Theoretical study of electron-attracting ability of the nitro group. Classical and reverse substituent effects.

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Supporting Information

Table S1 cSAR(X) values for *p*-nitrobenzene-X derivatives calculated using different atomic charges

X	VDD	Hirshfeld	Mulliken	Bader	Weinhold
NO_2	-0.102	-0.083	-0.198	-0.253	-0.164
CN	-0.125	-0.092	-0.144	-0.150	-0.149
CHO	-0.067	-0.052	-0.082	-0.080	-0.118
COOH	-0.061	-0.030	-0.098	-0.117	-0.124
COOMe	-0.038	-0.005	-0.063	-0.094	-0.112
COMe	-0.036	-0.014	-0.051	-0.053	-0.086
CF_3	-0.066	-0.045	-0.100	-0.135	-0.125
Cl	-0.006	0.026	-0.056	-0.114	0.019
H	0.033	0.030	0.032	0.031	0.040
Me	0.070	0.073	0.049	0.081	0.056
OMe	0.136	0.130	0.196	0.037	0.167
NH_2	0.180	0.166	0.182	0.117	0.183
NHMe	0.215	0.206	0.228	0.157	0.225

Table S2 Statistics of linear regressions between $cSAR(X)^{VDD}$ and cSAR(X) calculated by other methods, $cSAR(X) = a \cdot cSAR(X)^{VDD} + b$; *cc* – correlation coefficients

	a	*b*	*cc*
Hirshfeld *vs.* VDD	0.86	0.02	0.996
Mulliken *vs*. VDD	1.22	-0.02	0.981
Bader *vs*. VDD	1.01	-0.05	0.923
Weinhold *vs*. VDD	1.24	-0.03	0.982

Table S3 $cSAR(NO_2)$ values for *p*-nitrobenzene-X derivatives calculated using different atomic charges

X	VDD	Hirshfeld	Mulliken	Bader	Weinhold
NO_2	-0.102	-0.083	-0.198	-0.253	-0.164
CN	-0.113	-0.093	-0.202	-0.261	-0.161
CHO	-0.113	-0.096	-0.205	-0.272	-0.158
COOH	-0.119	-0.102	-0.209	-0.278	-0.175
COOMe	-0.130	-0.112	-0.218	-0.286	-0.176
COMe	-0.128	-0.109	-0.215	-0.284	-0.180
CF_3	-0.116	-0.096	-0.207	-0.266	-0.185
Cl	-0.148	-0.128	-0.233	-0.286	-0.201
H	-0.146	-0.128	-0.237	-0.299	-0.198
Me	-0.167	-0.147	-0.251	-0.307	-0.212
OMe	-0.195	-0.172	-0.280	-0.324	-0.262
NH_2	-0.219	-0.194	-0.296	-0.343	-0.283
NHMe	-0.236	-0.210	-0.315	-0.357	-0.305

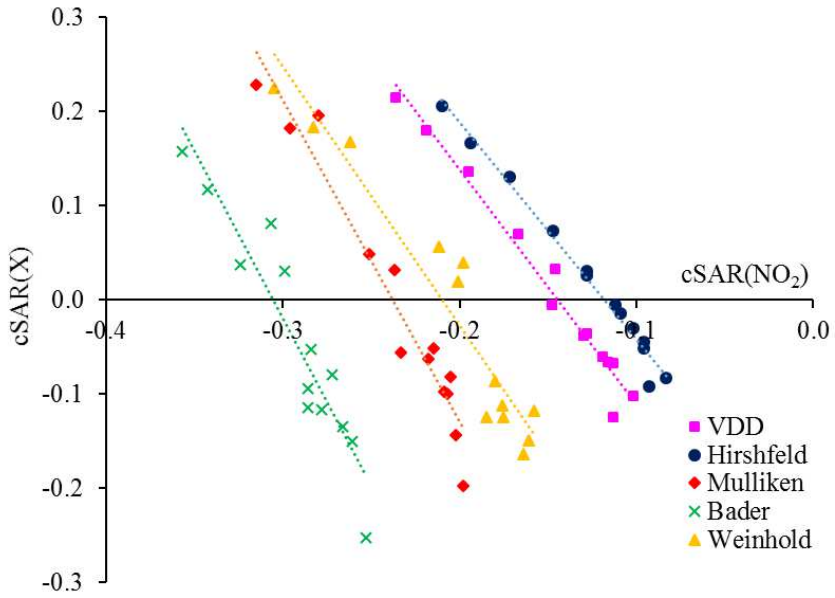

Figure S1 Correlations between cSAR(X) and cSAR(NO_2) for different atomic charge assessments for *p*-nitrobenzene-X derivatives with X = NO_2, CN, CHO, COOMe, COMe, CF_3, Cl, H, Me, OMe, NH_2 and NHMe. Correlation coefficients for VDD, Hirshfeld, Mulliken, Bader and Weinhold methods are -0.986, -0.992, -0.970, -0.940, -0.958, respectively

