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Linear Free Energy Relationships in Halogen Bonds

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Table S1 I···X and Br···X distance in Å in the complexes between the *p*- and *m*-substituted halobenzenes and NH_3 (X = N), NCH (X = N) and CNH (X = C)

	Hal = I	Hal = Br			
Substituent	NH_3 (*para*)	NH_3 (*para*)	NCH (*para*)	CNH (*para*)	NH_3 (*meta*)
NO_2	3.054	3.064	3.393	3.445	3.059
CN	3.068	3.077	3.404	3.455	3.069
CF_3	3.088	3.093	3.417	3.470	3.088
$COCH_3$	3.112	3.110	3.429	3.485	3.117
CO_2H	3.106	3.106	3.426	3.482	3.110
CHO	3.093	3.094	3.418	3.476	3.097
Cl	3.114	3.115	3.436	3.493	3.106
Br	3.111	3.113	3.434	3.49	3.101
SH	3.140	3.138	3.454	3.518	3.148
F	3.121	3.121	3.441	3.500	3.108
H	3.158	3.150	3.464	3.533	3.150
SCH_3	3.157	3.150	3.467	3.524	3.130
CH_3	3.168	3.160	3.472	3.543	3.160
OCH_3	3.170	3.162	3.477	3.546	3.157
OH	3.158	3.153	3.467	3.535	3.141
NH_2	3.189	3.175	3.487	3.560	3.169
$N(CH_3)_2$	3.210	3.186	3.497	3.571	3.184

Table S2. Interaction energies (all values in kJ mol^{-1}) of the complexes between the *p*- and *m*-substituted halobenzenes and NH_3, NCH and CNH.

		Hal = I		Hal = Br					
		NH_3		NH_3		NCH		CNH	
Subs.	Position	Ei	Ei (cp)	Ei	Ei (cp)	Ei	Ei (cp)	Ei	Ei (cp)
NO_2	*p*	–22.58	–19.30	–16.09	–13.03	–7.30	–6.46	–7.39	–6.91
CN	*p*	–21.62	–18.37	–15.20	–12.20	–6.81	–5.92	–6.84	–6.34
CF_3	*p*	–20.34	–17.15	–14.07	–11.13	–6.01	–5.12	–6.01	–5.50
$COCH_3$	*p*	–18.96	–15.86	–13.16	–10.30	–5.37	–4.57	–5.33	–4.92
CO_2H	*p*	–19.28	–16.17	–13.31	–10.43	–5.39	–4.57	–5.36	–4.93
CHO	*p*	–19.73	–16.62	–14.10	–11.22	–6.18	–5.32	–6.16	–5.71
Cl	*p*	–18.60	–15.48	–12.48	–9.64	–4.93	–4.02	–4.89	–4.38
Br	*p*	–18.76	–15.63	–12.63	–9.78	–5.02	–4.11	–4.98	–4.47
SH	*p*	–17.11	–14.04	–11.17	–8.42	–4.03	–3.15	–3.96	–3.47
F	*p*	–18.20	–15.07	–12.09	–9.24	–4.67	–3.76	–4.64	–4.11
H	*p*	–16.27	–13.30	–10.56	–7.88	–3.63	–2.75	–3.54	–3.05

SCH_3	*p*	–15.94	–13.00	–10.33	–7.67	–3.45	–2.64	–3.31	–2.88
CH_3	*p*	–15.66	–12.70	–9.95	–7.31	–3.19	–2.35	–3.08	–2.64
OCH_3	*p*	–15.03	–12.09	–9.69	–7.06	–3.09	–2.32	–2.98	–2.60
OH	*p*	–16.14	–13.10	–10.26	–7.55	–3.42	–2.53	–3.33	–2.84
NH_2	*p*	–14.57	–11.60	–8.85	–6.24	–2.45	–1.60	–2.34	–1.87
$N(CH_3)_2$	*p*	–13.81	–10.92	–8.18	–5.61	–1.96	–1.11	–1.81	–1.38
NO_2	*m*			–15.71	–12.64				
CN	*m*			–15.21	–12.24				
CF_3	*m*			–13.92	–10.94				
$COCH_3$	*m*			–12.52	–9.68				
CO_2H	*m*			–12.74	–9.86				
CHO	*m*			–13.48	–10.65				
Cl	*m*			–12.83	–10.01				
Br	*m*			–12.80	–9.96				
SH	*m*			–11.59	–8.87				
F	*m*			–12.64	–9.87				
H	*m*			–10.56	–7.88				
SCH_3	*m*			–10.68	–8.00				
CH_3	*m*			–9.81	–7.28				
OCH_3	*m*			–10.23	–7.58				
OH	*m*			–10.95	–8.33				
NH_2	*m*			–9.22	–6.74				
$N(CH_3)_2$	*m*			–8.51	–5.95				

