

DETERMINATION OF THE VALUES OF $\Delta_f H_{298.15}^0$ OF (Al) $_n$ CLUSTERS WITH $n = 3-10$

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Abstract: The values of $\Delta_f H_{298.15}^0$ of (Al) $_n$ clusters with $n = 3-10$ are determined on the basis of thermochemistry of the isodesmic reactions calculated using the results of the quantum mechanical modeling. As a result, the following values of $\Delta_f H_{298.15}^0$ are proposed: 551 ± 16 ($n = 3$), 668 ± 8 ($n = 4$), 720 ± 16 ($n = 5$), 769 ± 9 ($n = 6$), 776 ± 29 ($n = 7$), 853 ± 32 ($n = 8$), 931 ± 33 ($n = 9$), and 906 ± 33 kJ/mol ($n = 10$).

Keywords: aluminum; cluster; isodesmic reaction; enthalpy

Acknowledgments

The work was supported by the Russian Foundation for Basic Research (grant No. 16-08-00585 A).

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Received December 29, 2016

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