

Flavin Chemistry and Catalysis

144. T.C. Bruice; L. Main; S. Smith and P.Y. Bruice. Preequilibrium Complex Formation and Nucleophilic Addition (and Its Position) As Factors in Flavin-Catalyzed Oxidations. *J. Am. Chem. Soc.* **1971**, *93*, 7327.
153. L. Main; G.J. Kasperek and T.C. Bruice. Isoalloxazine(Flavin)Dehydrogenation of Dimethyl trans-1,2-Dihydrophthalate. *J. Chem. Soc., Chem. Commun.* **1972**, *14*, 847-8.
155. M. Brüstlein and T.C. Bruice. Demonstration of a Direct Hydrogen Transfer between NADH and a Deazaflavin. *J. Am. Chem. Soc.* **1972**, *94*, 6548.
157. L. Main; G.J. Kasperek and T.C. Bruice. Kinetics and Mechanism of the Isoalloxazine (Flavin) Dehydrogenation of Dimethyl Dihydrophthalates. *Biochem.* **1972**, *11*, 3991
160. L. Hevesi and T.C. Bruice. 5 vs. 4a-Addition to Isoalloxazine. *J. Am. Chem. Soc.* **1972**, *94*, 8277.
163. L. Hevesi and T.C. Bruice. Reaction of Sulfite with Isoalloxazines. *Biochem.* **1973**, *12*, 290.
167. T.C. Bruice; L. Hevisi and S. Shinkai. Mechanisms of Formation and Equilibria of 4a and 5 Adducts of an Isoalloxazine. Reaction of 10-(2',6'-Dimethylphenyl)-3-methylisoalloxazine- 6,8-disulfonate with Sulfite in Aqueous Media. *Biochem.* **1973**, *12*, 2083.
171. S. Shinkai and T.C. Bruice. The Question of Covalent Intermediate Formation in the Flavine-Catalyzed Carbonyl to Carbinol Oxidation-Reduction Reaction. *J. Am. Chem. Soc.* **1973**, *95*, 7526.
173. D.L. Elliot and T.C. Bruice. Evidence for an Intermediate Adduct in the Ethylenediaminetetraacetic Acid Mediated Photoreduction of Flavines. *J. Am. Chem. Soc.* **1973**, *95*, 7901.
180. S.B. Smith; M. Brüstlein and T. C. Bruice. Electrophilicity of the 8 Position of the Isoalloxazine (Flavine) Ring System. Comment on the Mechanism of Oxidation of Dihydroisoalloxazine. *J. Am. Chem. Soc.* **1974**, *96*, 3696.
185. D. Clerin and T.C. Bruice. A Kinetic Study of the Fate of a Covalent Intermediate of the Type Proposed to be Involved in Flavin Catalysis. *J. Am. Chem. Soc.* **1974**, *96*, 5571.
188. S. Shinkai; T. Kunitake and T.C. Bruice. The Importance of 1,2- Ene-diols in the Reduction of Lumiflavin by α -Ketols. *J. Am. Chem. Soc.* **1974**, *96*, 7140.
189. I. Yokoe and T.C. Bruice. Oxidation of Thiophenol and Nitroalkanes by an Electron Deficient Isoalloxazine. *J. Am. Chem. Soc.* **1975**, *97*, 450.
191. S.B. Smith and T.C. Bruice. Mechanisms of Isoalloxazine (Flavine) Hydrolysis. *J. Am. Chem. Soc.* **1975**, *97*, 2875.

192. R.F. Williams; S. Shinkai and T.C. Bruice. Radical Mechanisms for 1,5-Dihydroflavin Reduction of Carbonyl Compounds. *Proc. Natl. Acad. Sci. (USA)* **1975**, 72, 1763.
195. T.C. Bruice and Y. Yano. Radical Mechanisms for 1,5-Dihydro-5- methylflavine Reduction of Carbonyl Compounds. *J. Am. Chem. Soc.* **1975**, 97, 5263.
202. C. Kemal and T.C. Bruice. Simple synthesis of a 4a-hydroperoxy adduct of a 1,5-dihydroflavin: Preliminary studies of a model for bacterial luciferase. *Proc. Natl. Acad. Sci. (USA)* **1976**, 73, 995.