Table S3. Calculated properties of the isolated bromobenzenes

	para			*meta*		
X	C–Br	Br radius	σ hole	C–Br	Br radius	σ hole
NO_2	1.916	2.021	0.0347	1.920	2.020	0.0319
CN	1.919	2.023	0.0323	1.921	2.022	0.0308
CF_3	1.921	2.025	0.0285	1.923	2.025	0.0273
$COCH_3$	1.921	2.028	0.0256	1.928	2.030	0.0246
CO_2H	1.921	2.028	0.0257	1.926	2.029	0.0236
CHO	1.920	2.026	0.0288	1.926	2.027	0.0271
Cl	1.924	2.028	0.0234	1.924	2.028	0.0237
Br	1.924	2.028	0.0238	1.925	2.027	0.0239
SH	1.926	2.031	0.0192	1.928	2.032	0.0206
F	1.925	2.029	0.0224	1.924	2.028	0.0233
H	1.929	2.034	0.0174	1.929	2.034	0.0174
SCH_3	1.927	2.033	0.0167	1.930	2.035	0.0181

CH_3	1.930	2.035	0.0154	1.930	2.037	0.0155
OCH_3	1.928	2.035	0.0146	1.931	2.036	0.0166
OH	1.928	2.033	0.0164	1.928	2.033	0.0192
NH_2	1.930	2.037	0.0116	1.931	2.037	0.0135
$N(CH_3)_2$	1.930	2.039	0.0092	1.935	2.041	0.0106

Table S4. Br···N distance (Å) and interaction energies in the complexes between the 4-substituted 1-bromobicyclo[2.2.2]octanes and NH_3. In addition, the C-Br bond distance (Å), Br vdW radius (Å) and the MEP values (au) in the vdW surface along the C-Br bond of the isolated bromo derivatives are included.

X	E_i	E_i (cp)	Br···N	C–Br	Br radius	MEP-surface
NO_2	–7.97	–5.42	3.197	2.021	2.063	–0.0022
CN	–7.49	–4.96	3.202	2.024	2.065	0.0050
CF_3	–6.85	–4.39	3.214	2.025	2.067	0.0100
$COCH_3$	–5.70	–3.30	3.228	2.028	2.071	0.0067
CO_2H	–5.71	–3.31	3.228	2.029	2.071	0.0063
CHO	–6.32	–3.92	3.222	2.027	2.070	0.0029
Cl	–6.64	–4.17	3.213	2.025	2.068	0.0026
Br	–6.91	–4.46	3.211	2.025	2.067	0.0109
SH	–5.83	–3.43	3.226	2.029	2.071	–0.0014
F	–6.65	–4.22	3.220	2.025	2.067	0.0033
H	–4.19	–1.92	3.250	2.034	2.077	0.0056
SCH_3	–5.47	–3.09	3.233	2.030	2.073	–0.0004
CH_3	–4.44	–2.12	3.248	2.033	2.076	0.0067
OCH_3	–5.19	–2.85	3.237	2.030	2.073	0.0008
OH	–5.48	–3.09	3.231	2.029	2.071	0.0020
NH_2	–4.82	–2.48	3.240	2.031	2.074	–0.0026
$N(CH_3)_2$	–4.55	–2.28	3.248	2.031	2.075	0.0016

Table S5. Corrected interaction energy (kJ mol^{-1}) and Br···N distance (Å) in the complexes between the 3- and 4-substituted pyridines and BrCl and BrF

	Ei (cp)				Br···N distance			
	3-subst. pyridines		4-subst. pyridines		3-subst. pyridines		4-subst. pyridines	
	FBr	ClBr	FBr	ClBr	FBr	ClBr	FBr	ClBr
NO_2	–73.75	–47.1	–76.63	–49.17	2.304	2.437	2.284	2.420
CN	–75.55	–48.36	–78.86	–51.13	2.285	2.402	2.281	2.412
CF_3	–79.94	–52.4	–81.24	–53.33	2.29	2.413	2.282	2.407

