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Supplementary Materials: Effect of Intra- and Intermolecular Interactions on the Properties of *para*-Substituted Nitrobenzene Derivatives

Halina Szatylowicz, Olga A. Stasyuk, Célia Fonseca Guerra and Tadeusz M. Krygowski

Table S1. Characteristics of substituents in *p*-nitroaniline.

	E_{rel}/kcal/mol	cSAR (NO_2)	cSAR (NH_2)	d_{CN}_NO_2/Å	d_{CN}_NH_2/Å
PNA_0	0.00	−0.219	0.181	1.467	1.386
PNA_10	0.15	−0.219	0.180	1.466	1.386
PNA_20	0.58	−0.218	0.177	1.466	1.387
PNA_30	1.33	−0.216	0.174	1.466	1.388
PNA_40	2.39	−0.213	0.168	1.467	1.390
PNA_50	3.69	−0.208	0.162	1.470	1.392
PNA_60	5.12	−0.198	0.154	1.474	1.394
PNA_70	6.49	−0.188	0.147	1.480	1.397
PNA_80	7.53	−0.177	0.138	1.485	1.399
PNA_90	7.93	−0.170	0.134	1.488	1.400

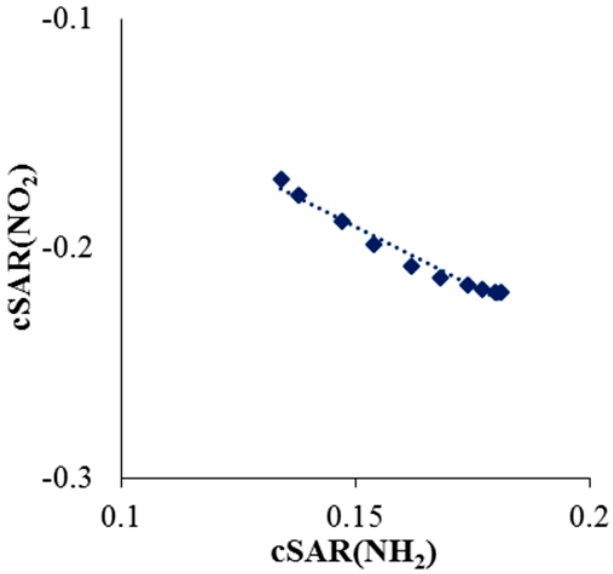

Figure S1. Dependence of cSAR(NO_2) on cSAR (NH_2) for free PNA, for linear regression *cc* = −0.985. cSAR(NO_2) = −1.039 cSAR(NH_2) − 0.035.

