

# HOMOGENEOUS PYROLYSIS OF 2-METHYLPENTANE UNDER PULSED ADIABATIC COMPRESSION

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**Abstract:** Thermal decomposition of 2-methylpentane has been studied in a rapid compression machine over a temperature range of 700–1150 °C. The main products (ethylene, methane, propylene, hydrogen, isobutene, acetylene) and minor products of reaction have been determined. Some of them like vinylacetylene, cyclopentadiene, isoprene, benzene, toluene, and some other compounds were identified for the first time. Soot has not been found in products. It is shown that the increase of the pyrolysis temperature along with the decrease of the residence time brings to a growth of selectivity of the ethylene formation and to a fall of selectivity of methane, propylene, and isobutene formation. Increase of C<sub>2</sub>–C<sub>5</sub> alkenes yields in 2-methylpentane pyrolysis compared to isopentane pyrolysis has been established.

**Keywords:** 2-methylpentane; 2-methylalkane; pyrolysis; rapid compression machine (RCM); alkenes; ethylene; isopentenes; isohexenes

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## Figure Captions

**Figure 1** Dependence of 2-methylpentane pyrolysis product yields on maximum compression ratio  $\varepsilon_{\max}$ . Identified compounds: 1 — ethylene; 2 — propylene; 3 — methane; 4 — acetylene; 5 — isobutene; 6 — 1,3-butadiene; 7 — ethane; 8 — hydrogen; 9 — benzene; 10 — but-1-ene; 11 — methylacetylene; 12 — sum of unidentified compounds; 13 — allene; 14 — propane; 15 — trans-pent-2-ene; 16 — 3-methylbut-1-ene; 17 — cis-pent-2-ene; 18 — cyclopentadiene; 19 — vinylacetylene; 20 — toluene; 21 — 2-methylbut-1-ene; 22 — isoprene; 23 — 2-methylbut-2-ene; 24 — pent-1-ene; 25 — sum of isohexenes (assumption); 26 — trans-but-2-ene; 27 — cis-but-2-ene; 28 — diacetylene; 29 — but-1-yne; 30 — sum of cyclohexane and methylcyclopentane; 31 — but-2-yne; 33 — n-butane; 34 — sum of linear isomers of hexene; 35 — isopentane; and 36 — n-pentane

**Figure 2** Selectivity of 2-methylpentane pyrolysis products: 1–36 — refer Fig. 1

**Figure 3** Total content of olefins C<sub>2</sub>–C<sub>5</sub> (1) and C<sub>2</sub>–C<sub>4</sub> (2) in the pyrolysis products of 2-methylpentane depending on maximum compression ratio  $\varepsilon_{\max}$

**Figure 4** Selectivity of the sum of olefins C<sub>2</sub>–C<sub>5</sub> (1) and C<sub>2</sub>–C<sub>4</sub> (2) in the pyrolysis products of 2-methylpentane

**Figure 5** Deviation of H (1) and C (2) element content in 2-methylpentane pyrolysis products from the initial value in the initial mixture

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## References

- Mukhina, T.N., N.L. Barabanov, S.E. Babash, V.A. Men'shikov, and G.L. Avrekh. 1987. *Pirolyzuvlevodorodnogo syr'ya* [Pyrolysis of hydrocarbon raw materials]. Moscow: Chemistry. 240 p.
- Burcat, A., E. Olchanski, and C. Sokolinski. 1999. 2-Methyl-pentane ignition kinetics in a shock-tube. *Combust. Sci. Technol.* 147(1):1–37. doi: 10.1080/00102209908924210.
- Sarathy, S. M., C. K. Westbrook, M. Mehl, W.J. Pitz, C. Togbe, P. Dagaut, H. Wang, M.A. Oehlschlager, U. Niemann, K. Seshadri, P.S. Veloo, C. Ji, F.N. Egolfopoulos, and T. Lu. 2011. Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from C<sub>7</sub> to C<sub>20</sub>. *Combust. Flame* 158(12):2338–2357. doi: 10.1016/j.combustflame.2011.05.007.
- Wang, Z., O. Herbinet, Z. Cheng, B. Husson, R. Fournet, F. Qi, and F. Battin-Leclerc. 2014. Experimental

