Supporting Information (SI)

Substituent Effect on the σ- and π-Electron Structure of the Nitro Group and the Ring in *Meta*- and *Para*-Substituted Nitrobenzenes

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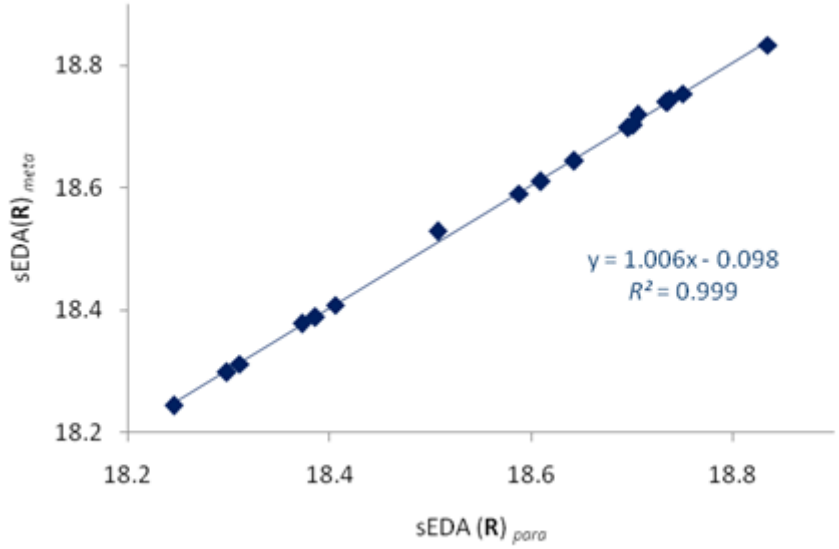

Fig. S1. Dependence of sEDA(**R**) for *meta*-substituted series on that for the *para*- systems.

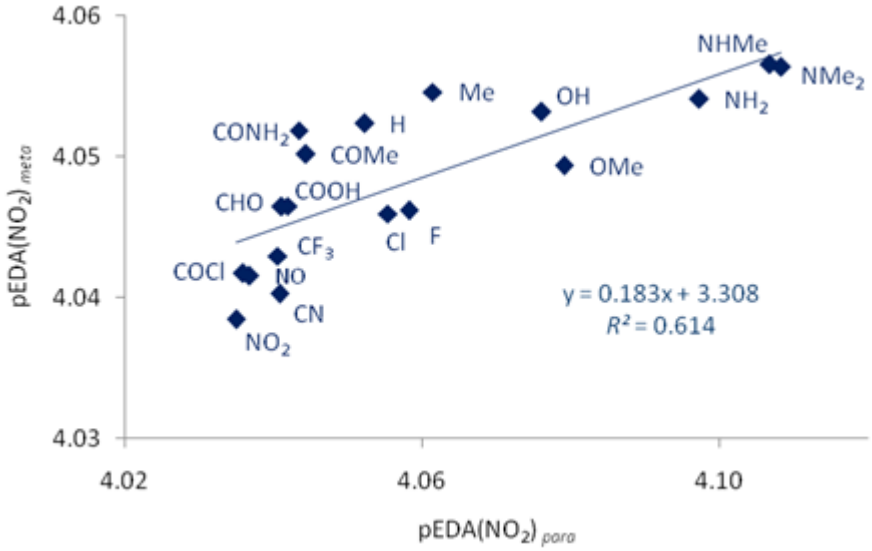

Fig. S2. Dependence of $pEDA(NO_2)_{meta}$ *vs* $pEDA(NO_2)_{para}$ for substituted nitrobenzene derivatives.

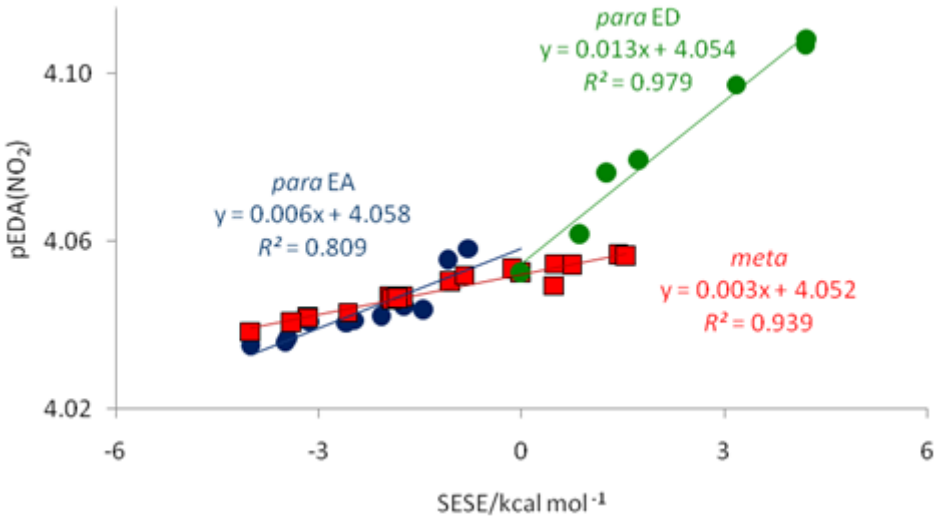

Fig. S3. Dependence of pEDA(NO_2) on SESE for *meta*- and *para*- substituted nitrobenzene derivatives with separation of the data for *para* derivatives into ED ($\sigma \leq 0$) and EA ($\sigma > 0$) substituents.

Table S1. σ, cSAR, SESE and HOMA values for *para*- and *meta*-substituted nitrobenzenes, B3LYP/6-311++G(d,p) results.

