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[Lab. of Pharm. Physical Chemistry]

**An INDO/S Study of Photochemical Reactivity of
2,4,6,8(1H,3H,7H,9H)-Pyrimido [5,4-g] pteridinetetrone 5-Oxide.**

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The specific photochemical reactivity of 2,4,6,8(1H,3H,7H,9H)-pyrimido [5,4-g] pteridinetetrone 5-oxide (1), an effective photochemical oxygen-atom transfer agent, was discussed based on the results of molecular orbital (INDO/S-CI) calculations of the excited states, in comparison with several simple aromatic N-oxides, pyridine 1-oxide (2), pyrazine 1-oxide (3), acridine 10-oxide (4), and phenazine 5-oxide (5). The lowest $\pi-\pi^*$ excited singlet ($S_1\pi-\pi^*$) state of 1 was most characterized by the high proportion of the $\psi_{a2}-\psi_{b2}^*$ transition for the CI state and by the marked decrease of the N-O bond order, distinct from those of 2-5. The low reactivity in photorearrangement of 1 was interpreted to result from the decrease of the N-O bond order in the $S_1\pi-\pi^*$ state.

[Regulatory Toxicology and Pharmacology, **13**, 185-194 (1991)]

[Lab. of Pharm. Physical Chemistry]

Quantum Chemical Study for Genotoxic and Antitumor Activities of Hydroxyanthraquinones.

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For anthraquinone and its mono- and dihydroxyl derivatives, and for their semiquinone anion radicals, semiempirical MNDO/H calculations were performed. From these calculations, it was found that the electrophilic frontier electron densities ($f^E\beta$) on the β position in anthraquinones were distinctly correlated with the genotoxic activity. On the other hand, calculations for the semiquinone anion radicals revealed the great stabilizations by the intramolecular hydrogen bond of the carbonyl group with α -hydroxyl groups. It has been suggested that this type of stabilization may be associated with the antitumor activity of several hydroxylantraquinone derivatives.

[Anal. Sci., **7**, 281-284 (1991)]

[Lab. of Pharm. Analytical Chemistry]

**Detection Method of Pyrroloquinoline Quinone (PQQ) and PQQ-
Adducts by Isotachopheresis.**

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A new detection method of PQQ and PQQ-adducts has been developed by isotachopheresis using UV and potential gradient detectors. Taking into account of the acid dissociation constants of PQQ, 0.01 M amidol hydrochloride containing 0.1% Triton X (pH 8.9) and 0.01 M sodium *n*-caproate (pH 7.5) were used as the leading and terminating electrolytes, respectively. The detection limit of both free PQQ and PQQ-acetone adduct (5-acetonyl-PQQ) was about 0.1 μ M in the sample injection of 10 μ l. Isotachopheretic behavior of the reaction products of free PQQ with nucleophilic agents such as alcohols, ketones, aldehydes, amino acids, and phenylhydrazines was investigated.