THERMODYNAMIC PROPERTIES OF TRIETHYLALUMINUM ISOMERS

A. A. Kroupnov and M. Ju. Pogosbekian

Institute of Mechanics, M. V. Lomonosov Moscow State University, 1 Michurinsky Prosp., Moscow 119192, Russian Federation

Abstract: A quantum-mechanical calculation of the structure and energy characteristics of triethylaluminum $Al(C_2H_5)_3$ (TEA) was carried out during which three of its isomers were found. The processes of isomerization of TEA are considered and the corresponding equilibrium constants and the equilibrium isomeric composition of TEA are obtained. The main thermodynamic properties (heat capacity, enthalpy of formation, entropy, and reduced Gibbs energy) of the found isomers and the equilibrium composition are calculated over a wide temperature range. An approximation of the reduced Gibbs energy was carried out in accordance with the analytical representation adopted in the reference book "Thermodynamic properties of individual substances" edited by L. V. Gurvich.

Keywords: triethylaluminum; isomerization; equilibrium; thermodynamic properties; quantum mechanics

DOI: 10.30826/CE22150412 **EDN:** RMLQMS

Figure Captions

Figure 1 Equilibrium constants for TEA isomerization processes: *1* — K_{12}; and *2* — K_{23}

Figure 2 Equilibrium composition of TEA: *1* — $Al(C_2H_5)_3$-iso1; *2* — $Al(C_2H_5)_3$-iso2; and *3* — $Al(C_2H_5)_3$-iso3

Figure 3 Reduced Gibbs energy (*a*), entrophy (*b*), heat capacity at constant pressure (*c*), and enthalphy (*d*) of TEA isomers: *1* — $Al(C_2H_5)_3$-iso1; *2* — $Al(C_2H_5)_3$-iso2; and *3* — $Al(C_2H_5)_3$-iso3

Table Captions

Table 1 Geometric structure of TEA isomers and their energies

Table 2 Thermodynamic properties of the $Al(C_2H_5)_3$-iso1 isomer ($\Delta_f H^0(0) = -631{,}991$ kJ/mol; $\Delta_f H^0(298{,}15) = -366{,}782$ kJ/mol)

Table 3 Thermodynamic properties of the $Al(C_2H_5)_3$-iso2 isomer ($\Delta_f H^0(0) = -640{,}511$ kJ/mol; $\Delta_f H^0(298{,}15) = -373{,}338$ kJ/mol)

Table 4 Thermodynamic properties of the $Al(C_2H_5)_3$-iso3 isomer ($\Delta_f H^0(0) = -639{,}552$ kJ/mol; $\Delta_f H^0(298{,}15) = -370{,}250$ kJ/mol)

Table 5 Thermodynamic properties of the equilibrium composition of TEA ($\Delta_f H^0(0) = -640{,}511$ kJ/mol; $\Delta_f H^0(298{,}15) = -371{,}93$ kJ/mol)

Table 6 Approximation coefficients for the reduced Gibbs energy $\Phi(T)$ for isomers and the equilibrium composition of TEA

References

1. Kuznetsov, N. M., S. M. Frolov, I. O. Shamshin, and P. A. Storozhenko. 2020. Kinetika vzaimodeystviya kapel' trietilalyuminiya s peregretym vodyanym parom: eksperiment, fiziko-khimicheskaya model' i skhema khimicheskikh reaktsiy [Kinetics of the interaction of triethylaluminum drops with superheated steam: Experiment, physicochemical model, and scheme of chemical reactions]. *Goren. Vzryv (Mosk.) — Combustion and Explosion*. 13(3):76–81.
2. Gurvich, L. V., I. V. Veyts, V. A. Medvedev, *et al.* 1978–1982. *Termodinamicheskie svoystva individual'nykh veshchestv* [Thermodynamic properties of individual substances]. Moscow: Nauka. 4 vols.
3. Linstrom, P. J., and W. G. Mallard. 2018. NIST Chemistry WebBook, NIST Standard Reference Database Number 69. National Institute of Standards and Technology. Available at: https://webbook.nist.gov/chemistry/ (accessed November 18, 2022).
4. Frisch, M. J., G. W. Trucks, H. B. Schlegel, *et al.* 2009. Gaussian 09. Gaussian, Inc., Wallingford CT.
5. Hohenberg, P., and W. Kohn. 1964. Inhomogeneous electron gas. *Phys. Rev.* 136(3B):B864–B871.
6. Kohn, W., and L. J. Sham. 1965. Self-consistent equations including exchange and correlation effects. *Phys. Rev.* 140(4A):A1133–A1138.
7. Lee, C., W. Yang, and G. G. Parr. 1988. Development of the Colle–Salvetti correlation-energy formula into a func-

tional of the electron density. *Phys. Rev. B* 37(2):785–789.

8. Kendall, R. A., T. H. Dunning, and R. J. Harrison. 1992. Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. *J. Chem. Phys.* 96(9):6796–6806.
9. Kroupnov, A. A., and M. J. Pogosbekian. 2021. Energeticheskie i strukturnye kharakteristiki nachal'noy stadii samovosplamaneniya trietilalyuminiya v vozdukhe [Energy and structural characteristics for initial stage of self-ignition triethyluminum in air]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 14(4):91–95.
10. Tel'noi, V. I., and I. B. Rabinovich. 1980. Thermochemistry of organic derivatives of non-transition elements. *Russ. Chem. Rev.* 49(7):603–622.
11. Smith, M. B. 1974. The heats of formation of aluminum alkyls and related compounds. *J. Organomet. Chem.* 76(2):171–201.

Received September 5, 2022

Contributors

Kroupnov Alexsander A. (b. 1960) — Candidate of Science in physics and mathematics, leading research scientist, Institute of Mechanics, M. V. Lomonosov Moscow State University, 1 Michurinsky Prosp., Moscow 119192, Russian Federation; kroupnov@imec.msu.ru

Pogosbekian Mikhail Ju. (b. 1970) — Candidate of Science in physics and mathematics, leading research scientist, Institute of Mechanics, M. V. Lomonosov Moscow State University, 1 Michurinsky Prosp., Moscow 119192, Russian Federation; pogosbekian@imec.msu.ru