X	**σ***	**cSAR(X)**	**cSAR(NO_2)**	**SESE kcal/mol**	**HOMA**
para-					
NO	0.91	-0.131	-0.147	-3.46	0.989
NO_2	0.78	-0.169	-0.169	-4.01	0.998
COCl	0.69	-0.175	-0.155	-3.49	0.984
CN	0.66	-0.151	-0.163	-3.12	0.980
CF_3	0.54	-0.113	-0.169	-2.58	0.994
COMe	0.50	-0.091	-0.179	-1.72	0.983
COOH	0.45	-0.128	-0.174	-2.08	0.988
CHO	0.42	-0.114	-0.162	-2.46	0.986
$CONH_2$	0.36	-0.065	-0.188	-1.45	0.988
Cl	0.23	0.016	-0.204	-1.09	0.996
F	0.06	0.100	-0.217	-0.77	0.998
H	0.00	0.042	-0.202	0.00	0.993
Me	-0.17	0.059	-0.220	0.87	0.984
OMe	-0.27	0.167	-0.263	1.74	0.974
OH	-0.37	0.163	-0.251	1.27	0.985
NH_2	-0.66	0.187	-0.286	3.17	0.955
NHMe	-0.70	0.225	-0.307	4.20	0.933
NMe_2	-0.83	0.219	-0.303	4.23	0.911
meta-					
NO	0.62	-0.152	-0.185	-3.14	0.989
NO_2	0.71	-0.167	-0.167	-4.00	0.997
COCl	0.53	-0.193	-0.181	-3.14	0.985
CN	0.56	-0.172	-0.174	-3.39	0.983
CF_3	0.43	-0.130	-0.183	-2.57	0.995
COMe	0.38	-0.113	-0.185	-1.04	0.986
COOH	0.37	-0.149	-0.192	-1.75	0.989
CHO	0.35	-0.136	-0.192	-1.93	0.987
$CONH_2$	0.28	-0.087	-0.196	-0.84	0.990
Cl	0.37	-0.010	-0.173	-1.93	0.996
F	0.34	0.075	-0.173	-1.82	0.996
H	0.00	0.019	-0.202	0.00	0.993
Me	-0.07	0.032	-0.198	0.48	0.987
OMe	0.12	0.126	-0.188	0.5	0.984
OH	0.12	0.129	-0.181	-0.14	0.991
NH_2	-0.16	0.163	-0.185	0.75	0.978
NHMe	-0.21	0.173	-0.191	1.43	0.960
NMe_2	-0.16	0.163	-0.194	1.55	0.945

* Hansch, C.; Leo, A.; Taft, R. W. *Chem. Rev.* **1991**, *91*, 165–195.

Table S2. The obtained pEDA and sEDA values for the nitro group -NO_2 and transmitting moiety **R** (benzene ring) parts for *para*- and *meta*-substituted nitrobenzenes.

	-NO_2		X-**R**-Y	
X	sEDA(NO_2)	pEDA(NO_2)	sEDA(**R**)	pEDA(**R**)
para-				
NO	13.1280	4.0368	18.5878	5.8300
NO_2	13.1248	4.0350	18.5070	5.8836
COCl	13.1272	4.0359	18.7379	5.8615
CN	13.1260	4.0408	18.6959	5.9102
CF_3	13.1279	4.0406	18.7007	5.9127
COMe	13.1315	4.0444	18.7344	5.8737
COOH	13.1308	4.0419	18.7339	5.8766
CHO	13.1300	4.0411	18.7501	5.8622
$CONH_2$	13.1345	4.0434	18.7052	5.9072
Cl	13.1288	4.0554	18.6094	5.9956
F	13.1288	4.0583	18.2450	5.9898
H	13.1343	4.0524	18.8341	5.9179
Me	13.1348	4.0615	18.6426	5.9319
OMe	13.1324	4.0791	18.2978	6.0356
OH	13.1312	4.0761	18.3105	6.0288
NH_2	13.1331	4.0973	18.4055	6.0664
NHMe	13.1336	4.1068	18.3854	6.0935
NMe_2	13.1343	4.1084	18.3723	6.1061
meta-				
NO	13.1241	4.0416	18.5910	5.8175
NO_2	13.1207	4.0384	18.5287	5.8776
COCl	13.1237	4.0417	18.7460	5.8516
CN	13.1230	4.0403	18.6983	5.9047
CF_3	13.1255	4.0430	18.7032	5.9082
COMe	13.1301	4.0502	18.7400	5.8636
COOH	13.1286	4.0465	18.7403	5.8683
CHO	13.1279	4.0465	18.7539	5.8512
$CONH_2$	13.1302	4.0518	18.7201	5.8899
Cl	13.1276	4.0459	18.6101	5.9959
F	13.1285	4.0462	18.2442	5.9958
H	13.1343	4.0524	18.8341	5.9179
Me	13.1358	4.0546	18.6440	5.9347
OMe	13.1342	4.0493	18.2980	6.0488
OH	13.1330	4.0532	18.3116	6.0373
NH_2	13.1371	4.0541	18.4084	6.0738
NHMe	13.1389	4.0566	18.3883	6.1114
NMe_2	13.1387	4.0563	18.3781	6.1134

Table S3. Statistical characteristic of received dependencies for *para*- and *meta*-substituted nitrobenzenes (Y = *a* X + *b*).