- investigation of the low temperature oxidation of the five isomers of hexane. *J. Phys. Chem. A* 118(30):5573–5594. doi: 10.1021/jp503772h.
5. Basevich, V. Ya., A. A. Belyaev, S. N. Medvedev, V. S. Posvyanskii, and S. M. Frolov. 2015. Detailed kinetic mechanism of the multistep oxidation and combustion of isopentane and isohexane. *Russ. J. Phys. Chem. B* 9(6):933–939. doi: 10.1134/S1990793115060159.
  6. Zhang, K., C. Banyon, U. Burke, G. Kukkadapu, S. W. Wagnon, M. Mehl, H. J. Curran, C. K. Westbrook, and W. J. Pitz. 2019. An experimental and kinetic modeling study of the oxidation of hexane isomers: Developing consistent reaction rate rules for alkanes. *Combust. Flame* 206:123–137. doi: 10.1016/j.combustflame.2019.04.011.
  7. Van Goethem, M. W. M., S. Barendregt, J. Grievink, J. A. Moulijn, and P. J. T. Verheijen. 2008. Towards synthesis of an optimal thermal cracking reactor. *Chem. Eng. Res. Des.* 86(7):703–712. doi: 10.1016/j.cherd.2008.03.020.
  8. Peard, M. G., F. J. Stubbs, and C. Hinshelwood. 1952. The kinetics of the thermal decomposition of branched-chain paraffin hydrocarbons. II. The isomeric hexanes. *P. R. Soc. A* 214(1118):339–343. doi: 10.1098/rspa.1952.0172.
  9. Chrysochoos, J., and W. A. Bryce. 1965. Surface effects in the uninhibited and the inhibited pyrolyses of isomeric hexanes. *Can. J. Chem.* 43(7):2092–2115. doi: 10.1139/v65-280.
  10. Doue, F., and G. Guiochon. 1969. Mechanism of pyrolysis of some normal and branched C<sub>6</sub> to C<sub>9</sub> alkanes. Composition of their pyrolysis products. *J. Phys. Chem.* 73(9):2804–2809. doi: 10.1021/j100843a003.
  11. Poutsma, M. L., and S. R. Schaffer. 1973. Comparison of thermal cracking of the isomeric hexanes with that catalyzed by potassium ion exchanged Y zeolite. *J. Phys. Chem.* 77(2):158–166. doi: 10.1021/j100621a004.
  12. Tanaka, S., Y. Arai, and S. Saito. 1975. Simulation of initial product distributions from pyrolysis of branched alkanes. *J. Chem. Eng. Jpn.* 8(4):305–309. doi: 10.1252/jcej.8.305.
  13. Tanaka, S., Y. Arai, and S. Saito. 1976. Simulation for high-conversion pyrolysis of branched alkanes. *J. Chem. Eng. Jpn.* 9(2):161–163. doi: 10.1252/jcej.9.161.
  14. McGivern, W. S., I. A. Awan, W. Tsang, and J. A. Manion. 2008. Isomerization and decomposition reactions in the pyrolysis of branched hydrocarbons: 4-methyl-1-pentyl radical. *J. Phys. Chem. A* 112(30):6908–6917. doi: 10.1021/jp8020003.
  15. Kolbanovskiy, Yu. A., V. S. Shchipachev, N. Ya. Chernyak, et al. 1982. *Impul'snoe szhatie gazov v khimii i tekhnologii* [Impulsive compression of gases in chemistry and technology]. Moscow: Nauka. 240 p.
  16. Bilera, I. V. 2017. Gomogennyy piroliz etana v reaktore adiabaticheskogo szhatiya [The high-temperature homogeneous pyrolysis of ethane in the adiabatic compression reactor]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 10(2):12–17.
  17. Bilera, I. V., and N. N. Buravtsev. 2013. Gomogennyy piroliz izobutana v usloviyakh adiabaticheskogo szhatiya [The homogeneous pyrolysis of isobutane under pulsed adiabatic compression]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 6:37–40.
  18. Bilera, I. V. 2014. Gomogennyy piroliz n-butana v usloviyakh adiabaticheskogo szhatiya [The homogeneous pyrolysis of n-butane under pulsed adiabatic compression]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 7:35–41.
  19. Bilera, I. V. 2015. Gomogennyy piroliz n-pentana v usloviyakh adiabaticheskogo szhatiya [The homogeneous pyrolysis of n-pentane under pulsed adiabatic compression]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 8:97–105.
  20. Bilera, I. V., and N. N. Buravtsev. 2016. Gomogennyy piroliz izopentana v usloviyakh adiabaticheskogo szhatiya [The homogeneous pyrolysis of isopentane under pulsed adiabatic compression]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 9(1):74–82.
  21. ScanView — an application and chromatogram database. Available at: <https://community.agilent.com> (accessed October 16, 2018).
  22. Yampol'skiy, Yu. P. 1990. *Elementarnye reaktsii i mehanizm piroliza uglevodorodov* [Elementary reactions and mechanism of pyrolysis of hydrocarbons]. Moscow: Chemistry. 216 p.
  23. Zamostny P., Z. Belohlav, L. Starkbaumova, and J. Patera. 2010. Experimental study of hydrocarbon structure effects on the composition of its pyrolysis products. *J. Anal. Appl. Pyrol.* 87(2): 207–216. doi:10.1016/j.jaat.2009.12.006.
  24. Yasunaga, K., H. Yamada, H. Oshita, K. Hattori, Y. Hidaka, and H. Curran. 2017. Pyrolysis of n-pentane, n-hexane and n-heptane in a single pulse shock tube. *Combust. Flame* 185:335–345. doi: 10.1016/j.combustflame.2017.07.027.

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