Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Material

Global and Local Reactivity Indices for Electrophilic/Nucleophilic Free Radicals

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Table S1. Electronic chemical potential μ°, chemical hardness η°, global electrophilicity, ω°, and global nucleophilicity, N°, in eV, for the series of 32 FRs ordered by decreasing nucleophilicity.

	Type	R_1	R_2	R_3	μ°	η°	ω°	N°
30	**VI**				-1.63	2.94	0.45	4.79
32	**I**	OMe	OMe	H	-1.35	3.61	0.25	4.74
31	**I**	NH_2	Me	Me	-1.67	3.58	0.39	4.43
29	**I**	NH_2	H	H	-1.93	3.92	0.48	4.00
28	**I**	OH	Me	Me	-2.11	3.84	0.58	3.86
19	**III**	NH_2			-2.82	2.54	1.56	3.80
22	**IV**	OMe	H	H	-2.70	3.04	1.20	3.68
26	**I**	OMe	H	H	-2.24	3.96	0.63	3.67
27	**I**	OH	H	H	-2.20	4.18	0.58	3.60
18	**III**	OMe			-3.07	2.64	1.79	3.50
25	**I**	Me	Me	Me	-2.57	3.88	0.85	3.38
24	**I**	Me	Me	H	-2.78	4.12	0.94	3.05
13	**III**	H			-3.47	2.80	2.15	3.02
21	**I**	Cl	Me	Me	-3.23	3.85	1.36	2.73
9	**IV**	CN	H	OMe	-3.95	2.59	3.01	2.65
17	**IV**	H	H	H	-3.54	3.41	1.84	2.64
8	**IV**	CN	OMe	H	-3.98	2.61	3.03	2.60
23	**I**	Me	H	H	-3.13	4.42	1.10	2.55
12	**I**	CN	OMe	H	-3.99	3.16	2.53	2.32
7	**III**	CN			-4.30	2.57	3.61	2.31
11	**I**	CN	OH		-4.12	3.28	2.59	2.13
4	**III**	NO_2			-4.58	2.46	4.28	2.08
20	**I**	H	H	H	-3.70	4.80	1.43	1.79
5	**IV**	CN	H	H	-4.74	2.91	3.86	1.69
16	**II**	Me			-4.19	4.46	1.97	1.47
15	**II**	H			-4.24	4.45	2.02	1.42
14	**II**	OMe			-4.33	4.51	2.08	1.31
6	**I**	CN	H	H	-5.29	3.70	3.79	0.75
3	**I**	COMe	CO_2Me		-5.67	3.10	5.18	0.67
10	**III**	CN			-5.00	4.52	2.77	0.62
2	**V**				-6.09	2.86	6.49	0.37
1	**I**	CN	CN	H	-6.35	3.08	6.54	0.00

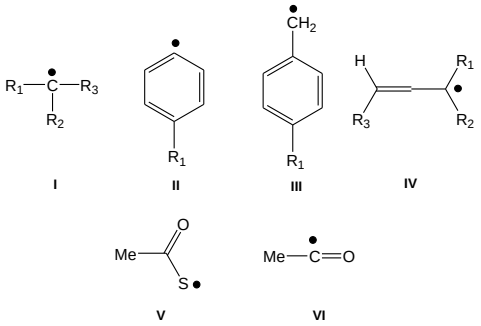

Table S2. UB3LYP/6-31G* Total (E, in au) and relative (ΔE, in kcal/mol) energies of the stationary points involved in the additions of the FRs **3** and **28** on the substituted ethylenes **33** and **35**.

	E	ΔE
3	-420.374721	
33	-632.202578	
TS11	-1052.544309	20.7
TS12	-1052.571909	3.4
IN11	-1052.554197	14.5
IN12	-1052.590956	-8.6
28	-193.697975	
35	-306.467760	
MC21	-500.180220	-9.1
MC22	-500.179186	-8.4
TS21	-500.172361	-4.2
TS22	-500.160760	3.1
IN21	-500.205880	-25.2
IN22	-500.186845	-13.2