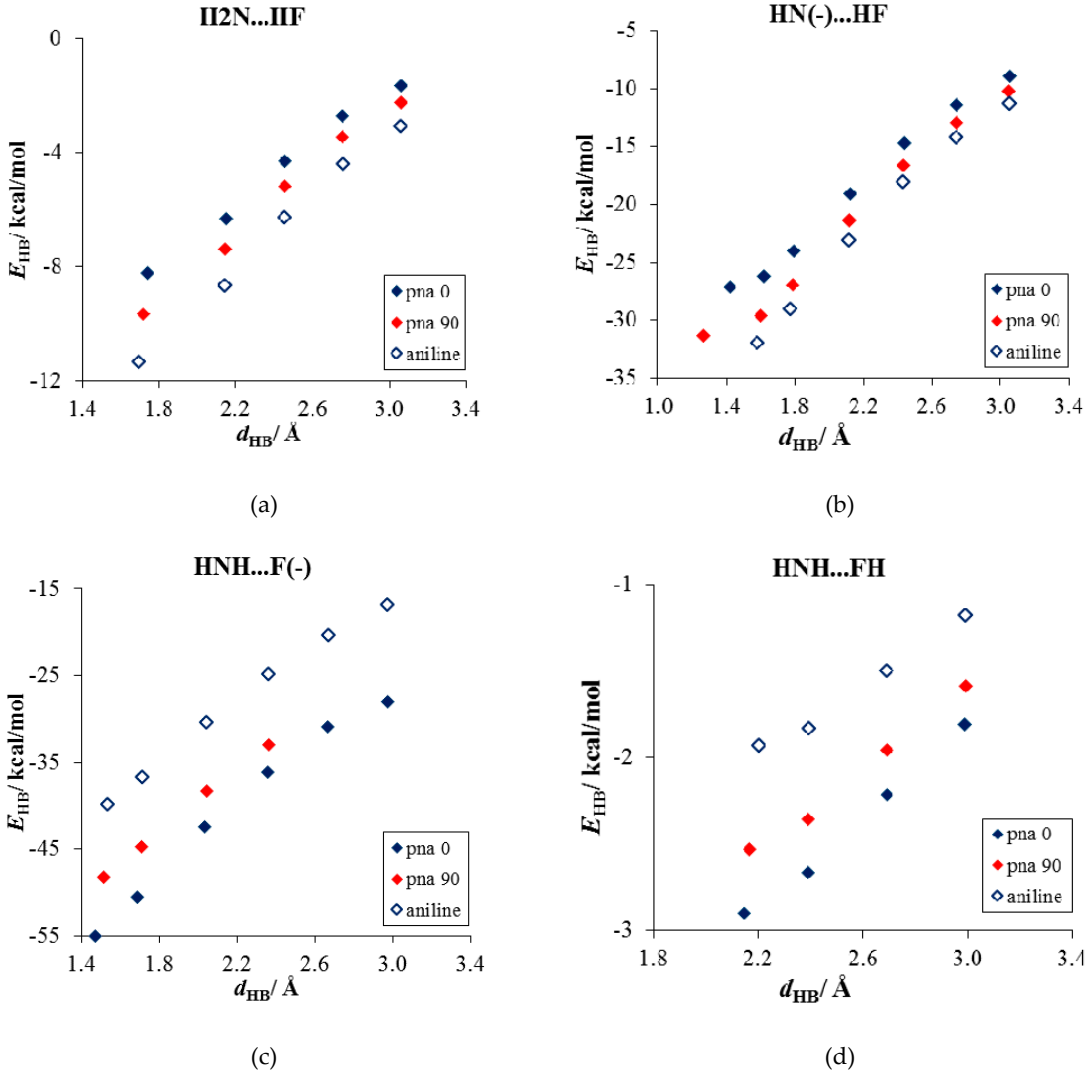

Figure S2. Relation between hydrogen bond energy, E_{HB}, and its length, d_{HB}, for the H-bonded complexes of aniline and *p*-nitroaniline (NO_2 group is coplanar and perpendicular to the ring plane) with HF or F^-.

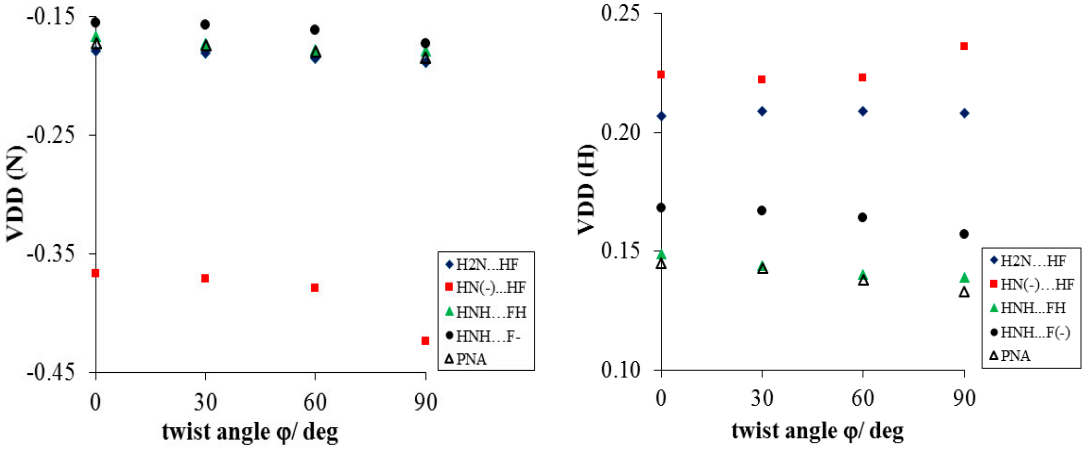

Figure S3. Dependences of VDD atomic charge at N and H atoms of the amino group on NO_2 rotation, ϕ, for fragment of *p*-nitroaniline. VDD(H) for $H_2N\cdots HF$ and $HN^-\cdots HF$ taken for the hydrogen in HF (in free HF VDD(H) = 0.204).