203. T.C. Bruice. Models and Flavin Catalysis. *Progress in Bioorganic Chemistry, Vol. 4*; E.T. Kaiser; Ed.; Wiley and Sons, **1976**; 1-87.
204. C. Kemal and T.C. Bruice. The Chemistry of an N5-Methyl-1,5- dihydroflavin and Its Aminium Cation Radical. *J. Am. Chem. Soc.* **1976**, 98, 3955.
207. T.C. Bruice. Some Physical Organic Studies Dealing with Flavin Catalysis. *Flavins Flavoproteins, Proc. Int. Symp., 5th* **1976**, Meeting Date 1975, 244-260.
209. R.F. Williams and T.C. Bruice. The Kinetics and Mechanisms of 1,5-Dihydroflavin Reduction of Carbonyl Compounds and Flavin Oxidation of Alcohols. 2. Ethyl Pyruvate, Pyruvamide and Pyruvic Acid. *J. Am. Chem. Soc.* **1976**, 98, 7752.
210. T.C. Bruice and J.P. Taulane. The Kinetics and Mechanisms of 1,5-Dihydroflavin Reduction of Carbonyl Compounds and Flavin Oxidation of Alcohols. 3. Oxidation of Benzoin by Flavin and Reduction of Benzil by 1,5-Dihydroflavin. *J. Am. Chem. Soc.* **1976**, 98, 7769.
211. R.F. Williams; S.S. Shinkai and T.C. Bruice. Kinetics and Mechanisms of the 1,5-Dihydroflavin Reduction of Carbonyl Compounds and the Flavin Oxidation of Alcohols. 4. Interconversion of Formaldehyde and Methanol. *J. Am. Chem. Soc.* **1977**, 99, 921.
212. C. Kemal; T.W. Chan and T.C. Bruice. Chemiluminescent reactions and electrophilic oxygen donating ability of 4a- hydroperoxyflavins: General synthetic method for the preparation of N5-alkyl-1,5-dihydroflavins. *Proc. Natl. Acad. Sci. (USA)* **1977**, 74, 405.
213. T.W. Chan and T.C. Bruice. One and Two Electron Transfer Reactions of Glucose Oxidase. *J. Am. Chem. Soc.* **1977**, 99, 2387.
219. T.C. Bruice; T.W. Chan; J.P. Taulane; I. Yokoe; D.L. Elliott; R.F. Williams and M. Novak. Changes in the Chemistry of an Isoalloxazine Brought About by Substitution at the 7 and 8 Positions by a Strongly Electronegative Substituent. *J. Am. Chem. Soc.* **1977**, 99, 6713.
220. R.L. Chan and T.C. Bruice. The Chemistry of an Electron- Deficient 5-Deazaflavin. 8-Cyano-10-methyl-5- deazaisoalloxazine. *J. Am. Chem. Soc.* **1977**, 99, 6721.
221. C. Kemal and T.C. Bruice. Chemiluminescence Accompanying the Decomposition of 4a-Flavin Alkyl Peroxide. Model Studies of Bacterial Luciferase. *J. Am. Chem. Soc.* **1977**, 99, 7064.

222. C. Kemal; T.W. Chan and T.C. Bruice. Reactions of $3O_2$ with Dihydroflavins. 1. N3,5-Dimethyl-1,5-Dihydrolumiflavin and 1,5-Dihydroisoalloxazines. *J. Am. Chem. Soc.* **1977**, *99*, 7272.
223. T.W. Chan and T.C. Bruice. Reaction of Nitroxides with 1,5-Dihydroflavins and N3,5-Dimethyl-1,5-Dihydrolumiflavin. *J. Am. Chem. Soc.* **1977**, *99*, 7287.
224. M. Novak and T.C. Bruice. Oxidation of 9-Hydroxy- and 9-Methoxyfluorene Carbanions by Flavin. Proof of Radical Mechanism. *J. Am. Chem. Soc.* **1977**, *99*, 8079.
231. T.W. Chan and T.C. Bruice. Importance of C4a- and N5-Covalent Adducts in the Flavin Oxidation of Carbanions. *Biochem.* **1978**, *17*, 4784.