$COCH_3$	–84.98	–56.48	–86.59	–57.6	2.289	2.405	2.27	2.385
CO_2H	–84.45	–56.14	–85.58	–56.58	2.285	2.402	2.271	2.391
CHO	–81.18	–53.34	–83.41	–54.72	2.286	2.405	2.273	2.397
Cl	–82.94	–54.95	–85.51	–57.17	2.302	2.434	2.279	2.394
Br	–82.31	–54.76	–85.23	–56.9	2.287	2.404	2.279	2.394
SH	–88.45	–59.68	–91.34	–62.26	2.276	2.391	2.268	2.372
F	–83.44	–55.52	–85.75	–57.53	2.268	2.37	2.282	2.396
H	–91.78	–62.82	–91.78	–62.82	2.269	2.375	2.269	2.375
SCH_3	–93.66	–64.4	–94.91	–65.29	2.266	2.375	2.264	2.363
CH_3	–94.96	–65.67	–94.92	–65.57	2.293	2.412	2.263	2.363
OCH_3	–95.05	–65.75	–96.41	–66.77	2.267	2.371	2.266	2.359
OH	–90.78	–61.95	–93.31	–64.19	2.276	2.379	2.269	2.369
NH_2	–97.25	–67.62	–101.01	–71.11	2.265	2.364	2.254	2.343
$N(CH_3)_2$	–102.45	–72.63	–105.47	–75.1	2.255	2.345	2.245	2.329

Table S6. MEP minima (au) associated to the lone pair of the pyridine

X	4-X substituted	3-X substituted
NO_2	–0.0728	–0.0721
CN	–0.0755	–0.0736
CF_3	–0.0801	–0.0796
$COCH_3$	–0.0863	–0.0879
CO_2H	–0.0857	–0.0854
CHO	–0.0816	–0.0826
Cl	–0.0872	–0.0839
Br	–0.0865	–0.0828
SH	–0.0942	–0.0888
F	–0.0884	–0.0860
H	–0.0958	–0.0958
SCH_3	–0.0986	–0.0937
CH_3	–0.0994	–0.0984
OCH_3	–0.1014	–0.0967
OH	–0.0981	–0.0926
NH_2	–0.1069	–0.1013
$N(CH_3)_2$	–0.1115	–0.1054

Table S7. Ei(cp)energies (kJ mol^{-1}) of the complexes between the 4-substituted-1-bromobenzenes and 4-substituted pyridines calculated at the B97D/6-311+G(d) computational level. The substituents in the 1-bromobenzene derivatives are indicated in the columns and the substituents of the pyridines are indicated in each row.