	Y	X	a	b	R^2	Y_{SEE}*	F**
Fig. 1	$HOMA_{meta}$	$HOMA_{para}$	0.561 ± 0.024	0.436 ± 0.024	0.970	0.002	522.76
Fig. 2	$pEDA(\mathbf{R})_{meta}$	$pEDA(\mathbf{R})_{para}$	1.100 ± 0.013	-0.598 ± 0.077	0.998	0.005	7256.26
Fig. 3	$pEDA(\mathbf{R})_{p,m}$	$sEDA(\mathbf{R})_{p,m}$					
N			-1.4199 ± 0.073	32.18 ± 1.35	0.979	0.020	374.14
O			-2.676 ± 0.547	55.00 ± 10.01	0.749	0.022	29.94
C			-0.775 ± 0.066	20.39 ± 1.24	0.907	0.009	137.40
Fig. 4 a	$pEDA(NO_2)$	$pEDA(\mathbf{R})$					
para ED			0.286 ± 0.032	2.361 ± 0.191	0.942	0.006	81.51
para EA			0.127 ± 0.023	3.293 ± 0.135	0.775	0.004	31.05
meta			0.040 ± 0.011	3.808 ± 0.066	0.452	0.004	13.21
Fig. 4 b	$pEDA(NO_2)$	$pEDA(\mathbf{R})$					
para R<0			0.475 ± 0.029	1.209 ± 0.175	0.982	0.003	270.72
para R≥0			0.100 ± 0.052	3.454 ± 0.303	0.320	0.004	3.76
meta			0.040 ± 0.011	3.808 ± 0.066	0.452	0.004	13.21
Fig. 5	$pEDA(NO_2)$	σ					
para ED			-0.070 ± 0.006	4.053 ± 0.003	0.963	0.005	130.22
para EA			-0.027 ± 0.004	4.057 ± 0.003	0.810	0.003	38.37
meta			-0.019 ± 0.002	4.053 ± 0.001	0.892	0.002	132.55
Fig. 6	$pEDA(NO_2)$	cSAR(X)					
para ED			0.286 ± 0.040	4.040 ± 0.007	0.911	0.0071	51.26
para EA			0.087 ± 0.008	4.051 ± 0.001	0.928	0.0021	115.82
meta			0.034 ± 0.006	4.049 ± 0.001	0.650	0.0035	29.74
Fig. 7	$sEDA(NO_2)$	σ					
para			-0.004 ± 0.001	13.131 ± 0.001	0.532	0.0022	18.21
meta			-0.019 ± 0.001	13.135 ± 0.001	0.967	0.001	468.47
Fig. 8	$sEDA(NO_2)_{meta}$	$sEDA(NO_2)_{para}$	1.616 ± 0.186	-8.083 ± 2.442	0.825	0.0024	75.43
Fig. 9	$pEDA(NO_2)$	$sEDA(NO_2)$					
para R<0			9.537 ± 1.017	-121.158 ± 13.350	0.946	0.0055	88.01
para R≥0			1.246 ± 0.307	-12.317 ± 4.035	0.673	0.0030	16.44
meta			0.997 ± 0.063	-9.041 ± 0.827	0.940	0.0014	250.32
Fig. S1	$sEDA(\mathbf{R})_{meta}$	$sEDA(\mathbf{R})_{para}$	1.006 ± 0.007	-0.098 ± 0.137	0.999	0.0057	18372
Fig. S2	$pEDA(NO_2)_{meta}$	$pEDA(NO_2)_{para}$	0.183 ± 0.036	3.308 ± 0.146	0.614	0.0037	25.51
Fig. S3	$pEDA(NO_2)$	SESE					
para ED			0.013 ± 0.001	4.054 ± 0.002	0.975	0.0035	229.94
para EA			0.006 ± 0.001	4.058 ± 0.003	0.809	0.0034	38.20
meta			0.003 ± 0.0002	4.052 ± 0.001	0.939	0.0015	247.79

* Standard Error of Y Estimation; ** 95% confidence level

Table S4. Cartesian coordinates of equilibrium geometries of *meta*- and *para*- substituted nitrobenzene derivatives.

p-NO-Ph-NO2 E = -566.19723464 a.u.

6	1.127192	-1.052404	-0.000224
6	-0.254176	-1.157825	-0.000222
6	-1.013917	0.013488	-0.000019
6	-0.445378	1.282057	0.000220
6	0.941797	1.378922	0.000289
6	1.714480	0.217638	0.000039
1	1.761156	-1.930278	-0.000418
1	-0.753763	-2.116738	-0.000374
1	-1.081236	2.156203	0.000350
1	1.440631	2.340810	0.000512
7	-2.496121	-0.101394	-0.000046
8	-3.141901	0.936801	-0.000662
8	-2.973992	-1.226864	0.000672
7	3.149238	0.435608	0.000099
8	3.821069	-0.570032	-0.000129

m-NO-Ph-NO2 E = -566.19774395 a.u.

6	0.539950	2.016070	0.000018
6	-0.753319	1.487838	0.000007
6	-0.919621	0.106733	-0.000002
6	0.161379	-0.764584	-0.000002
6	1.440959	-0.215404	0.000007
6	1.640868	1.170359	0.000017
1	0.676771	3.090695	0.000027
1	-1.625883	2.127016	0.000011
1	0.022272	-1.837681	-0.000012
7	-2.293513	-0.452399	-0.000016
8	-2.405799	-1.669475	-0.000082
8	-3.224594	0.340923	0.000026
1	2.654121	1.553592	0.000024
7	2.520338	-1.182386	0.000009
8	3.633348	-0.708471	0.000022

p-NO2-Ph-NO2 E = -641.43174721 a.u.

