THERMOCHEMISTRY OF REACTIONS OF $C_6H_5CH_2C_6H_4O^\bullet$ AND $C_6H_5CH^\bullet C_6H_4$ WITH O_2 AS WELL AS OF REACTIONS OF THEIR UNIMOLECULAR DECOMPOSITION

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Abstract: The thermochemical properties of the products of the reactions of $C_6H_5CH_2C_6H_4O^\bullet$ and $C_6H_5CH^\bullet C_6H_4$ radicals with molecular oxygen as well as the products of their monomolecular decomposition are determined using the modern molecular modeling approaches. Based on the calculated values, the thermochemistry of the considered reactions as well as the values of their activation barriers are reported.

Keywords: $C_{13}H_{11}O$; peroxy radical; enthalpy

DOI: 10.30826/CE21140303

Figure Caption

The values of $\Delta_f H^\circ_{298.15}(\mathrm{C_6H_5CH{=}C_6H_4{=}O, CORR})$ (*a*) and $\Delta_f H^\circ_{298,15}(\mathrm{C_6H_5CH(O_2^\bullet)C_6H_4OH, CORR})$ (*b*), determined using the considered quantum mechanical approaches

Table Captions

Table 1 The structures of considered compounds and their B3LYP ($i = 1$) values of $H^\circ_0((Y_n)_i)$, $H^\circ_{298.15}((Y_n)_i)$, and $G^\circ_{298.15}((Y_n)_i)$ in Hartree

Table 2 Literature values of $\Delta_f H^\circ_{298.15}(Y_n, \mathrm{TAB})$ and $S^\circ_{298.15}(Y_n, \mathrm{TAB})$

Table 3 The values of $\Delta_r H^\circ_{298.15}((Y_n)_i, \mathrm{CALC})_{\mathrm{atom}}$ and $\Delta_r H^\circ_{298.15}((Y_n)_i, \mathrm{CORR})_{\mathrm{atom}}$ determined in the present work

Table 4 Parameters of the linear callibration dependencies $(-\Delta_r H^\circ_{298.15}((Y_n)_i, \mathrm{CORR})_{\mathrm{atom}} = (A_1)_i + (B_1)_i(-\Delta_r H^\circ_{298.15}((Y_n)_i, \mathrm{CALC})_{\mathrm{atom}}))$ used in the present study as well as their root mean squared (RMSE) and standard (SE) errors [7]

Table 5 The values of $\Delta_f H^\circ_{298.15}((Y_n)_i, \mathrm{CORR})_{\mathrm{atom}}$ and $\Delta_f H^\circ_{298.15}(Y_n, \mathrm{CORR})$ calculated in the present work for the considered compounds (see Table 1)

Table 6 The values of $\Delta_{\mathrm{R}n} H^\circ_{298.15}$, $\Delta_{\mathrm{R}n} S^\circ_{298.15}$, and $\Delta_{\mathrm{R}n} G^\circ_{298.15}$ determined in the present work for the reactions (R1)–(R6)

Table 7 The values of $S^\circ_{298.15}((Y_n)_i)$ and $S^\circ_{298.15}((Y_n)_1, \mathrm{IRot})$ calculated with and without accounting for internal rotations

Acknowledgments

The author is grateful to the Ministry of Science and Higher Education of the Russian Federation (AAAA-A20-120011390097-9 and AAAA-A20-120011390099-3) for support of this work.

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Received August 15, 2021

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