Supplementary information

Perturbed reactivity descriptors in the two parabolas model of fractional electron number

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Substituted ethenes

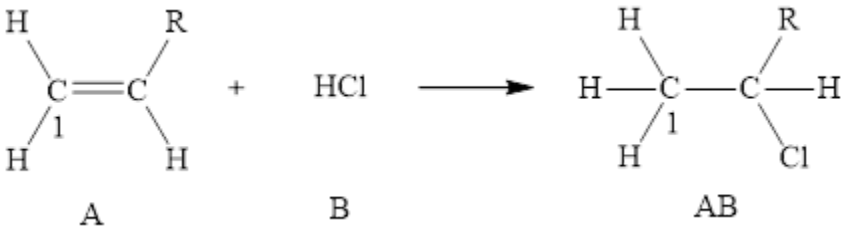

Table S-1. Frontier orbitals information for the substituted ethenes. Calculations done with the exchange-correlation density functional PBE0 and the basis set 6-311G**.

R	ε_A^{HOMO} [a]	ε_A^{LUMO} [a]	ε_{AB}^{HOMO} [a]	ε_{AB}^{LUMO} [a]	f_{kA}^{HOMO} [b]	f_{kA}^{LUMO} [b]
NH_2	-0.216	0.047	-0.278	0.021	0.380	0.246
OH	-0.247	0.038	-0.310	0.023	0.422	0.336
CH_3	-0.268	0.024	-0.306	0.030	0.423	0.368
OCH_3	-0.236	0.033	-0.302	0.024	0.379	0.327
$NHCH_3$	-0.207	0.044	-0.263	0.022	0.345	0.289
NHOH	-0.228	0.024	-0.272	0.027	0.325	0.288
$N(CH_3)_2$	-0.204	0.043	-0.251	0.021	0.318	0.231
$NHNH_2$	-0.212	0.039	-0.266	0.023	0.358	0.195
CH_2CH_3	-0.269	0.020	-0.304	0.032	0.417	0.349
F	-0.281	0.018	-0.322	0.024	0.431	0.363
H	-0.287	0.013	-0.308	0.030	0.431	0.389
	ε_B^{HOMO} [a]	ε_B^{LUMO} [a]			$f_{k,B}^{HOMO}$ [c]	$f_{k,B}^{LUMO}$ [c]
HCl	-0.350	0.006			0.044	0.489

[a] Orbital energies in hartrees.
[b] Condensed to atom Fukui functions shown for species A correspond to the C1 atom.
[c] Condensed to atom Fukui functions shown for species B correspond to the H atom.

Table S-2. Perturbation parameters values for the substituted ethenes. Second and third columns correspond to the two-parameter case. Fourth to seventh columns correspond to the four-parameter case.

R	γ	ξ	γ^{Do}	ξ^{Do}	γ^{Ac}	ξ^{Ac}
NH_2	1.03	0.99	1.11	0.95	0.91	1.05
OH	0.90	1.05	1.01	1.00	0.76	1.13
CH_3	0.91	1.05	0.85	1.08	0.99	1.01
OCH_3	0.88	1.06	0.96	1.02	0.77	1.13
$NHCH_3$	1.07	0.97	1.09	0.96	1.05	0.97
NHOH	0.97	1.02	0.86	1.08	1.12	0.94
$N(CH_3)_2$	1.14	0.93	1.08	0.96	1.22	0.90
$NHNH_2$	1.04	0.98	1.03	0.99	1.06	0.97
CH_2CH_3	0.90	1.05	0.81	1.11	1.01	1.00
F	0.88	1.06	0.88	1.07	0.88	1.06
H	0.93	1.04	0.78	1.12	1.10	0.95

Table S-3. Determination coefficient values for the isolated, two-parameter, and four-parameter cases, for the substituted ethenes.