6	-0.694835	1.220246	0.000001
6	0.694843	1.220246	-0.000006
6	1.362630	0.000000	0.000000
6	0.694843	-1.220246	-0.000001
6	-0.694835	-1.220246	0.000006
6	-1.362628	0.000000	0.000011
1	-1.259318	2.142159	0.000010
1	1.259329	2.142158	0.000001
1	1.259329	-2.142158	0.000010
1	-1.259318	-2.142159	0.000020
7	2.849119	0.000000	0.000007
8	3.411459	-1.085239	0.000028
8	3.411459	1.085239	-0.000054
7	-2.849119	0.000000	0.000009
8	-3.411466	-1.085231	0.000043
8	-3.411466	1.085231	-0.000044

m-NO2-Ph-NO2 E = -641.43175978 a.u.

6	0.000031	2.235397	0.000017
6	-1.208050	1.543074	0.000002
6	-1.183565	0.151753	0.000000
6	0.000000	-0.572920	0.000014
6	1.183574	0.151736	0.000025
6	1.208098	1.543053	0.000029
1	0.000043	3.318167	0.000018
1	-2.158827	2.058249	-0.000009
1	-0.000007	-1.653206	0.000013
7	-2.470450	-0.590357	-0.000014
8	-2.416761	-1.810581	0.000025
8	-3.498702	0.071307	0.000012
1	2.158890	2.058205	0.000039
7	2.470440	-0.590389	0.000044
8	3.498684	0.071293	-0.000061
8	2.416709	-1.810614	-0.000074

p-COCl-Ph-NO2 E = -1009.86566899 a.u.

6	-0.430154	-1.004339	0.000012
6	0.952005	-1.151483	0.000010
6	1.744383	-0.010203	0.000010
6	1.205202	1.272375	0.000011
6	-0.175016	1.409855	0.000011
6	-0.998979	0.273678	0.000012
1	-1.063288	-1.880206	0.000013
1	1.415820	-2.127889	0.000009
1	1.861107	2.131729	0.000011
1	-0.628945	2.392229	0.000011
7	3.222626	-0.164916	0.000010
8	3.895115	0.856121	0.000014
8	3.670065	-1.302695	-0.000006
6	-2.469119	0.522671	0.000013
8	-2.986318	1.590657	-0.000032
17	-3.514347	-0.964084	-0.000023

m-COCl-Ph-NO2 E = -1009.86622707 a.u.

6	-0.730584	2.400327	0.000005
6	-1.778009	1.482530	0.000019
6	-1.473369	0.125682	0.000046
6	-0.168042	-0.345740	0.000050
6	0.873865	0.583038	0.000038
6	0.586833	1.957534	0.000015
1	-0.945184	3.461863	-0.000014
1	-2.812641	1.797412	0.000012
1	0.017375	-1.409565	0.000066
7	-2.584478	-0.858430	0.000056
8	-2.288921	-2.044439	0.000001
8	-3.725442	-0.417468	-0.000010
1	1.408176	2.662871	0.000005
6	2.313602	0.200180	0.000048
8	3.225781	0.960288	-0.000050
17	2.646265	-1.583054	-0.000077

p-CN-Ph-NO2 E = -529.13627009 a.u.

6	1.083499	1.217051	0.000023
6	-0.304638	1.218741	0.000036
6	-0.974703	0.000000	0.000030
6	-0.304638	-1.218741	0.000011
6	1.083499	-1.217051	-0.000002
6	1.781606	0.000000	0.000004
1	1.630458	2.151096	0.000029
1	-0.868623	2.141100	0.000051
1	-0.868623	-2.141100	0.000008
1	1.630458	-2.151095	-0.000018
7	-2.458727	0.000000	0.000047
8	-3.022339	-1.085138	-0.000043
8	-3.022339	1.085138	-0.000058
6	3.213312	0.000000	-0.000010
7	4.368175	0.000000	-0.000021

m-CN-Ph-NO2 E = -529.13583835 a.u.

6	-0.425243	2.131613	-0.000008
6	0.811564	1.492641	0.000018
6	0.843081	0.102180	0.000038
6	-0.309851	-0.669600	0.000032
6	-1.546106	-0.014195	0.000006
6	-1.600920	1.388378	-0.000013
1	-0.471520	3.213543	-0.000023
1	1.739858	2.047104	0.000024
1	-0.242125	-1.748413	0.000048
7	2.158655	-0.585870	0.000069
8	2.156057	-1.808050	-0.000062
8	3.159798	0.116004	-0.000054
1	-2.564078	1.883210	-0.000033
6	-2.758226	-0.776762	0.000002
7	-3.740765	-1.383358	-0.000003

p-CF3-Ph-NO2 E = -774.02024112 a.u.

6	-0.334959	1.212989	-0.026454
6	1.054975	1.217838	-0.012842
6	1.724959	0.000004	-0.005048
6	1.054944	-1.217808	-0.013252
6	-0.334992	-1.212907	-0.026922
6	-1.025431	0.000054	-0.035676
1	-0.878695	2.148655	-0.038928
1	1.617923	2.140712	-0.009880
1	1.617852	-2.140706	-0.010544
1	-0.878735	-2.148566	-0.039792
7	3.209256	-0.000014	0.007316
8	3.773469	-1.085092	0.013012
8	3.773510	1.085048	0.011903
6	-2.533931	0.000008	0.000160
9	-3.054961	-1.087188	-0.606290
9	-3.055019	1.088161	-0.604518
9	-2.995839	-0.001052	1.274011

m-CF3-Ph-NO2 E = -774.02024669 a.u.