	NO_2	CN	CF_3	$COCH_3$	CO_2H	CHO	Cl	Br	SH	F	H	SCH_3	CH_3	OCH_3	OH	NH_2	NMe_2
NO_2	–11.05	–10.63	–10.02	–9.72	–9.84	–10.15	–9.47	–9.54	–8.90	–9.29	–8.63	–8.58	–8.37	–8.29	–8.51	–7.92	–7.65
CN	–11.40	–10.94	–10.41	–9.93	–10.05	–10.41	–9.64	–9.72	–9.01	–9.45	–8.71	–8.66	–8.43	–8.34	–8.58	–7.93	–7.70
CF_3	–11.99	–11.46	–10.79	–10.24	–10.36	–10.79	–9.88	–9.97	–9.12	–9.87	–8.67	–8.71	–8.40	–8.31	–8.59	–7.86	–7.47
$COCH_3$	–12.82	–12.18	–11.37	–10.66	–10.72	–11.40	–10.23	–10.34	–9.32	–9.95	–8.88	–8.89	–8.46	–8.32	–8.68	–7.68	–7.24
CO_2H	–12.78	–12.15	–11.22	–10.59	–10.86	–11.28	–10.22	–10.32	–9.30	–9.94	–8.87	–8.74	–8.45	–8.27	–8.67	–7.72	–7.26
CHO	–12.16	–11.60	–10.86	–10.32	–10.41	–10.87	–9.93	–10.03	–9.14	–9.69	–8.76	–8.70	–8.40	–8.16	–8.57	–7.76	–7.39
Cl	–12.87	–12.22	–11.39	–10.71	–10.82	–11.41	–10.24	–10.35	–9.31	–9.95	–8.87	–8.77	–8.44	–8.28	–8.66	–7.67	–7.33
Br	–12.80	–12.16	–11.36	–10.67	–10.78	–11.38	–10.21	–10.32	–9.29	–9.93	–8.97	–8.77	–8.43	–8.28	–8.65	–7.68	–7.21
SH	–13.92	–13.15	–12.12	–11.31	–11.43	–12.19	–10.74	–10.87	–9.49	–10.39	–9.08	–8.97	–8.57	–8.38	–8.82	–7.65	–7.08
F	–13.01	–12.34	–11.49	–10.80	–10.92	–11.53	–10.32	–10.44	–9.36	–10.03	–8.92	–8.82	–8.48	–8.32	–8.70	–7.69	–7.32
H	–14.11	–13.31	–12.17	–11.42	–11.54	–12.32	–10.82	–10.96	–9.66	–10.46	–9.11	–8.99	–8.57	–8.37	–8.84	–7.60	–7.02
SCH_3	–14.65	–13.80	–12.54	–11.60	–11.96	–12.75	–11.13	–11.27	–9.90	–10.74	–9.30	–9.13	–8.73	–8.54	–9.03	–7.77	–7.31
CH_3	–14.70	–13.84	–12.71	–11.79	–11.90	–12.77	–11.12	–11.27	–9.86	–10.73	–9.26	–9.16	–8.56	–8.48	–8.97	–7.63	–7.01
OCH_3	–15.00	–14.11	–12.85	–11.92	–12.17	–12.98	–11.28	–11.43	–9.97	–10.87	–9.35	–9.44	–8.75	–8.64	–9.05	–7.96	–7.30
OH	–14.44	–13.61	–12.50	–11.63	–11.75	–12.54	–11.00	–11.14	–9.70	–10.63	–9.21	–9.11	–8.66	–8.83	–8.91	–7.69	–7.28
NH_2	–15.93	–14.81	–13.61	–12.58	–12.66	–13.73	–11.64	–11.79	–10.30	–11.18	–9.60	–9.47	–8.79	–8.70	–9.27	–7.72	–6.98
NMe_2	–16.79	–15.69	–14.23	–13.01	–13.24	–14.38	–12.20	–12.39	–10.62	–11.70	–9.86	–9.79	–9.11	–8.82	–9.46	–8.06	–7.18

List of equations.

$\sigma_I = (0.996\pm0.038)\ \sigma_F$, n = 16, $R^2 = 0.978$

Dist (N···Br, 4X-1Br-Benzene:NH_3)= -0.92±0.04 + 1.17±0.01*Dist(N···Br, 4X-1Br-Benzene:NCH), R_2= 0.998, n=17

Dist (N···Br, 4X-1Br-Benzene:NH_3)= -0.18±0.07 + 0.94±0.02*Dist(C···Br, 4X-1Br-Benzene:CNH), R^2= 0.993, n=17

Dist (N···Br, 4X-1Br-Benzene:NCH)= 0.63±0.06 + 0.80±0.02*Dist(C···Br, 4X-1Br-Benzene:CNH), R^2= 0.992, n=17

Dist (N···Br, 4X-1Br-Benzene:NH_3)= 0.08±0.13 + 0.97±0.04*Dist(N···Br, 3X-1Br-Benzene:NH_3), R^2= 0.97, n=17

Ei(cp) (4X-1Br-Benzene:NH_3)= 2.03±0.03 + 0.936±0.002*Ei (4X-1Br-Benzene:NH_3), R_2= 0.9999, n=17

Ei(cp) (4X-1Br-Benzene:NCH)= 0.83±0.03 + 0.994±0.006*Ei (4X-1Br-Benzene:NCH), R_2= 0.9992, n=17

Ei(cp) (4X-1Br-Benzene:CNH)= 0.42±0.03 + 0.991±0.006*Ei (4X-1Br-Benzene:CNH), R_2= 0.9993, n=17

Ei(cp) (3X-1Br-Benzene:NH_3)= 1.83±0.07 + 0.922±0.006*Ei (3X-1Br-Benzene:NH_3), R_2= 0.9993, n=17

Eq. [6], Ei(cp) (4X-1Br-Benzene:NH_3)= –197.±3.+ 60.1±0.9*Dist(N···Br, 4X-1Br-Benzene:NH_3), R_2= 0.996, n=17, SD=0.13

Eq. [7], Ei(cp) (4X-1Br-Benzene:NH_3)= –8.6±0.2 –4.5±0.4*σ_p (X), R_2= 0.916, n=17, SD=0.63

Eq. [8], Ei(cp) (4X-1Br-Benzene:NH_3)= –7.9±0.2–6.0±0.4*σ_F (X) –5.7±0.3*σ_R (X), R_2= 0.982, n=16, SD=0.29

Eq. [9], Ei(cp) (4X-1Br-Benzene:NH_3)= –921.±54.– 474±28*Dist(C-Br, 4X-1Br-Benzene), R_2= 0.950, n=17, SD=0.49.

