DETERMINATION OF THE VALUES OF $\Delta_f H^0_{298.15}$ OF Al_2O_3 AND ITS CLUSTERS ($(Al_2O_3)_n$) WITH $n = 2$ AND 4

G. A. Poskrebyshev and A. N. Ermakov

V. L. Talrose Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, 38-2 Leninsky Prosp., Moscow 119334, Russian Federation

Abstract: The values of $\Delta_f H^0_{298.15}$ of Al_2O_3 and its clusters ($(Al_2O_3)_n$) with $n = 2$ and 4 are determined on the basis of thermochemistry of the isodesmic reactions calculated using the results of the quantum mechanical modeling at B3LYP/6-311++G(d,p) level of theory. As a result, the following values of $\Delta_f H^0_{298.15}$ are proposed for the most thermochemically favorable conformers, considered in the present study, in the singlet state: -502 ± 42 ($^1Al_2O_3$), -1976 ± 18 ($^1(Al_2O_3)_2$) and -4792 ± 23 ($^1(Al_2O_3)_4$) kJ/mol.

Keywords: aluminum oxides; cluster; isodesmic reaction; enthalpy

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Contributors

Poskrebyshev Gregory A. (b. 1965) — Candidate of Science in chemistry, leading scientist, V. L. Talrose Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, 38-2 Leninsky Prosp., Moscow 119334, Russian Federation; gposkr@chph.ras.ru

Ermakov Alexander N. (b. 1943) — Doctor of Science in chemistry, head of laboratory, V. L. Talrose Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, 38-2 Leninsky Prosp., Moscow 119334, Russian Federation; polclouds@yandex.ru