6	-0.463284	2.300012	-0.002482
6	-1.626054	1.535700	0.006086
6	-1.510001	0.150467	-0.003676
6	-0.279630	-0.494002	-0.020706
6	0.871927	0.287567	-0.030844
6	0.784299	1.681279	-0.019586
1	-0.530140	3.380884	0.001399
1	-2.607315	1.989650	0.017169
1	-0.235747	-1.573866	-0.033781
7	-2.743517	-0.673604	0.001057
8	-2.611088	-1.889116	-0.013401
8	-3.814940	-0.083641	0.019580
1	1.688007	2.277513	-0.033251
6	2.225330	-0.377588	-0.001829
9	2.200193	-1.604692	-0.559179
9	2.675846	-0.529676	1.267346
9	3.155353	0.347978	-0.660405

p-COMe-Ph-NO2 E = -589.56245588 a.u.

6	0.671766	1.159831	0.000077
6	-0.718381	1.204410	0.000038
6	-1.421016	0.005429	-0.000006
6	-0.780161	-1.230823	-0.000011
6	0.606841	-1.258288	0.000029
6	1.346666	-0.067645	0.000076
1	1.222868	2.091489	0.000112
1	-1.257236	2.141657	0.000038
1	-1.367362	-2.138716	-0.000045
1	1.142191	-2.199316	0.000027
7	-2.903347	0.045717	-0.000049
8	-3.498411	-1.023173	-0.000069
8	-3.440378	1.145559	-0.000077
6	2.852132	-0.164957	0.000125
8	3.389686	-1.253843	-0.000051
6	3.668729	1.110656	-0.000009
1	3.445402	1.717774	-0.882326
1	3.445599	1.717819	0.882327
1	4.725328	0.849254	-0.000120

m-COMe-Ph-NO2 E = -589.56353922 a.u.

6	0.152974	2.284460	-0.000016
6	1.326461	1.533471	-0.000022
6	1.224522	0.146977	-0.000022
6	-0.001548	-0.508026	-0.000015
6	-1.173839	0.250635	-0.000009
6	-1.084384	1.650285	-0.000009
1	0.209573	3.366316	-0.000016
1	2.302778	1.998359	-0.000027
1	-0.013361	-1.588533	-0.000015
7	2.464306	-0.664069	-0.000029
8	2.344940	-1.882762	0.000033
8	3.532284	-0.066857	0.000034
1	-2.004923	2.221037	-0.000004
6	-2.541917	-0.381902	-0.000002
8	-3.533706	0.319346	0.000017
6	-2.647671	-1.892451	0.000018
1	-2.159889	-2.318650	-0.881665
1	-2.159863	-2.318630	0.881696
1	-3.700188	-2.169922	0.000037

p-COOH-Ph-NO2 E = -625.50837803 a.u.

6	-0.673429	-1.187688	0.000161
6	0.716290	-1.209549	0.000108
6	1.401369	0.000570	0.000071
6	0.746579	1.228369	0.000083
6	-0.641695	1.238511	0.000134
6	-1.355217	0.034726	0.000181
1	-1.230221	-2.114878	0.000196
1	1.269082	-2.138583	0.000095
1	1.321876	2.143620	0.000053
1	-1.188695	2.172661	0.000149
7	2.885714	-0.018567	0.000014
8	3.464807	1.058793	-0.000214
8	3.437380	-1.110419	-0.000229
6	-2.845907	0.108250	0.000262
8	-3.480695	1.134530	-0.000128
8	-3.430397	-1.112995	-0.000193
1	-4.388736	-0.971261	-0.000479

m-COOH-Ph-NO2 E = -625.50888814 a.u.

6	0.101571	2.266227	0.000060
6	1.286316	1.534907	0.000075
6	1.211832	0.145356	-0.000038
6	0.001104	-0.534641	-0.000159
6	-1.179195	0.211324	-0.000183
6	-1.125499	1.610147	-0.000064
1	0.138711	3.348714	0.000144
1	2.254252	2.017144	0.000171
1	-0.014412	-1.614739	-0.000247
7	2.470265	-0.638993	-0.000024
8	2.378053	-1.858611	-0.000061
8	3.523888	-0.016221	0.000183
1	-2.055627	2.164894	-0.000085
6	-2.520690	-0.440193	-0.000351
8	-3.570118	0.156660	0.000135
8	-2.446019	-1.790932	0.000196
1	-3.353834	-2.129000	0.000523

p-CHO-Ph-NO2 E = -550.22867287 a.u.

6	0.918227	1.368595	0.000021
6	-0.469174	1.276092	0.000011
6	-1.043381	0.010099	-0.000003
6	-0.284130	-1.159000	-0.000006
6	1.098541	-1.050984	0.000003
6	1.704757	0.212253	0.000018
1	1.393280	2.343971	0.000033
1	-1.101857	2.152648	0.000013
1	-0.781662	-2.118914	-0.000015
1	1.726358	-1.933708	0.000001
7	-2.524150	-0.099888	-0.000010
8	-3.007004	-1.223602	-0.000034
8	-3.167861	0.940523	-0.000043
6	3.187027	0.335697	0.000027
1	3.566565	1.378266	0.000039
8	3.949261	-0.601866	0.000023

m-CHO-Ph-NO2 E = -550.22952463 a.u.

