Rate Constants for the β -Elimination of Tosyl Radical from a Variety of Substituted Carbon-Centered Radicals

Vitaliy I. Timokhin,^{†,‡} Stéphane Gastaldi,[†] Michèle P. Bertrand,^{*,†}
and Chryssostomos Chatgililoglu^{\$}

*Laboratoire de Chimie Moléculaire Organique – UMR 6517, Boite 562 – Faculté des
Sciences St Jérôme, Université d'Aix-Marseille III, Av. Escadrille Normandie–Niemen, 13397
Marseille Cedex 20, France, and ISOF, Consiglio Nazionale delle Ricerche, Via P. Gobetti
101, 40129 Bologna, Italy*

Supporting Information

Table of Contents :

¹ H, ¹³ C and DEPT NMR spectra data of compounds 2a , 2a' , 2b-2e , 5a-5e	S2-S34
Kinetic data for compounds 2a , 2a' , 2b-2e	S35-S36

S7

15.1493
14.6547
21.4913
22.0877
23.7678
25.5642

38.5320

135.1539
133.1829
130.4119
130.2664
129.8955
129.7282
128.8991
128.5064
128.3318
127.3718

S13

21.7402
21.6778

44.7861

64.2437

129.7681
129.7057
129.3313
128.5013
128.3328
127.9209
127.4404
127.3656
127.0473
124.7945

—65.2676

S19

—21.9059

—67.0204

134.5284
130.5574
130.4846
128.7609
128.4773

S20

S22

S25

S28

S34

Table S1. kinetic experiments with compound **2a**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
293	0.398	0.53	1.0 ± 0.1	0.13 ± 0.01
	0.513	0.651		
	0.62	0.756		

Table S2. kinetic experiments with compound **2a'**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
293	0.108	0.221	1.6 ± 0.2	0.06 ± 0.04
	0.21	0.426		
	0.275	0.479		
	0.338	0.594		

Table S3. kinetic experiments with compound **2c**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
403	0.037	0.029	0.26 ± 0.01	0.017 ± 0.004
	0.108	0.048		
	0.21	0.063		
	0.338	0.104		
	0.62	0.179		

Table S4. kinetic experiments with compound **2d**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
293	0.0074	0.968	159 ± 39	0.002 ± 0.53
	0.011	2.13		
	0.015	2.27		
	0.018	2.83		

Table S5. kinetic experiments with compound **2e**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
293	0.091	0.24	4.4 ± 0.4	- 0.14 ± 0.07
	0.126	0.42		
	0.177	0.62		
	0.189	0.77		
	0.256	0.96		

Table S6. kinetic experiments with compound **2b**

T, K	[Bu ₃ SnH] ₀ , M	[5]/[4]	k _H /k _f , M ⁻¹	intercept
293	0.0028	0.861	325 ± 47	-0.04 ± 0.17
	0.0037	1.2		
	0.0041	1.27		
353	0.03	0.351	19.8 ± 1.5	-0.29 ± 0.08
	0.044	0.539		
	0.059	0.906		
	0.073	1.18		
373	0.03	0.183	10.6 ± 0.5	-0.16 ± 0.04
	0.066	0.524		
	0.094	0.812		
	0.129	1.24		
393	0.03	0.128	7.5 ± 1.1	-0.13 ± 0.08
	0.059	0.233		
	0.087	0.572		
	0.115	0.725		
410	0.101	0.156	3.2 ± 0.8	-0.18 ± 0.09
	0.115	0.19		
	0.129	0.21		
	0.143	0.3		