

Metal-free oxygenation of cyclohexane with oxygen catalyzed by 9-mesityl-10-methylacridinium and hydrogen chloride under visible light irradiation†

Kei Ohkubo,^a Atsushi Fujimoto^a and Shunichi Fukuzumi^{*a,b}

^a *Department of Material and Life Science, Graduate School of Engineering, Osaka University and ALCA, Japan Science and Technology Agency (JST), 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan. Fax: +81-6-6879-7370; Tel: +81-6-6879-7368; E-mail: fukuzumi@chem.eng.osaka-u.ac.jp*

^b *Department of Bioinspired Science, Ewha Womans University, Seoul, 120-750, Korea.*

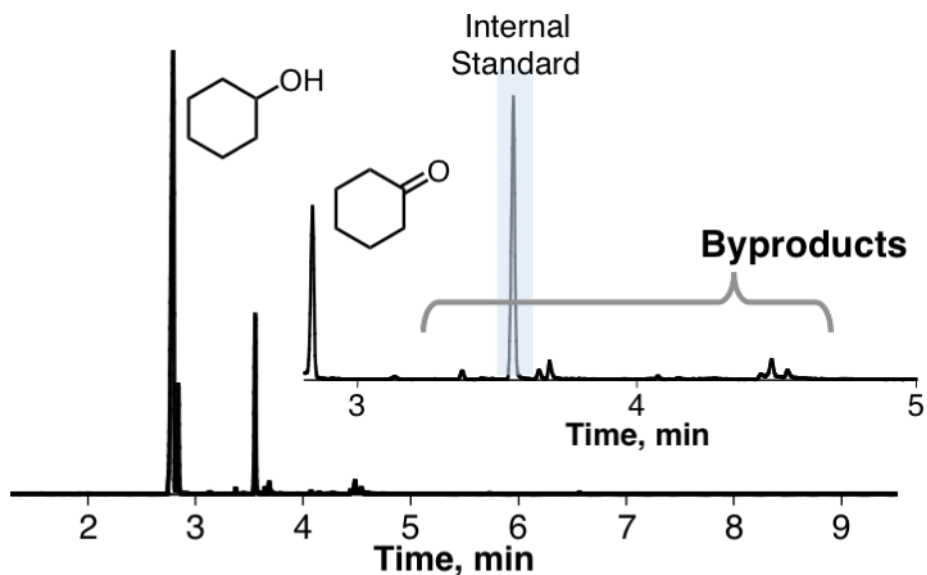


Fig. S1 GC mass chart of the reaction mixture after photooxygenation of an O₂-saturated MeCN solution containing cyclohexane (45 mM), HCl (2.0 mM) and Acr⁺-Mes (1.0 mM) irradiated by a xenon lamp (500 W, $\lambda > 390$ nm) for 3h. Internal standard: benzonitrile.

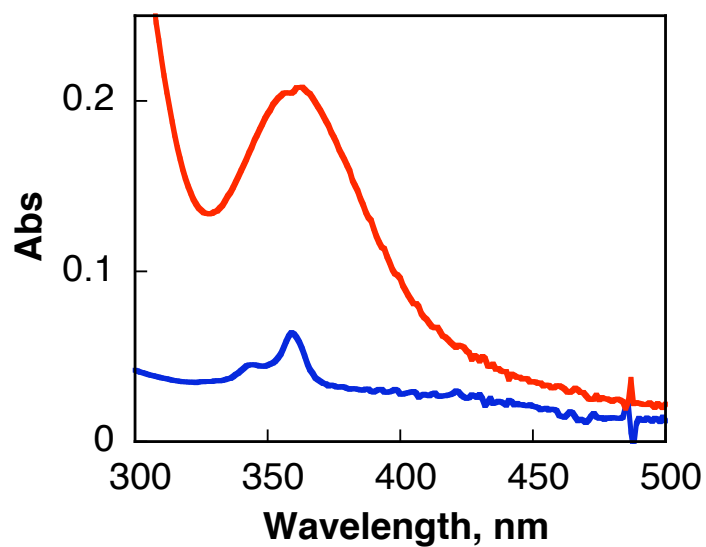


Fig. S2 UV-vis spectra of the reaction mixture after photooxygenation of cyclohexane (45 mM) with HCl (2.0 mM) and Acr⁺-Mes (1.0 mM) for 3h photoirradiation by a xenon lamp (500 W, $\lambda > 390$ nm) in MeCN in the absence (blue) and presence of NaI (red).