6	0.473759	2.043685	0.000008
6	-0.807928	1.493112	0.000034
6	-0.942212	0.108896	0.000035
6	0.158521	-0.738647	0.000004
6	1.435720	-0.177467	-0.000022
6	1.590195	1.216095	-0.000020
1	0.592675	3.120399	0.000009
1	-1.693645	2.113725	0.000055
1	0.011692	-1.811654	0.000002
7	-2.301406	-0.481538	0.000060
8	-2.386907	-1.702275	-0.000020
8	-3.252532	0.287895	-0.000006
1	2.593299	1.626022	-0.000040
6	2.623555	-1.070920	-0.000054
8	3.767805	-0.682007	-0.000018
1	2.389237	-2.155144	-0.000001

p-CONH2-Ph-NO2 E = -605.63149195 a.u.

6	-0.664111	1.183750	-0.142481
6	0.726285	1.204783	-0.137583
6	1.408633	0.001436	-0.002257
6	0.746712	-1.217187	0.112339
6	-0.641686	-1.223475	0.094801
6	-1.357058	-0.026382	-0.018520
1	-1.200249	2.115504	-0.277661
1	1.280781	2.126899	-0.242625
1	1.317427	-2.130378	0.208825
1	-1.192467	-2.152775	0.164605
7	2.890551	0.018311	0.012297
8	3.467728	-1.052461	0.143802
8	3.446119	1.102741	-0.106505
6	-2.862143	-0.117194	-0.035580
8	-3.432141	-1.140263	-0.371654
7	-3.541600	1.015034	0.325271
1	-4.545240	0.936347	0.394136
1	-3.096348	1.756470	0.840279

m-CONH2-Ph-NO2 E = -605.63245365 a.u.

6	0.113222	2.258051	0.118014
6	1.300330	1.531384	0.081621
6	1.223104	0.145647	0.001694
6	0.009101	-0.530693	-0.038657
6	-1.175242	0.205223	0.006978
6	-1.113438	1.602368	0.074307
1	0.148142	3.339163	0.176530
1	2.267770	2.013417	0.109490
1	0.022564	-1.607842	-0.132025
7	2.475787	-0.642763	-0.050426
8	2.376830	-1.862867	-0.097732
8	3.533696	-0.028435	-0.039335
1	-2.044341	2.155481	0.086307
6	-2.542734	-0.428608	-0.043924
8	-3.526341	0.217964	-0.361584
7	-2.612303	-1.757786	0.266448
1	-1.865736	-2.239840	0.738401
1	-3.532320	-2.170058	0.298154

p-Cl-Ph-NO2 E = -896.49596098 a.u.

6	0.962307	1.216265	0.000019
6	-0.427121	1.216616	0.000038
6	-1.102176	0.000000	0.000040
6	-0.427120	-1.216616	0.000021
6	0.962307	-1.216265	0.000002
6	1.643939	0.000000	0.000001
1	1.512716	2.147819	0.000018
1	-0.987877	2.141075	0.000051
1	-0.987877	-2.141075	0.000023
1	1.512717	-2.147818	-0.000012
7	-2.579610	0.000000	0.000061
8	-3.147114	-1.084973	-0.000052
8	-3.147114	1.084973	-0.000055
17	3.393447	0.000000	-0.000022

m-Cl-Ph-NO2 E = -896.49463417 a.u.

6	0.325985	2.148981	-0.000004
6	-0.915491	1.520406	0.000043
6	-0.948829	0.130811	0.000074
6	0.203356	-0.648274	0.000056
6	1.427419	0.008752	0.000009
6	1.501531	1.400670	-0.000021
1	0.381341	3.230760	-0.000027
1	-1.840213	2.079742	0.000058
1	0.133842	-1.726440	0.000079
7	-2.263524	-0.556055	0.000126
8	-2.264210	-1.779269	-0.000100
8	-3.266330	0.144661	-0.000105
1	2.467877	1.888352	-0.000057
17	2.904841	-0.933602	-0.000014

p-F-Ph-NO2 E = -536.14237329 a.u.

6	-1.392136	1.219231	-0.000004
6	-0.002872	1.218269	-0.000001
6	0.671621	0.000000	0.000009
6	-0.002872	-1.218269	0.000009
6	-1.392136	-1.219231	0.000006
6	-2.057501	0.000000	0.000000
1	-1.957952	2.141870	-0.000009
1	0.560265	2.141154	-0.000003
1	0.560265	-2.141153	0.000013
1	-1.957953	-2.141869	0.000008
7	2.147960	0.000000	0.000005
8	2.716101	-1.084941	-0.000010
8	2.716101	1.084941	-0.000007
9	-3.404731	0.000000	-0.000002

m-F-Ph-NO2 E = -536.14070853 a.u.

6	1.101323	1.828256	0.000005
6	-0.244785	1.472030	0.000004
6	-0.569669	0.120030	-0.000002
6	0.393034	-0.884254	-0.000003
6	1.718118	-0.484729	-0.000003
6	2.095466	0.851461	0.000002
1	1.379458	2.874988	0.000010
1	-1.031468	2.212848	0.000007
1	0.115627	-1.928710	-0.000006
7	-1.998318	-0.277006	0.000000
8	-2.253253	-1.473602	0.000009
8	-2.833504	0.616872	-0.000006
1	3.147027	1.109525	0.000002
9	2.678969	-1.432503	-0.000006

Ph-NO2 E = -436.87472548 a.u.