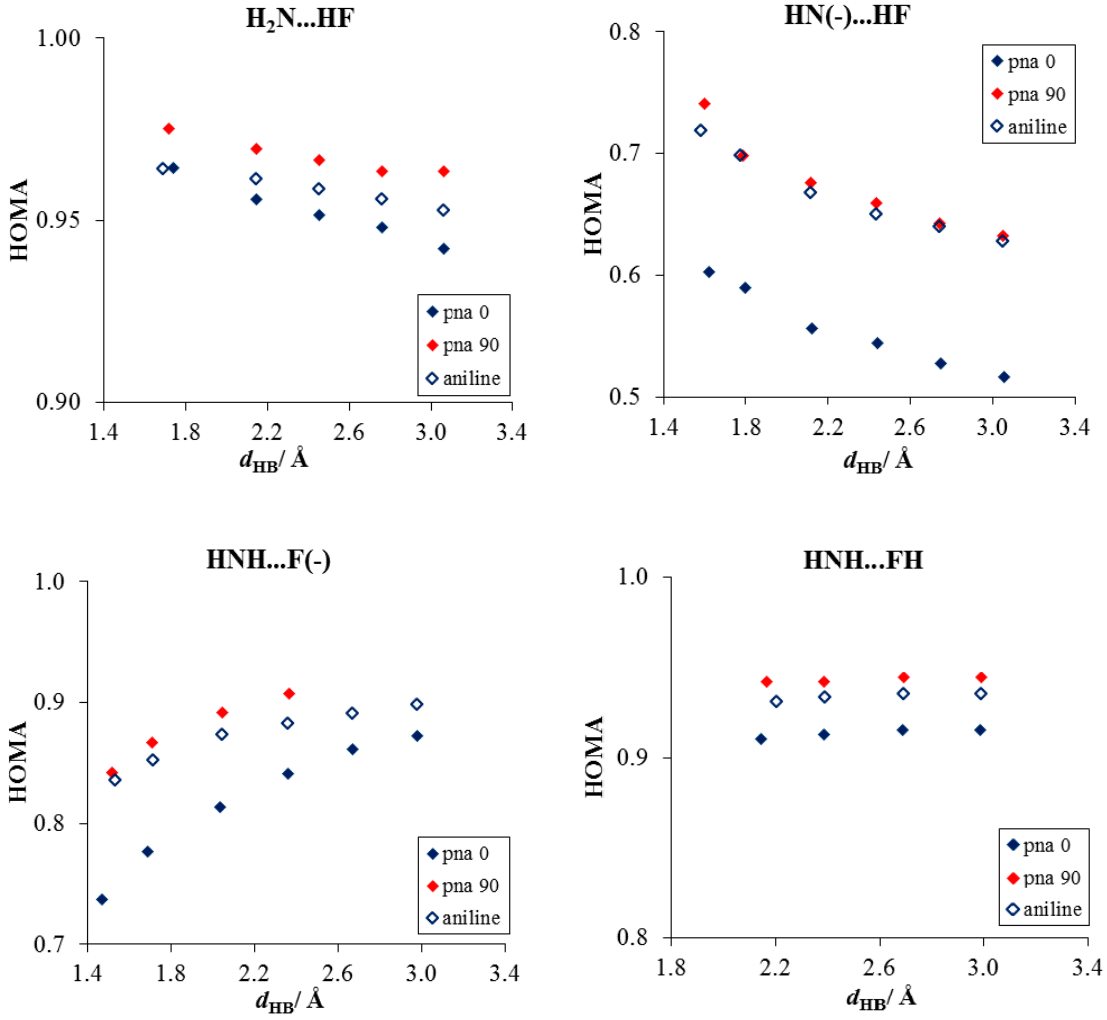

Figure S4. Dependences of HOMA values on H-bond length for different types of aniline and *p*-nitroaniline complexes (for HNH···F⁻ interactions only modeled systems are presented).

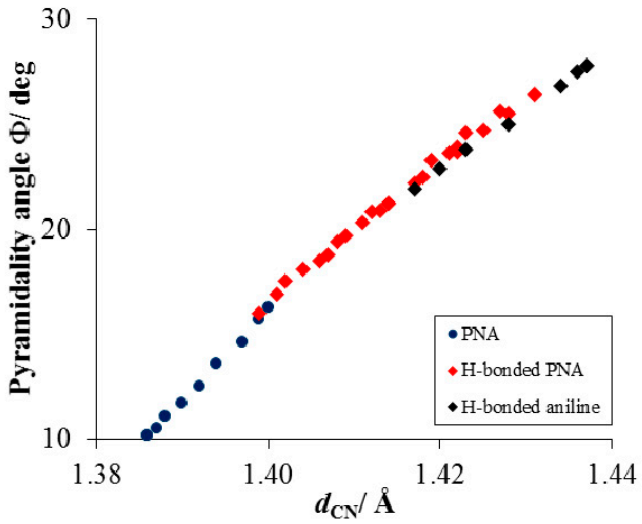

Figure S5. Correlation between angle of pyramidality of NH_2 group, Φ, and C7-N14 bond length, d_{CN} (*cc* = 0.998).

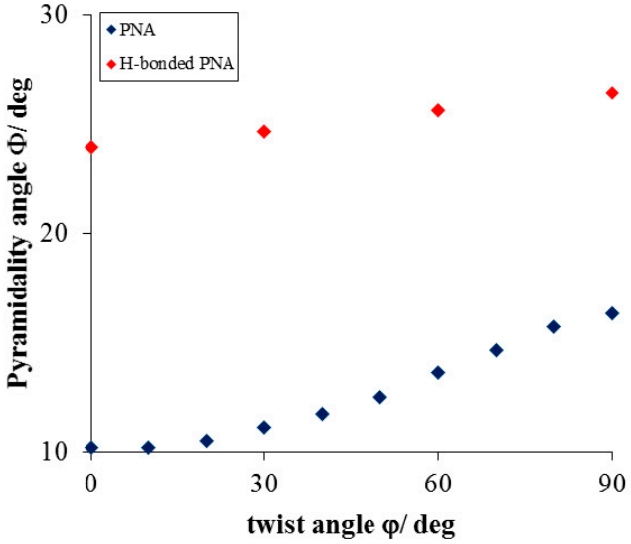

Figure S6. Dependence of pyramidality angle, Φ, of NH_2 group on rotation of NO_2 group, ϕ, for $H_2N\cdots HF$ interactions.