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Note

Enthalpy of formation of L-serine in the solid state

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Carrying on our studies on thermochemical properties of nitrogen compounds, we report here the enthalpy of combustion and formation of crystalline L-serine. Despite its biological importance, no thermochemical data have been reported for the compound except in the paper of Hutchens et al.[1] where an estimated value of ΔH_f^0 (c, 298.15 K) is given. Such data will be necessary if quantitative studies on energetics of biochemical reactions are made.

EXPERIMENTAL

Apparatus and procedure

The apparatus and experimental procedure are similar to those described previously[2] except the outer jacket temperature which is now controlled by an electronic regulator to ± 0.002°C at 24.78°C. The samples were burnt in a Parr 1004 C stainless-steel combustion bomb with platinum lining. The internal volume of the bomb is 350.6 ml. This bomb was initially filled with oxygen at 30 atm. Air Liquide ultrahigh purity grade oxygen (N 45) was used without further treatment. The sample pellets were weighed to an accuracy better than 0.005 mg and corrections for air buoyancy applied.

10 ml of water were placed in the bomb and a cotton thread was used as fuse, its heat of combustion has been found to be $-(16.502 \pm 0.041)$ kJ g^{-1} (mean and standard deviation).

The extent of combustion was based on the mass of the sample. All calculations, including conversion of time and temperature measurements to initial and final temperature, correction for heat exchange between calorimeter and jacket and reduction to the standard state, were carried out with a computer. The computer programme followed the procedure of Hubbard et al.[3].

Materials

L-serine was obtained from Koch-Light and had a claimed purity better than

99%. It was further purified by recrystallization from its aqueous solution and dried under vacuum (P # 10^{-2} Torr) until the weight loss of the sample was negligible.

The calorimeter was calibrated with benzoic acid, NBS sample 39i, which had a heat of combustion ΔU_c^0 (c) = − (26.414 ± 0.003) kJ g^{-1}.

RESULTS

Units of measure and auxiliary quantities

All data reported are based on the 1973 atomic weights[4]. For reducing weights in air to weights in vacuum and correcting to standard states, the values for density ρ, specific heat cp and $(\partial u/\partial p)_T$ for the substances were summarized in Table 1.

TABLE 1

PHYSICAL PROPERTIES FOR THE SUBSTANCES AT 298.15 K

Substance	ρ(g ml^{-1})	cp(J K^{-1} g^{-1})	$-(\partial u/\partial p)_T$/(J atm^{-1} g^{-1})[a]
L-serine	1.561	1.322	(0.013)
Benzoic acid	1.320	1.209	0.012
Fuse	1.5	1.7	0.029

[a] 1 atm   101.325 k Pa.

The density of L-serine was measured with a pycnometer filled with oil. The specific heat value of L-serine was measured using the drop method and a Tian-Calvet calorimeter. The value of $(\partial u/\partial p)_T$ in parentheses is estimated. All other values are taken from the literature.

Calorimetric results

The apparent energy equivalent of the calorimeter U (calor.), was determined from twelve calibration runs. The average value was (15108.2 ± 1.7) J K^{-1} where the uncertainty is expressed as the standard deviation of the mean. Ten satisfactory combustion experiments were obtained for L-serine, some of them were carried out in the presence of benzoic acid as an auxiliary material. No difference was observed in the results (Table 2). Another observation was done. Since the rise of temperature ΔT for a run is included in the value of ΔT obtained in calibration experiments, there is apparently no effect on the result if initial and final temperatures are not the same for all runs.

Derived results

Values of the enthalpy of combustion ΔH_c^0 (c, 298.15 K) derived from the mass of the sample and current best values[5] of the enthalpies of formation of gaseous carbon dioxide [ΔH_f^0 (g, 298.15 K)] = − (393.51 ± 0.13) kJ mol^{-1} and liquid water

TABLE 2

SUMMARY OF COMBUSTION EXPERIMENTS FOR L-SERINE

Mean values and standard deviations of the means: ΔU_c^0 (c, 298.15 K) = − (1448.83 ± 0.18) kJ mol^{-1}
ΔH_c^0 (c, 298.15 K) = − (1448.21 ± 0.18) kJ mol^{-1}
ΔH_f^0 (c, 298.15 K) = − (732.73 ± 0.28) kJ mol^{-1}

m(sub) (g)	m(aux sub) (g)	m(cot) (g)	m(Pt) (g)	m(HNO_3) (mol)	θ_i (°C)	θ_f (°C)	ΔT (K)	$-\Delta U_{IBP}$ (J)	$-w_1$ [a] (J)	w_2 [a] (J)	$-\Delta U_c^0$ (kJ mol^{-1})	$-\Delta H_c^0$ (kJ mol^{-1})	$-\Delta H_f^0$ (kJ mol^{-1})
1.710698		0.001574	3.816444	9.80 10^{-4}	23.47449	25.04038	1.56400	23714	26	92	1449.58	1448.96	731.97
1.228715		0.001476	3.563886	6.67	23.87852	25.00282	1.12312	17029	24	63	1448.96	1448.34	732.59
1.801381		0.001506	3.563851	9.62	23.47441	25.12053	1.64596	24958	25	93	1449.14	1448.52	732.41
1.776854		0.001643	3.563776	9.24	23.47460	25.09920	1.62247	24601	27	91	1448.10	1447.48	733.45
1.942814		0.001461	3.563772	9.60	23.29548	25.07141	1.77348	26891	24	96	1448.13	1447.51	733.43
1.633124		0.001323	3.563733	8.23	23.55134	25.04484	1.49143	22614	22	81	1448.59	1447.97	732.96
1.663147	0.302879	0.001668	3.816426	9.96	23.29548	25.34259	2.04820	31058	8028	104	1448.67	1448.05	732.89
1.645001	0.354147	0.001442	3.816550	10.09	23.29529	25.41437	2.12060	32156	9378	107	1448.37	1447.75	733.19
1.355780	0.242974	0.001623	3.816596	8.90	23.34674	25.01444	1.66448	25238	6445	89	1449.87	1449.25	731.67
1.738167	0.229926	0.001469	3.816595	10.15	23.29540	25.28397	1.98932	30165	6097	104	1448.87	1448.25	732.68

[a] w_1 = heat of combustion of fuse and auxiliary material, w_2 = corrections to standard states.

[ΔH_f^0 (1, 298.15 K)] = − (285.830 ± 0.042) kJ mol^{-1} were combined to derive values of the enthalpy of formation in the condensed state ΔH_f^0 (c, 298.15 K). These are listed in Table 2.

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