6	-0.429858	-1.218855	-0.000023
6	-1.821496	-1.210420	-0.000003
6	-2.515993	0.000000	0.000018
6	-1.821496	1.210420	0.000017
6	-0.429858	1.218856	-0.000003
6	0.241912	0.000000	-0.000021
1	0.135307	-2.140725	-0.000038
1	-2.362746	-2.149103	-0.000004
1	-2.362747	2.149103	0.000033
1	0.135307	2.140725	-0.000006
7	1.722822	0.000000	-0.000052
8	2.290994	1.084686	0.000023
8	2.290994	-1.084686	0.000032
1	-3.600054	0.000000	0.000033

p-Me-Ph-NO2 E = -476.20367952 a.u.

6	-1.347322	1.204092	-0.009965
6	0.042314	1.214918	-0.004052
6	0.720065	0.000170	-0.000251
6	0.041516	-1.214621	-0.004394
6	-1.347648	-1.203145	-0.010301
6	-2.064813	0.000856	-0.010115
1	-1.883703	2.146622	-0.016851
1	0.602290	2.139963	-0.005425
1	0.601180	-2.139852	-0.006051
1	-1.884507	-2.145484	-0.017390
6	-3.571935	-0.000275	0.014963
1	-3.979115	-0.858997	-0.523086
1	-3.939570	-0.055274	1.045452
1	-3.979554	0.909256	-0.430617
7	2.195837	-0.000230	0.003075
8	2.765858	-1.085092	0.004620
8	2.766524	1.084267	0.005023

m-Me-Ph-NO2 E = -476.20306087 a.u.

6	-0.960585	1.913313	0.000011
6	0.364976	1.488012	0.000017
6	0.609244	0.120336	-0.000010
6	-0.416520	-0.821287	-0.000029
6	-1.744387	-0.394420	-0.000031
6	-1.998407	0.984638	-0.000016
1	-1.182931	2.973889	0.000022
1	1.191719	2.184316	0.000032
1	-0.165142	-1.873525	-0.000051
7	2.011177	-0.355854	-0.000003
8	2.202745	-1.565739	0.000021
8	2.898828	0.487928	0.000047
6	-2.881421	-1.386986	-0.000020
1	-3.516706	-1.256405	-0.881004
1	-2.513166	-2.413950	-0.000462
1	-3.516167	-1.256983	0.881441
1	-3.025830	1.334479	-0.000028

p-OMe-Ph-NO2 E = -551.43383693 a.u.

6	-0.803145	1.423648	0.000286
6	0.571847	1.289430	0.000219
6	1.131714	0.009535	-0.000071
6	0.332668	-1.127258	-0.000307
6	-1.051323	-0.993789	-0.000257
6	-1.625878	0.284740	0.000053
1	-1.270236	2.400379	0.000528
1	1.220426	2.154541	0.000399
1	0.796796	-2.103946	-0.000536
1	-1.666176	-1.882865	-0.000478
8	-2.957411	0.524607	0.000100
6	-3.861730	-0.578343	0.000379
1	-3.733530	-1.194280	0.895724
1	-4.857838	-0.140746	0.000812
1	-3.734266	-1.194142	-0.895170
7	2.592247	-0.137882	-0.000122
8	3.054344	-1.274662	-0.000224
8	3.269840	0.884862	-0.000153

m-OMe-Ph-NO2 E = -551.43066491 a.u.

6	0.393055	2.027428	0.000002
6	-0.891474	1.501631	-0.000045
6	-1.021366	0.113976	-0.000045
6	0.066473	-0.742666	-0.000014
6	1.353398	-0.193640	0.000029
6	1.515789	1.196179	0.000037
1	0.531290	3.102130	0.000006
1	-1.771024	2.128593	-0.000074
1	-0.070413	-1.814634	-0.000021
7	-2.381602	-0.476785	-0.000106
8	-2.474481	-1.697202	-0.000197
8	-3.333155	0.293754	-0.000175
1	2.502485	1.638718	0.000064
8	2.372979	-1.091740	0.000044
6	3.712447	-0.608604	0.000373
1	3.920543	-0.013672	0.895741
1	4.344673	-1.494286	0.000527
1	3.920988	-0.013674	-0.894894

p-OH-Ph-NO2 E = -512.12416486 a.u.

6	1.384225	-1.202249	0.000101
6	-0.003262	-1.210729	0.000084
6	-0.688909	0.000614	-0.000023
6	-0.010995	1.219747	-0.000111
6	1.373716	1.226224	-0.000100
6	2.075396	0.015044	0.000008
1	1.931155	-2.139633	0.000187
1	-0.558675	-2.138435	0.000149
1	-0.575504	2.141975	-0.000187
1	1.929197	2.155426	-0.000175
7	-2.157720	-0.006781	-0.000032
8	-2.734683	1.075432	0.000032
8	-2.724430	-1.094896	0.000004
8	3.431852	0.086232	0.000012
1	3.814932	-0.797918	0.000113

m-OH-Ph-NO2 E = -512.12191218 a.u.

6	-1.066869	1.852769	0.000001
6	0.277878	1.484648	-0.000084
6	0.577361	0.128667	-0.000075
6	-0.402928	-0.859628	0.000009
6	-1.739247	-0.467061	0.000095
6	-2.071605	0.891996	0.000090
1	-1.333195	2.902945	-0.000003
1	1.074051	2.214898	-0.000153
1	-0.110089	-1.902131	0.000008
7	1.996179	-0.295637	-0.000163
8	2.229229	-1.498650	-0.000001
8	2.851187	0.579542	-0.000091
1	-3.117706	1.172775	0.000157
8	-2.768437	-1.361407	0.000180
1	-2.429691	-2.263256	0.000213

p-NH2-Ph-NO2 E = -492.25620192 a.u.