232. R.L. Chan and T.C. Bruice. Characterization and One- and Two- Electron Redox Chemistry of 1,5-Dicarbonyl-1,5-dideazaisoalloxazines (Flavins). *J. Am. Chem. Soc.* **1978**, *100*, 7375.
234. G. Tollin; R.L. Chan; T.R. Malefyt and T.C. Bruice. Some One Electron Reduction Products of Flavin Analogs: Cyanoisoalloxazines and Deazaisoalloxazines. *Photochem. Photobiol.* **1979**, *29*, 233-43.
235. C. Kemal and T.C. Bruice. Transfer of O_2 from a 4a-Hydroperoxyflavin Anion to a Phenolate Ion. A Flavin-Catalyzed Dioxygenation Reaction. *J. Am. Chem. Soc.* **1979**, *101*, 1635.
236. S. Ball and T.C. Bruice. 4a-Hydroperoxyflavin N-Oxidation of Tertiary Amines. *J. Am. Chem. Soc.* **1979**, *101*, 4017.
241. A. Miller and T.C. Bruice. Oxidations by a 4a-Hydroperoxyisoalloxazine hindered in the 9a and 10a Positions. *J. Chem. Soc., Chem. Comm.* **1979**, *20*, 896-7.
242. M. Novak; A. Miller; T.C. Bruice and G. Tollin. The Mechanism of Flavin 4a Substitution Which Accompanies Photolytic Decarboxylation of α -substituted Acetic Acids. *J. Am. Chem. Soc.* **1980**, *102*, 1465.
243. M. Novak and T.C. Bruice. Mechanistic Investigation of the Oxidation of the Carbanion of Methyl 2-Methoxy-2-phenylacetate by an Isoalloxazine. *J. Chem. Soc., Chem. Commun.* **1980**, *9*, 372-4.
244. T.C. Bruice and A. Miller. Products of the Decomposition of the Anion of a 4a-Hydroperoxyisoalloxazine Hindered in the 9a and 10a Positions. *J. Chem. Soc., Chem. Commun.* **1980**, *15*, 693-4.
245. S. Muto and T.C. Bruice. Dioxygen Transfer from 4a-Hydroperoxyflavin Anion. 2. Oxygen Transfer to the 10 Position of 9-Hydroxyphenanthrene Anions and to 3,5-Di-tert-butylcatechol Anion. *J. Am. Chem. Soc.* **1980**, *102*, 4472.
246. M. Iwata; T.C. Bruice; H.L. Carrell and J.P. Glusker. Reactions of 4a-Peroxides and 4a-Pseudobases of N10- and N5-Phenethylflavins. *J. Am. Chem. Soc.* **1980**, *102*, 5036.
247. T.C. Bruice. Mechanisms of Flavin Catalysis. *Accts. Chem. Res.* **1980**, *13*, 256-262.

248. S. Ball and T.C. Bruice. Oxidation of Amines by a 4a- Hydroperoxyflavin. *J. Am. Chem. Soc.* **1980**, *102*, 6498.
250. Bruice, Thomas C.. Carbon acid oxidations and oxygen activation by flavins. *Advances in Chemistry Series* **1980**, *191*(*Biomimetic Chem.*), 89-118.
251. S. Muto and T.C. Bruice. Dioxygen Transfer from 4a- Hydroperoxyflavin Anion. 3. Oxygen Transfer to the 3-Position of Substituted Indoles. *J. Am. Chem. Soc.* **1980**, *102*, 7559.
252. P.T. Shepherd and T.C. Bruice. Formation of a Non- chemiluminescent Excited-State Species in the Decomposition of 4a-(Alkylperoxy)flavins. *J. Am. Chem. Soc.* **1980**, *102*, 7774.
253. E.J. Nanni; D.T. Sawyer; S.S. Ball and T.C. Bruice. Redox Chemistry of N5-Ethyl-4a-hydroperoxy-3-methylflavin in Dimethylformamide. Evidence for the Formation of the N5- Ethyl-4a-hydroperoxy-3-methylflavin Anion via Radical-Radical Coupling with Superoxide Ion. *J. Am. Chem. Soc.* **1981**, *103*, 2797.
