

The Energy of Isomerization of Normal Pentane into Tetramethylmethane

Frederick D. Rossini and John W. Knowlton

Citation: The Journal of Chemical Physics 6, 168 (1938); doi: 10.1063/1.1750218

View online: http://dx.doi.org/10.1063/1.1750218

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The Energy of Isomerization of Normal Pentane into Tetramethylmethane1

In 1935, one of the writers estimated² a value for the heat of combustion of gaseous tetramethylmethane by extrapolating the values, then newly obtained in the National Bureau of Standards thermochemical laboratory,3 for the heats of combustion of methane, ethane (monomethylmethane), propane (dimethylmethane), and isobutane (trimethylmethane). Combination of this value with that for normal pentane yielded a value for the energy of isomerization of gaseous normal pentane into gaseous tetramethylmethane, corresponding to $\Delta H = \Delta E$ $=-4.9\pm1.0$ kilocalories per mole at 25°C. New experimental measurements of the heat of combustion of tetramethylmethane have just been completed and it seems desirable to report the results here briefly, because of the immediate importance to science and industry of the energy content of this molecule. This importance ranges from consideration of the amount of hindrance to rotation of the methyl groups in the molecule to problems in the commercial production of 2,2,4-trimethylpentane, the standard "100 octane number" automotive fuel.

The new measurements have been made according to the regular procedure of this laboratory on a sample of tetramethylmethane kindly made available to us by Professor Frank C. Whitmore of The Pennsylvania State College. The synthesis and purifications were carried out by Mr. E. Rohrmann, and a "best" sample was obtained by fractional distillation by Dr. G. H. Messerly and Professor J. G. Aston. The new experimental value for the heat of combustion of tetramethylmethane, at 25°C and 1 atmosphere, is

$$C(CH_3)_4(gas) + 8O_2(gas) = 5CO_2(gas) + 6H_2O(liq.)$$

 $\Delta H = -3516.41 \pm 0.94$ NBS international kilojoules per mole.

Combining this value (which becomes 840.58 ±0.23 kilocalories per mole, using the conventional factor 1/4.1833) with the value previously reported for normal pentane,3 one obtains for the energy of isomerization of normal pentane into tetramethylmethane, at 25°C,

 $n - C_5H_{12}(gas) = C(CH_3)_4(gas)$ $\Delta H = \Delta E = -19.59 \pm 1.24$ kilojoules, or -4.68 ± 0.30 kilocalories, per mole.

The uncertainty in this energy of isomerization, as given by the earlier estimated value (see above), is thus reduced by over two-thirds. In view of the accord of the former estimated value with that obtained directly from the experimental data, the method of extrapolation used in obtaining the former estimated value appears to be a reliable one.

The new calorimetric measurements on the heat of combustion of tetramethylmethane will be described in detail in a forthcoming paper⁵ which will also include new data on 2-methylbutane.

> FREDERICK D. ROSSINI JOHN W. KNOWLTON

National Bureau of Standards, Washington, D. C., January 27, 1938.

¹ Publication approved by the Director of the National Bureau of Standards, United States Department of Commerce.

² F. D. Rossini, J. Chem. Phys. 3, 438 (1935),

³ F. D. Rossini, Nat. Bur. Stand. J. Research 6, 37 (1931); 12, 735

(1934)

⁵ F. D. Rossini, Chem. Rev. 18, 233 (1936).
⁵ J. W. Knowlton and F. D. Rossini, Nat. Bur. Stand. J. Research. Forthcoming publication.

Note

In my recent paper¹ I failed to give reference to D. G. Bourgin, "Sound Absorption and Velocity in Mixtures."2 which has since come to my attention. With the change in this paper from his earlier f_{ij} symbol to the newer k_{ij} , a symbol exactly equivalent to my $(f_{ij}^{\sigma})_k$, Bourgin has eliminated an approximation made in his earlier papers as he explained in Appendix A. I wish to commend this last paper for its clarity and general organization as well as for its completeness.

HAROLD L. SAXTON

Department of Physics, The Pennsylvania State College, State College, Pennsylvania, February 15, 1938.

¹ Saxton, J. Chem. Phys. **6**, 30 (1938). ² Bourgin, Phys. Rev. **50**, 355 (1936).