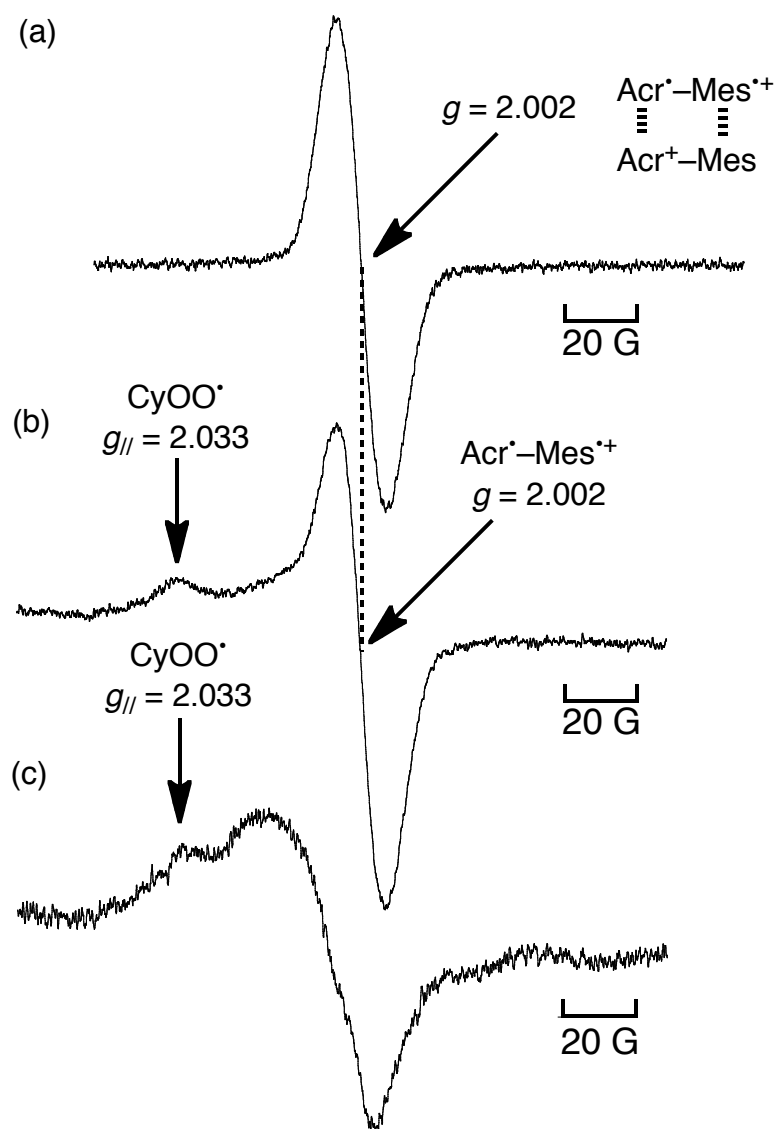


Fig. S3 ESR spectra of (a) $(\text{Acr}^\bullet\text{-Mes}^{\bullet+})(\text{Acr}^+-\text{Mes})$ generated by photoirradiation (1000-W Hg lamp) of Acr^+-Mes (10 mM) in deaerated MeCN, (b) $\text{Acr}^\bullet\text{-Mes}$ and cyclohexyl peroxy radical generated by photoirradiation of Acr^+-Mes (10 mM) with HCl (60 mM) and cyclohexane (1.0 M) in O_2 -saturated MeCN, (c) cyclohexyl peroxy radical generated by photoradiation of cyclohexane (1.0 M) with $t\text{BuOO}t\text{Bu}$ (0.50 M) in O_2 -saturated MeCN. The measurements were carried out at 77 K.