Supporting information

Photoinduced ω-bond dissociation in the higher excited singlet (S2) and lowest triplet (T1) states of a benzophenone derivative in solution

Minoru Yamaji, a,* Susumu Inomata, a Satoru Nakajima, b Kimio Akiyama, b Seiji Tobita a and Bronislaw Marciniak c

a Department of Chemistry, Gunma University, Kiryu 376-8515, Japan
b Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan
c Faculty of Chemistry, Adam Mickiewicz University, Poznan 60-780, Poland

Figure S1 shows absorption spectra of BBPS, p-methylbenzophenone (MBP) and thioanisol (TA). The absorption spectrum of BBPS can be reproduced by using those of MBP and TA in a 1:1 ratio. The molar absorption coefficient (ε) of BBPS at 266 nm was 20000 dm3 mol−1 cm−1 while those of MBP and TA were 17300 and 2800 dm3 mol−1 cm−1 at 266 nm, respectively. A sum of ε values of MBP and TA at 266 nm is close to that of BBPS, indicating that electronic conjugation between the benzoylbenzyl and phenyl thiyl moiety in BBPS is appreciably negligible. Therefore, it can be considered that upon 266 nm photolysis of BBPS, the benzoylbenzyl moiety mainly absorbs the light. Absorption of TA at 308 nm is indeed absent. The agreement in the Φrad(S2) values obtained upon laser excitation at 266 nm and 308 nm strongly supports that excitation of the phenylthiyl moiety of BBPS does not contribute to the C-S bond cleavage.
Figure S1  Absorption spectra of BBPS (black line), $p$-methylbenzophenone (MBP; red line) and thioanisol (TA; blue line) in ACN at 295 K.