Descriptor	Cases	R^2
μ_{kA}^{-}	Non-perturbed	0.9425
μ_{kA}^{Do}	Two-parameter	0.9768
μ_{kA}^{Do}	Four-parameter	0.9498
η_{kA}^{-}	Non-perturbed	0.5681
η_{kA}^{Do}	Two-parameter	0.9040
η_{kA}^{Do}	Four-parameter	0.9645

Substituted anilines

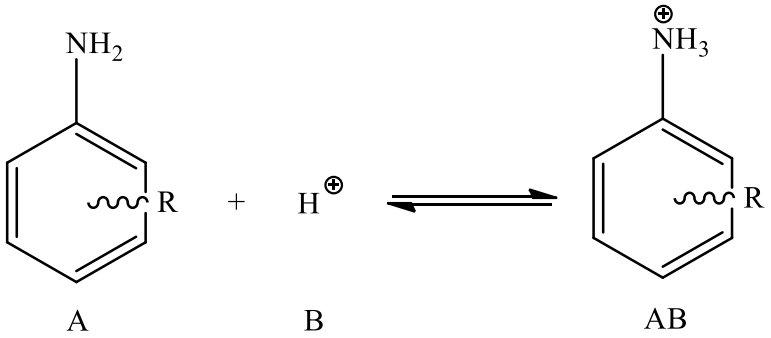

Table S-4. Frontier orbitals information for the substituted anilines. Calculations done with the exchange-correlation density functional PBE0 and the basis set 6-311G**.

R	ε_A^{HOMO} [a]	ε_A^{LUMO} [a]	ε_{AB}^{HOMO} [a]	ε_{AB}^{LUMO} [a]	f_{kA}^{HOMO} [b]	f_{kA}^{LUMO} [b]
H	-0.214	0.004	-0.434	-0.179	0.260	0.008
m-NH_2	-0.200	0.017	-0.361	-0.165	0.126	0.025
m-Br	-0.226	-0.011	-0.404	-0.186	0.248	0.007
m-CN	-0.238	-0.046	-0.438	-0.212	0.272	0.009
m-Cl	-0.226	-0.010	-0.415	-0.187	0.252	0.007
m-F	-0.223	-5.57e-5	-0.429	-0.190	0.251	0.019
m-OH	-0.211	0.010	-0.397	-0.178	0.196	0.027
m-OCH_3	-0.208	0.013	-0.387	-0.173	0.190	0.028
m-NO_2	-0.240	-0.080	-0.445	-0.230	0.280	0.004
p-NH_2	-0.185	0.006	-0.359	-0.156	0.171	0.008
p-Br	-0.219	-0.012	-0.401	-0.186	0.217	0.007
p-CN	-0.236	-0.032	-0.437	-0.215	0.232	0.071
p-Cl	-0.219	-0.012	-0.414	-0.187	0.229	0.007
p-F	-0.216	-0.009	-0.429	-0.184	0.246	0.007
p-OH	-0.198	-4.9e-4	-0.396	-0.170	0.207	0.008
p-OCH_3	-0.210	-6.4e-4	-0.384	-0.164	0.239	0.008
p-NO_2	-0.244	-0.069	-0.439	-0.228	0.258	0.039

[a] Orbital energies in hartrees.

[b] Condensed to atom Fukui functions shown for species A correspond to the N atom of the amino group.

Table S-5. Perturbation parameters values for the substituted anilines.

R	γ	ξ
H	0.71	1.17
m-NH_2	1.21	0.90
m-Br	0.98	1.01
m-CN	0.70	1.18
m-Cl	0.90	1.05
m-F	0.87	1.07
m-OH	1.02	0.99
m-OCH_3	1.06	0.97
m-NO_2	0.49	1.34
p-NH_2	0.88	1.06
p-Br	0.93	1.04
p-CN	0.84	1.09
p-Cl	0.83	1.09
p-F	0.68	1.19
p-OH	0.75	1.14
p-OCH_3	0.90	1.05
p-NO_2	0.67	1.20

Table S-6. Determination coefficient values for the substituted anilines.

Descriptor	Cases	R^2
μ_{kA}^{-}	Non-perturbed	0.5165
μ_{kA}^{Do}	Two-parameter	0.8415