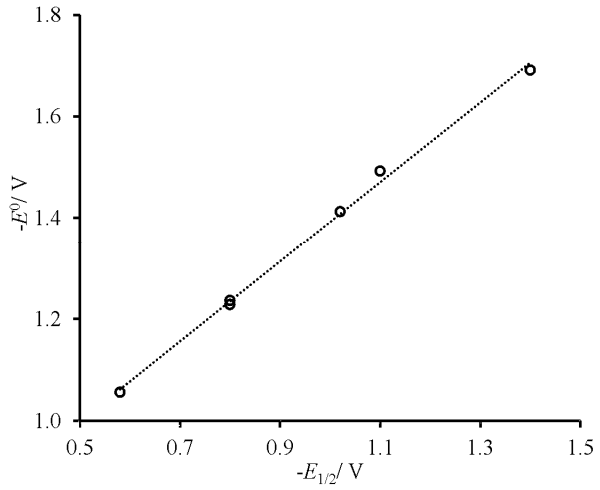

Figure S2 Relationship between formal reduction potentials, E^0, and polarographic half-wave potentials, $E_{1/2}$, for *p*-nitrobenzene-X derivatives (*cc* = 0.998)

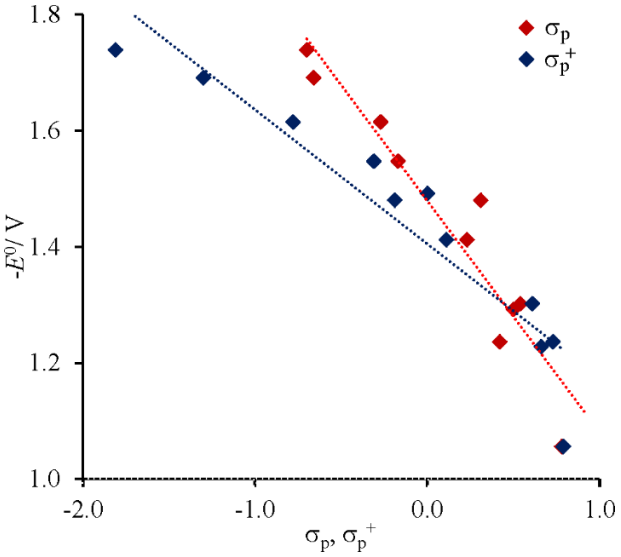

Figure S3 Relationships between formal reduction potentials and substituent constants (σ_p, σ_p^+) for *p*-nitrobenzene-X derivatives (*cc* = -0.956 and -0.940, respectively)

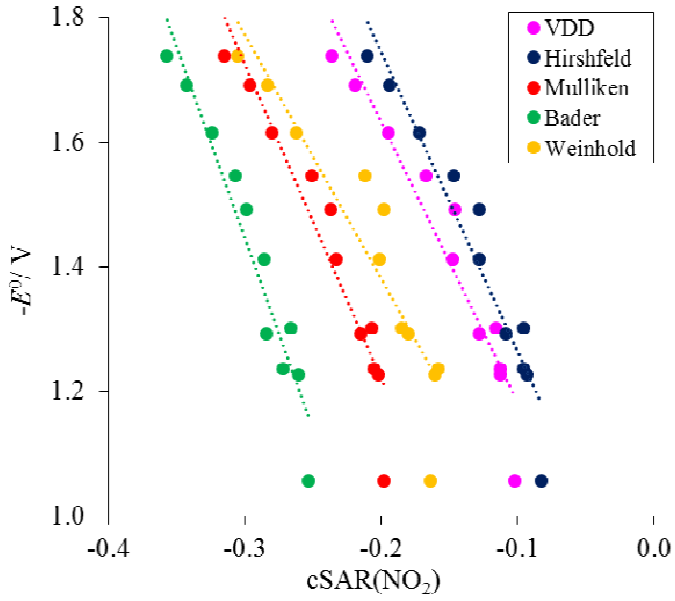

Figure S4 Relationships between formal reduction potentials (E^0) and cSAR values, calculated by VDD, Hirshfeld, Mulliken, Bader and Weinhold approaches, of the nitro group for *p*-nitrobenzene-X derivatives with X = NO_2, CN, CHO, COOMe, COMe, CF_3, Cl, H, Me, OMe, NH_2 and NHMe (*cc* = -0.957, -0.962, -0.953, -0.965, -0.926, respectively)

