

## The Difference in the Heats of Formation of the Two Isomers of Butane. An Estimate of the Heat of Formation of Tetramethylmethane (Neopentane)

Frederick D. Rossini

Citation: [The Journal of Chemical Physics](#) **3**, 438 (1935); doi: 10.1063/1.1749701

View online: <http://dx.doi.org/10.1063/1.1749701>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/3/7?ver=pdfcov>

Published by the [AIP Publishing](#)

---

### Articles you may be interested in

[An improved estimate of the heat of formation of H<sub>2</sub>O<sub>2</sub>](#)

J. Chem. Phys. **99**, 10082 (1993); 10.1063/1.465515

[Enthalpy difference of rotational isomers in liquid butane and pentane from infrared spectra](#)

J. Chem. Phys. **73**, 2013 (1980); 10.1063/1.440298

[Heats of Formation of Two Isomers of Difluorodiazine](#)

J. Chem. Phys. **38**, 169 (1963); 10.1063/1.1733457

[Errata: Thermodynamics of Gaseous Hydrocarbons: Ethane, Ethylene, Propane, Propylene, nButane, Isobutane, 1Butene, Cis and Trans 2Butenes, Isobutene, and Neopentane \(Tetramethylmethane\)](#)

J. Chem. Phys. **5**, 752 (1937); 10.1063/1.1750114

[Thermodynamics of Gaseous Hydrocarbons: Ethane, Ethylene, Propane, Propylene, n Butane, Isobutane, 1Butene, Cis and Trans 2Butenes, Isobutene, and Neopentane \(Tetramethylmethane\)](#)

J. Chem. Phys. **5**, 473 (1937); 10.1063/1.1750059



Using the ordinary expression for the absolute rate of a bimolecular reaction, we find for the interchange reaction  $\text{CH}_3\text{I} + \text{I}^-$  in alcohol an activation energy of 16.5 Kcal. as an upper limit. This is of interest in connection with the recent theoretical discussion<sup>1</sup> of such reactions by Ogg and Polanyi.

F. JULIUSBURGER  
B. TOPLEY  
J. WEISS

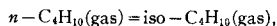
The Sir William Ramsay Laboratories  
of Inorganic and Physical Chemistry,  
University College,  
Gower Street,  
London, W.C. 1,  
May 17, 1935.

<sup>1</sup> See Ogg and Polanyi, *Trans. Faraday Soc.* **31**, 604 (1935).

#### The Difference in the Heats of Formation of the Two Isomers of Butane. An Estimate of the Heat of Formation of Tetramethylmethane (Neopentane)<sup>1</sup>

Data recently obtained in this laboratory on the heat of combustion of isobutane can be combined with similar data on normal butane<sup>2</sup> to yield a reliable value for the difference in the energies of formation of the two isomers.

The calorimetric experiments on both normal butane and isobutane were made with the same apparatus and procedure, and both hydrocarbons used in the measurements were of established purity. For these reasons, the reliability of the relatively small difference in the two values of the heats of combustion will be determined by the "precision" uncertainty of the calorimetric combustion experiments, rather than by the "accuracy" uncertainty. In the two series of calorimetric combustion experiments, the "precision" uncertainties were  $\pm 0.12$  and  $\pm 0.09$  kilocalorie per mole for normal butane and isobutane, respectively. Taking the resulting uncertainty in the difference of the two heats of combustion as the square root of the sum of the squares of the foregoing quantities, the data yield, at 25°C and 1 atmosphere, for the reaction,



$$\Delta H_{298,1} = -1.63 \pm 0.15 \text{ kilocalories per mole.}$$

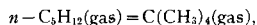
Since for these isomers, at room temperature and a pressure of 1 atmosphere, the difference in the values of  $PV$ , and of  $E(p=1) - E(p=0)$ , is not significant, one may write for the same reaction

$$\Delta H_{298,1}^0 = E_{298,1}^0 = -1.63 \pm 0.15 \text{ kilocalories per mole.}$$

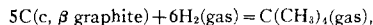
$\Delta H$  and  $\Delta E$  are, respectively, the increments in the heat content and in the internal or intrinsic energy.

The value of the heat of combustion of isobutane (trimethylmethane) can be used in conjunction with the values already reported<sup>2, 3</sup> for methane, ethane (monomethylmethane), and propane (dimethylmethane) to deduce a fairly reliable value for the heat of combustion of tetramethylmethane (neopentane). By plotting  $(Q_c - A)/n$  (where  $Q_c$  is the heat of combustion,  $A$  is a constant whose value was taken as 52.00, and  $n$  is the number of carbon atoms in the molecule) against  $n$ , one obtains a smooth curve which can be extrapolated to  $n=5$  with some confidence. Assigning a reasonable limit of error, one obtains for the heat of combustion of gaseous tetramethylmethane,  $\text{C}(\text{CH}_3)_4$ , in oxygen to form gaseous carbon dioxide and liquid water, at 25°C and a constant pressure of 1 atmosphere, the value  $840.4 \pm 1.0$  kilocalories per mole. This value is about 6 kilocalories per mole less than the one experimental value extant in the literature, that of Thomsen<sup>4</sup> reported in 1886. Thomsen's tetramethylmethane was impure, his samples having the empirical formulas of  $\text{C}_5\text{H}_{11.54}$  and  $\text{C}_5\text{H}_{11.78}$ , instead of  $\text{C}_5\text{H}_{12}$ . This thermochemical constant will be redetermined experimentally as soon as material of the necessary purity is obtained.

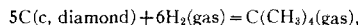
Combination of the foregoing value for tetramethylmethane with the values recently reported for normal pentane,<sup>2, 3</sup> yields the following:



$$\Delta H_{298,1}^0 = \Delta E_{298,1}^0 = -4.9 \pm 1.0 \text{ kilocalories per mole;}$$



$$\Delta H_{298,1}^0 = -40.7 \pm 1.2 \text{ kilocalories per mole;}$$



$$\Delta H_{298,1}^0 = -41.8 \pm 1.2 \text{ kilocalories per mole.}$$

FREDERICK D. ROSSINI

National Bureau of Standards,  
Washington, D. C.,  
June 10, 1935.

<sup>1</sup> Publication approved by the Director of the National Bureau of Standards, U. S. Department of Commerce.

<sup>2</sup> Rossini, *Bur. Standards J. Research* **12**, 735 (1934).

<sup>3</sup> Rossini, *J. Research Nat. Bur. Standards* **13**, 21 (1934).

<sup>4</sup> Thomsen, *Thermochemische Untersuchungen*, Vol. IV (Barth, Leipzig, 1886).