Eq. [10], Ei(cp) (4X-1Br-Benzene:NH_3)= –859±30.– 418±15*Dist(Br-radius, 4X-1Br-Benzene), R_2= 0.982, n=17, SD=0.29.

Eq. [11], Ei(cp) (4X-1Br-Benzene:NH_3)= –2.82±0.05 –292.±2.* σ hole(4X-1Br-Benzene), R_2= 0.999, n=17, SD=0.06

Eq. [12], Ei(cp) (3X-1Br-Benzene:NH_3)= –170.±8. + 51.±3.*Dist(N···Br, 3X-1Br-Benzene:NH_3), R_2= 0.965, n=17, SD=0.36

Eq. [13], Ei(cp) (3X-1Br-Benzene:NH_3)= –7.4±0.2–7.4±0.2*σ_m (X),
R_2= 0.942, n=17, SD=0.46

Eq. [14], Ei(cp) (3X-1Br-Benzene:NH_3)= –7.7±0.2–6.4±0.4*σ_F (X) –4.2±0.3*σ_R (X),
R_2= 0.974, n=16, SD=0.31

Eq. [15], Ei(cp) (3X-1Br-Benzene:NH_3)= –890±65.– 457±34*Dist(C-Br, 3X-1Br-Benzene),
R_2= 0.925, n=17, SD=0.53.

Eq. [16], Ei(cp) (3X-1Br-Benzene:NH_3)= –670.±20.– 325.±10.*Dist(Br-radius, 3X-1Br-Benzene),
R_2= 0.986, n=17, SD=0.23.

Eq. [17], Ei(cp) (3X-1Br-Benzene:NH_3)= –2.5±0.2–312±7* σ hole(3X-1Br-Benzene),
R_2= 0.991, n=17, SD=0.18

Eq. [18], Ei(cp) (3/4X-1Br-Benzene:NH_3)= –183.±5.+ 56.±2.*Dist(N···Br, 3/4X-1Br-Benzene:NH_3), R_2= 0.976, n=34, SD=0.31

Eq. [19], Ei(cp) (3/4X-1Br-Benzene:NH_3)= –8.3±0.1–5.0±0.4*σ_m/σ_p (X),
R_2= 0.852, n=34, SD=0.77

Eq. [20], Ei(cp) (3/4X-1Br-Benzene:NH_3)= –7.8±0.1–6.2±0.3*σ_F (X) –5.0±0.3*σ_R (X),
R_2= 0.975, n=32, SD=0.35

Eq. [21], Ei(cp) (3/4X-1Br-Benzene:NH_3)= –829±61.– 426±32*Dist(C-Br, 3/4X-1Br-Benzene),
R_2= 0.850, n=34, SD=0.77.

Eq. [22], Ei(cp) (3/4X-1Br-Benzene:NH_3)= –750±26.– 365±13.*Dist(Br-radius, 3/4X-1Br-Benzene), R_2= 0.963, n=34, SD=0.38.

Eq. [23], Ei(cp) (3X-1Br-Benzene:NH_3)= –2.68±0.09–300±4*σ hole(3/4X-1Br-Benzene),
R_2= 0.994, n=34, SD=0.15

Eq. [24], Ei(cp) (3/4X-1Br-Benzene:NH_3/NCH/CNH)= 21±5–290±208*σ hole(3/4X-1Br-Benzene) –0.028±0.006*PA(NH_3/NCH/CNH) –0.7±0.3*σ hole*PA, R_2= 0.927, n=68, SD=0.86

Eq. [25], Ei(cp) (3/4X-1Br-Benzene:NH_3/NCH/CNH)= 4.7±0.2–117±7*σ hole(3/4X-1Br-Benzene) –60±2*MEP minimum(NH_3/NCH/CNH) + 1470±70*σ hole*MEP, R_2= 0.998, n=68, SD=0.11

Eq. [26], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= 1.99±0.03.– 0.930±0.004* Ei(1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3), R_2= 0.9997, n=17, SD=0.02.