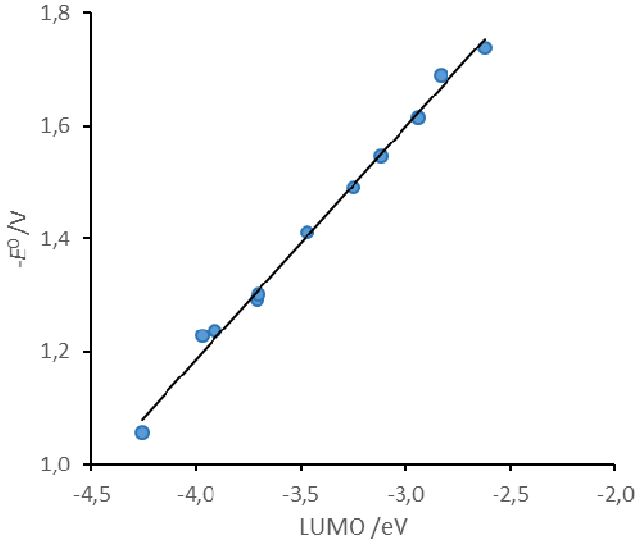

Figure S5 Correlation between formal reduction potentials and energies of LUMO orbitals for *p*-nitrobenzene-X derivatives (*cc* = 0.994)

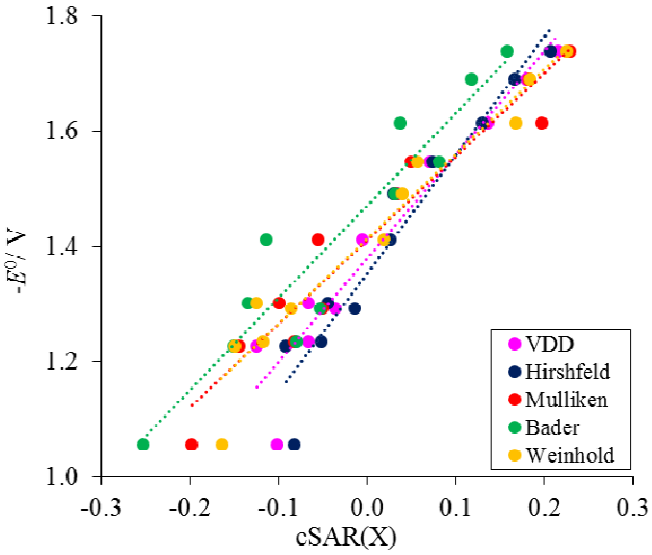

Figure S6 Relationships between formal reduction potentials (E^0) and cSAR values, calculated by VDD, Hirshfeld, Mulliken, Bader and Weinhold approaches, of the substituent X for *p*-nitrobenzene-X derivatives with X = NO_2, CN, CHO, COOMe, COMe, CF_3, Cl, H, Me, OMe, NH_2 and NHMe (*cc* = 0.962, 0.965, 0.967, 0.945, 0.972, respectively)

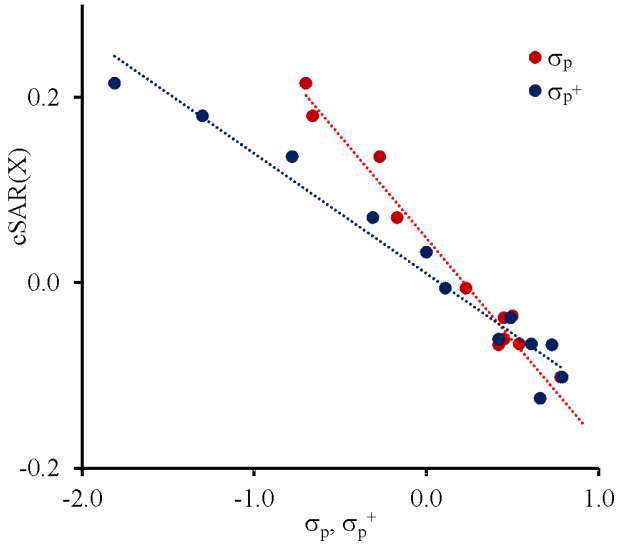

Figure S7 Relationships between cSAR(X) and substituent constants (σ_p, σ_p^+) for *p*-nitrobenzene-X derivatives (*cc* = -0.985 and -0.979, respectively)