6	1.363350	-1.212501	-0.004283
6	-0.019759	-1.213383	-0.002868
6	-0.708289	0.000000	-0.001871
6	-0.019763	1.213380	-0.002694
6	1.363352	1.212505	-0.004077
6	2.081337	0.000005	-0.003598
1	1.901893	-2.153941	-0.008902
1	-0.577844	-2.139721	-0.001587
1	-0.577841	2.139721	-0.001288
1	1.901882	2.153953	-0.008503
7	-2.169435	0.000000	0.002427
8	-2.744979	1.085719	0.004028
8	-2.744976	-1.085721	0.004516
7	3.457812	-0.000004	-0.046341
1	3.945780	0.849447	0.187821
1	3.945770	-0.849452	0.187847

m-NH2-Ph-NO2 E = -492.25234157 a.u.

6	-1.021733	1.874784	0.004576
6	0.316835	1.490283	0.004081
6	0.589277	0.126844	-0.001703
6	-0.403783	-0.843716	-0.007353
6	-1.747019	-0.446471	-0.006398
6	-2.040225	0.928537	-0.001640
1	-1.274923	2.928428	0.009682
1	1.124160	2.207574	0.009039
1	-0.124745	-1.889006	-0.015647
7	2.001973	-0.319951	0.001195
8	2.219730	-1.525857	0.004959
8	2.871340	0.541973	0.000581
1	-3.076012	1.251771	-0.006939
7	-2.763852	-1.391833	-0.066724
1	-2.528523	-2.329491	0.220775
1	-3.675476	-1.097289	0.248094

p-NHMe-Ph-NO2 E = -531.57175089 a.u.

6	-1.030082	-0.987393	0.000062
6	0.348203	-1.125443	0.000059
6	1.159492	0.007032	-0.000014
6	0.597743	1.287436	-0.000086
6	-0.774080	1.427945	-0.000081
6	-1.622176	0.294752	-0.000005
1	-1.649251	-1.874493	0.000116
1	0.807159	-2.104743	0.000111
1	1.248087	2.151422	-0.000143
1	-1.212316	2.420455	-0.000135
7	2.609957	-0.143338	-0.000017
8	3.295135	0.878110	-0.000083
8	3.073106	-1.282607	0.000050
7	-2.979055	0.461498	0.000001
6	-3.944210	-0.619622	0.000090
1	-3.844979	-1.252411	0.889194
1	-4.946284	-0.191617	0.000119
1	-3.845062	-1.252490	-0.888968
1	-3.328934	1.404498	-0.000062

m-NHMe-Ph-NO2 E = -531.56734365 a.u.

6	-1.467014	0.317165	0.000045
6	-0.308873	-0.477378	0.000040
6	0.935451	0.143521	-0.000041
6	1.102478	1.521394	-0.000117
6	-0.053751	2.302773	-0.000111
6	-1.312176	1.720989	-0.000032
1	-0.354377	-1.555869	0.000096
1	2.092164	1.953060	-0.000179
1	0.031958	3.383143	-0.000169
7	2.141209	-0.719234	-0.000045
8	3.235798	-0.169964	-0.000120
8	1.976420	-1.933914	0.000026
7	-2.722342	-0.241116	0.000121
1	-3.509006	0.384189	0.000111
6	-2.980398	-1.665915	0.000183
1	-2.565030	-2.155932	-0.888305
1	-2.564972	-2.155865	0.888680
1	-4.058540	-1.825210	0.000225
1	-2.196306	2.350653	-0.000029

p-NMe2-Ph-NO2 E = -570.88429535 a.u.

6	-0.577402	-1.213476	-0.000082
6	0.804762	-1.210299	-0.000064
6	1.497742	-0.000001	-0.000044
6	0.804763	1.210298	-0.000019
6	-0.577401	1.213476	-0.000037
6	-1.312830	0.000000	-0.000098
1	-1.091548	-2.163742	-0.000089
1	1.360166	-2.138355	-0.000061
1	1.360167	2.138354	0.000025
1	-1.091547	2.163742	0.000013
7	2.955042	0.000000	-0.000023
8	3.532684	1.085948	0.000053
8	3.532687	-1.085946	0.000010
7	-2.684091	0.000000	-0.000178
6	-3.420013	-1.256960	0.000220
1	-3.195098	-1.857764	0.888811
1	-4.487156	-1.044257	0.000081
1	-3.195005	-1.858326	-0.887957
6	-3.420013	1.256960	0.000077
1	-3.194781	1.858339	-0.888032
1	-4.487156	1.044258	-0.000342
1	-3.195321	1.857753	0.888736

m-NMe2-Ph-NO2 E = -570.88002766 a.u.

6	-0.161811	2.262402	0.007875
6	-1.365436	1.563374	0.012029
6	-1.285808	0.175922	-0.008044
6	-0.085681	-0.520385	-0.036013
6	1.133092	0.189355	-0.055720
6	1.061741	1.602647	-0.020151
1	-0.174164	3.346117	0.031046
1	-2.324829	2.058516	0.036019
1	-0.122136	-1.598022	-0.042327
7	-2.543399	-0.610056	0.007417
8	-2.456633	-1.832736	-0.003064
8	-3.600081	0.008470	0.029285
1	1.967651	2.192395	-0.015100
7	2.344134	-0.474112	-0.115186
6	3.581715	0.269951	0.061517
1	3.653164	0.743472	1.051139
1	4.423549	-0.411351	-0.051294
1	3.685683	1.048992	-0.699602
6	2.379136	-1.921373	0.040757
1	1.779063	-2.414596	-0.729233
1	3.406036	-2.264998	-0.073471
1	2.012866	-2.248580	1.023932