Eq. [27], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= –2.1±0.1.–4.6±0.4*σ_F (X),
R_2= 0.897, n=17, SD=0.34.

Eq. [28], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= –210±7 + 64±2*Dist(N···Br, 1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3), R_2= 0.984, n=17, SD=0.13

Eq. [29], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= –588±27.+ 288±13*Dist(C-Br, 1-Bromo-4-X-bicyclo[2.2.2]octanes), R_2= 0.969, n=17, SD=0.19.

Eq. [30], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= –527±18 + 253±9*Dist(Br-radius, 1-Bromo-4-X-bicyclo[2.2.2]octanes), R_2= 0.983, n=17, SD=0.14.

Eq. [31], Ei(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)= –2.63±0.03 –254±5*MEP(1-Bromo-4-X-bicyclo[2.2.2]octanes), R_2= 0.993, n=17, SD=0.09.

Ei(cp) (4X-1Br-Benzene:NH_3)= (-7.±1.) + 2.1±0.3* E_i(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes: NH_3), R^2 = 0.74, n=17.

Eq. [32], E_i(cp) (4X-1Br-Benzene:NH_3) = –(7.9±0.2) – (4.1±1.5)σ_F – (5.6±0.3)σ_R– (1.7±1.4)σ_I, R^2 = 0.986, n=17

Eq, [33], E_i(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3) = –(2.2±0.1) – (2.9±1.0)σ_F – (0.9±0.2)σ_R– (1.7±0.9)σ_I, R^2 = 0.973, n=17.

Eq. [34], E_i(cp) (4X-1Br-Benzene:NH_3)-coded = (0.38±0.04) – (1.1±0.4)σ_F – (1.51±0.08)σ_R– (0.5±0.4)σ_I, R^2 = 0.986

Eq. [35], E_i(cp) (1-Bromo-4-X-bicyclo[2.2.2]octanes:NH_3)-coded = (0.84±0.06) – (1.6±0.6)σ_F – (0.5±0.1)σ_R– (1.0±0.5)σ_I, R^2 = 0.973

Eq. [36], Ei(cp) (FBr:3X-pyridines)= –94.8±0.8 + 31±2*σ_m(X),
R^2= 0.921, n=17, SD=2.30

Eq. [37], Ei(cp) (FBr:4X-pyridines)= –90.9±0.6 + 16±1*σ_p(X),
R^2= 0.907, n=17, SD=2.45

Eq. [38], Ei(cp) (FBr:3/4X-pyridines)= –91.6±0.6 + 19±2.*σ_m/σ_p(X),
R^2= 0.834, n=34, SD=3.24

Eq. [39], Ei(cp) (ClBr:3X-pyridines)= –65.6±0.7 + 28. ±2.*σ_m(X),
R^2= 0.921, n=17, SD=2.05

Eq. [40], Ei(cp) (ClBr:4X-pyridines)= –61.9±0.5+ 15.0±1*σ_p(X),
R^2= 0.920, n=17, SD=2.06

Eq. [41], Ei(cp) (ClBr:3/4X-pyridines)= –62.6±0.5 + 18.±1.*σ_m/σ_p(X),
R^2= 0.834, n=34, SD=2.81

Eq. [42], Ei(cp) (FBr/ClBr:3/4X-pyridines)= 34±5 + 570±54*MEP mínima(3/4X-pyridines) – 628±70*σ hole(FBr/ClBr) + 2402±776*MEP*σ hole, R^2= 0.996, n=68, SD=1.07

Eq. [43], Ei(cp) (4X-1Br-benzenes:4X-pyridines)= –9.88±0.04 –4.00±0.08*σ_p(4X-1Br-benzenes) +1.13±0.08*σ_p(4X-pyridines) + 2.21±0.18*σ_p(4X-1Br-benzenes)*σ_p(4X-pyridines),
R^2= 0.902, n=289, SD=0.60

Eq. [44], Ei(cp) (4X-1Br-benzenes:4X-pyridines)= –12.0±0.2 – 332±10*σ hole(4X-1Br-benzenes) – 78±2*MEP minimum (4X-pyridines) + 6351±105*σ hole(4X-1Br-benzenes)*MEP(4X-pyridines), R^2= 0.995, n=289, SD=0.13