254. S. Ball and T.C. Bruice. The Chemistry of 1-Carba-1-deaza-N5- ethyl-N3-methylflavins. Influence of the N1 upon the Reactivity of Flavin 4a-Hydroperoxides. *J. Am. Chem. Soc.* **1981**, *103*, 5494.
258. A. Wessiak and T.C. Bruice. On the Nature of the Intermediate between 4a-Hydroperoxyflavin and 4a-Hydroxyflavin in the Hydroxylation Reaction of p-Hydroxybenzoate Hydroxylase. Synthesis of 6-Aminopyrimidine-2,4,5(3H)-triones and the Mechanism of Aromatic Hydroxylation by Flavin Monooxygenases. *J. Am. Chem. Soc.* **1981**, *103*, 6996.
259. Shepherd, Peter T.; Bruice, Thomas C.. Chemiluminescence derived from 4a-(alkylperoxy) flavins. *Biolumin. Chemilumin.*, [*Int. Symp. Anal. Appl. Biolumin. Chemilumin.*], 2nd **1981**, Meeting Date 1980, 391-4.
260. Bruice, Thomas C.. A progress report on studies of the activation of molecular oxygen by dihydroflavins. *Developments in Biochemistry* **1982**, *21*(*Flavins Flavoproteins*), 265-77.
261. G. Eberlein and T.C. Bruice. One- and Two-Electron Reduction of Oxygen by 1,5-Dehydroflavins. *J. Am. Chem. Soc.* **1982**, *104*, 1449.
263. S. Muto and T.C. Bruice. Dioxygen Transfer from 4a- Hydroperoxyflavin Anion. 4. Dioxygen Transfer to Phenolate Anion as a Means of Aromatic Hydroxylation. *J. Am. Chem. Soc.* **1982**, *104*, 2284.
266. E.B. Skibo and T.C. Bruice. Preparation and Study of a Low- Potential Flavin Analogue. *J. Am. Chem. Soc.* **1982**, *104*, 4982.
268. Bruice, Thomas C.. 4a-Peroxyflavins. *Oxidases Relat. Redox Syst., Proc. Int. Symp.*, 3rd **1982**, Meeting Date 1979, 423-46.
272. T.C. Bruice. Leaving Group Tendencies and the Rates of Monooxygen Donation by Hydrogen Peroxide, Organic Hydroperoxides, and the Peroxycarboxylic Acids. *J. Am. Chem. Soc., Chem. Commun.* **1983**, *1*, 14-15.

273. T.C. Bruice; J.B. Noar; S.S. Ball and U.V. Venkataram. Mono-oxygen Donation Potential of 4a-Hydroperoxyflavins as Compared with Those of a Pericarboxylic Acid and other Hydroperoxides. Monooxygen Donation to Olefin, Tertiary Amine, Alkyl Sulfide, and Iodide Ion. *J. Am. Chem. Soc.* **1983**, *105*, 2452.
274. E.B. Skibo and T.C. Bruice. High- and Low-Potential Flavin Mimics (Based on the Pyrimidino[5,4-g]pteridine and Imidazo[4,5-g]pteridine System). 1. General Chemistry. *J. Am. Chem. Soc.* **1983**, *105*, 3304.
275. E.B. Skibo and T.C. Bruice. High- and Low-Potential Flavin Mimics. 2. 3,7,10-Trimethyl-(1H,3H,5H,7H,9H,10H)-pyrimido[5,4,-g]-pteridine-2,4,6,8-tetrone Dianion Reduction of Carbonyl, Nicotinamides, and Alkyl Disulfide Functional Groups. *J. Am. Chem. Soc.* **1983**, *105*, 3316.
277. A. Wessiak and T.C. Bruice. Synthesis and Study of a 6-Amino-5-oxo-3H,5H-uracil and Derivatives. The Structure of an Intermediate Proposed in Mechanisms of Flavin and Pterin Oxygenases. *J. Am. Chem. Soc.* **1983**, *105*, 4809.
280. G. Eberlein and T.C. Bruice. The Chemistry of a 1,5-Diblocked Flavin. 1. Interconversion of the Reduced, Radical and Oxidized Forms of 1,10-Ethano-5-ethyllumiflavin. *J. Am. Chem. Soc.* **1983**, *105*, 6679.
