



Erratum

Erratum to "Photochemistry of the gaseous hydrogen peroxide—carbon monoxide system. III. Calculated energetics for possible HO₂–CO complexes"

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The publisher regrets that structures II and III were omitted from the Abstract. It is reprinted here in full.

Abstract

At 298 K, HO₂ radicals formed by secondary reactions in the photochemistry of the H₂O₂-CO system do not react with CO, whereas OH radicals formed in the primary process do. To explain the non-reactivity of HO₂, we made Hartree-Fock calculations of the energies needed to form three probable HO₂-CO intermediate radical complexes:

The values of ΔE for the reaction $HO_2 + CO \rightarrow R$ and ΔH_i° for R obtained at 298 K are as follows:

| | R | | | | |
|--|-----|----------|-----------|-----------|------------|
| | I | II (sym) | II (anti) | III (sym) | III (anti) |
| $\Delta E (kJ)$ | 89 | 6 | 9 | -280 | -259 |
| $\Delta H_{\rm f}^{\circ}$ (kJ mol ⁻¹) | -22 | - 105 | -102 | -391 | -370 |

From the high-temperature rate data, we conclude that the first stage of the reaction is the formation of complex I with ΔE the same or almost the same as the activation energy for the reaction to yield products CO_2 and OH, and that every collision of the reactants with sufficient energy yields the complex.

Keywords: Hydrogen peroxide–carbon monoxide; Energetics; HO_2 –CO complexes

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