9 462.17

Stand. dev. of mean 0.56

$\Delta E_c^\circ/M = -9\,462.2 \text{ cal} \cdot \text{g}^{-1}$

$\Delta E_c^\circ/M = -9\,465.0 \text{ cal} \cdot \text{g}^{-1}$

Table 9. 2-Ethyl-hexanol-1.

$t_h = 25.0^\circ\text{C}$, $t_i = 24.1^\circ\text{C}$, $P(\text{Gas}) = 30.0 \text{ atm}$, $V(\text{Bomb}) = 0.2751 \text{ l}$, $V(\text{water}) = 0.000820 \text{ l}$, $\varepsilon^\circ(\text{calor}) = 5\,927.63 \pm 0.24 \text{ cal} \cdot \text{deg}^{-1}$, $m(\text{Pt}) = 29.758 \text{ g}$, $\Delta E_c^\circ/M$ (Oil) = $-1\,0979.6 \pm 0.9 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_c^\circ/M$ (Fuse) = $-3\,971 \pm 4 \text{ cal} \cdot \text{g}^{-1}$, $\Delta E_\Sigma = 1.31 \text{ cal}$, $M' = 130.232 \text{ g} \cdot \text{mole}^{-1}$

m' g	m'' g	m''' g	$m^i(\text{cont})$ g	Δt deg	$\Delta E(\text{HNO}_3)$ cal	$-\Delta E_c^\circ/M$ cal · g ⁻¹
0.427374	0.100038	0.004245	42.11	0.89256	1.42	9 684.30
0.401689	0.114704	0.004867	42.10	0.87829	1.45	9 687.24
0.459568	0.062875	0.004255	42.10	0.87654	1.32	9 688.60
0.459179	0.064999	0.004276	41.85	0.87974	1.22	9 687.57
0.450269	0.079140	0.004574	41.87	0.89176	1.74	9 687.88
0.447457	0.076646	0.004430	41.88	0.88214	1.85	9 684.34
0.407624	0.100577	0.004097	41.85	0.86099	2.17	9 682.99

Mean 9 686.13

Stand. dev. of mean 0.83

$\Delta E_c^\circ/M = -9\,686.1 \text{ cal} \cdot \text{g}^{-1}$

Table 10. Thermochemical data, referring to the liquid standard state at 25°C.

Compound	$-\Delta E_c^\circ/M$ cal · g ⁻¹	$-\Delta E_c^\circ$ kcal · mole ⁻¹	$-\Delta H_c^\circ$ kcal · mole ⁻¹	$-\Delta H_f^\circ$ kcal · mole ⁻¹
2-Butenal	7 791.4 ± 1.2	546.12 ± 0.09	546.71 ± 0.09	34.45 ± 0.09
Butanal	8 203.4 ± 2.3	591.53 ± 0.17	592.42 ± 0.17	57.06 ± 0.17
Butanol-1	8 594.6 ± 1.3	637.07 ± 0.10	638.25 ± 0.10	79.55 ± 0.10
2-Ethyl-2-hexenal	9 242.4 ± 1.3	1 166.39 ± 0.17	1 168.17 ± 0.17	62.46 ± 0.17
2-Ethyl-hexanal	9 465.0 ± 1.4	1 213.56 ± 0.18	1 215.63 ± 0.18	83.32 ± 0.18
2-Ethyl-hexanol-1	9 686.1 ± 1.4	1 261.44 ± 0.19	1 263.81 ± 0.19	103.46 ± 0.19

The uncertainties given are the final overall standard deviations.

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