281. G. Eberlein and T.C. Bruice. The Chemistry of a 1,5-Diblocked Flavin. 2. Proton and Electron Transfer Steps in the Reaction of Dihydroflavins with Oxygen. *J. Am. Chem. Soc.* **1983**, *105*, 6685.
284. A. Wessiak; J.B. Noar and T.C. Bruice. The possibility that the spectrum of intermediate two, seen in the course of reaction of flavoenzyme phenol hydroxylases, may be attributable to iminol isomers of a flavin-derived 6-arylamino-5-oxo(3H,5H)uracil. *Proc. Natl. Acad. Sci. (USA)* **1984**, *81*, 332.
285. L.-C. Yuan and T.C. Bruice. Redox Reactions of a Tetrahydro-/Hexahydropyrido[2,3-d³:6,5-d']dipyrimidine Tetrone Couple. A High vs. Low Potential 5-Carba-5-deazaflavin Mimic. *J. Am. Chem. Soc.* **1984**, *106*, 1530.
287. O.L. Farnig and T.C. Bruice. Carbon-Carbon Double Bond Formation Accompanying Hydride Transfer from a Carbanion to a 5-Carbalumiflavin. *J. Chem. Soc., Chem. Commun.* **1984**, *3*, 185-6.
288. T.C. Bruice. Oxygen-Flavin Chemistry. *Isr. J. Chem.* **1984**, *24*, 54.
291. A. Wessiak; L.M. Schopfer; L.C. Yuan; T.C. Bruice; and V. Massey. Use of riboflavin-binding protein to investigate steric and electronic relationships in flavin analogs and models. *Proc. Natl. Acad. Sci.* **1984**, *81*, 4246.
292. U.V. Venkataram and T.C. Bruice. Determination of the Kinetic pK_a of a Flavin 4a-Pseudobase from a Study of the Hydrolysis of 4a-Hydroxy-5-ethyl-3-methyl-lumiflavin in H₂O. The Oxygen Donation Potential of 4a-Hydroperoxyflavins. *J. Chem. Soc., Chem. Commun.* **1984**, *14*, 899-900.
293. U.V. Venkataram and T.C. Bruice. On the Mechanism of Flavin-Catalyzed Dehydrogenation α , β to an Acyl Function. The Mechanism of 1,5-Dihydroflavin Reduction of Malemides. *J. Am. Chem. Soc.* **1984**, *106*, 5703.

296. G. Eberlein; T.C. Bruice; R.A. Lazarus; R. Henrie and S.J. Benkovic. The Interconversion of the 5,6,7,8-Tetrahydro-, 7,8-Dihydro-, and Radical Forms of 6,6,7,7-Tetramethyldihydropterin. A Model for the Biopterin Center of Aromatic Amino Acid Mixed Function Oxidases. *J. Am. Chem. Soc.* **1984**, *106*, 7916.
297. Bruice, Thomas C. Flavin oxygen chemistry brought to date. *Flavins Flavoproteins, Proc. Int. Symp., 8th* **1984**, 45-55.
317. E.B. Skibo and T.C. Bruice. High- and Low-Potential Flavin Mimics. 3. 3,7,10-Trimethyl-(1H,3H,5H,7H,9H,10H)- pyrimido[5,4-g]pteridine-2,4,6,8-tetrone-Mediated Reduction of Carbon-Carbon Double Bonds α - β to an Acyl Function. *J. Am. Chem. Soc.* **1986**, *108*, 1650.
363. S.-R. Keum; D.H. Gregory; and T.C. Bruice. Oxidation of Aminophenols by 4a-Hydroperoxy-5-ethylflavin Anion. Flavoenzyme Hydroxylase Mechanism. *J. Am. Chem. Soc.* **1990**, *112*, 2711.
366. T.W. Kaaret and T.C. Bruice. Electrochemical Luminescence with N(5)-Ethyl-4a-Hydroxy-4a,5-Dihydroflavin. The Mechanism of Bacterial Luciferase. *Photochem. Photobiol.* **1990**, *51*, 629.
464. Y-J. Zheng & T. C. Bruice. Identifying the Intermediate in the Dioxygen Transfer from 4a-Hydroperoxyflavin Anion to Phenolate and Indole Anions. *Bioorganic Chem.* **1998**, *25*, 331.