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Á. I. Kiss
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QUANTUMSPECTROSCOPY

No 5. Singlet transition energies, MIM wave functions, PPP charge densities and bond orders of the mono- and disubstituted halogenbenzenes

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SINGLET TRANSITION ENERGIES, MIM WAVE FUNCTIONS, PPP CHARGE DENSITIES AND BOND ORDERS OF THE MONO- AND DISUBSTITUTED HALOGENBENZENES

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TABLE 1. Singlet transition energies of mono- and dihalogenbenzenes calculated by MIM method using point charge charged sphere and Mataga-Nishimoto approximation as well as β_{CX} variation. The ground state energies have negative sign which is omitted.

$E_{exp.}$	Point			Sphere			Mataga-Nishimoto		
(eV)	B=-1.0	B=-1.5	B=-2.0	B=-1.0	B=1.5	B=-2.0	B=-1.0	B=-1.5	B=-2.0
				Fluorobenzene					
	0.093	0.207	0.364	0.076	0.171	0.302	0.072	0.161	0.285
4.750	4.836	4.779	4.697	4.838	4.782	4.703	4.847	4.804	4.742
6.107	5.931	5.778	5.612	6.013	5.933	5.825	6.024	5.956	5.863
6.80	6.658	6.574	6.480	6.662	6.582	6.491	6.687	6.630	6.559
6.80	6.575	6.520	6.491	6.670	6.615	6.568	6.682	6.632	6.587
				1,2- difluorobenzene					
	0.153	0.340	0.595	0.151	0.335	0.587	0.134	0.299	0.526
	4.762	4.627	4.455	4.780	4.662	4.510	4.810	4.725	4.613
	5.847	5.554	5.212	5.902	5.661	5.354	5.973	5.824	5.608
	6.356	6.190	6.045	6.462	6.295	6.145	6.587	6.458	6.330
	6.613	6.547	6.507	6.641	6.574	6.526	6.679	6.625	6.573
				1,3- difluorobenzene					
	0.152	0.336	0.583	0.150	0.331	0.575	0.134	0.296	0.517
4.768	4.762	4.628	4.458	4.780	4.663	4.512	4.810	4.726	4.613
6.107	5.841	5.533	5.165	5.896	5.638	5.302	5.971	5.810	5.568
	6.356	6.184	6.016	6.462	6.293	6.129	6.587	6.458	6.329
	6.609	6.538	6.492	6.638	6.563	6.510	6.678	6.618	6.560
				1,4- difluorobenzene					
	0.152	0.334	0.579	0.150	0.330	0.571	0.133	0.295	0.513
4.643	4.734	4.550	4.304	4.762	4.611	4.399	4.804	4.703	4.556
6.205	5.932	5.731	5.456	5.939	5.747	5.480	5.981	5.843	5.637
	6.399	6.232	6.112	6.506	6.344	6.211	6.621	6.506	6.385
	6.612	6.537	6.490	6.618	6.543	6.494	6.650	6.581	6.527
				chlorobenzene					
	0.094	0.210	0.369	0.088	0.196	0.345	0.075	0.168	0.298
4.678	4.826	4.756	4.657	4.829	4.762	4.667	4.842	4.792	4.720
5.740	5.919	5.759	5.590	5.967	5.840	5.690	6.016	5.939	5.834
6.525	6.621	6.513	6.403	6.632	6.530	6.423	6.674	6.605	6.522
6.525	6.562	6.510	6.484	6.616	6.554	6.515	6.673	6.619	6.573
				1,2- dichlorobenzene					
	0.166	0.367	0.640	0.163	0.361	0.630	0.144	0.321	0.562
4.592	4.752	4.609	4.428	4.770	4.644	4.483	4.802	4.708	4.585
5.661	5.809	5.497	5.147	5.868	5.601	5.281	5.953	5.779	5.536
	6.330	6.157	6.001	6.438	6.264	6.105	6.565	6.426	6.290
	6.588	6.525	6.490	6.619	6.550	6.508	6.667	6.606	6.555
				1,3- dichlorobenzene					
	0.165	0.362	0.626	0.162	0.356	0.617	0.143	0.317	0.551
4.592	4.753	4.609	4.431	4.770	4.644	4.484	4.802	4.708	4.585
5.610	5.800	5.466	5.083	5.859	5.569	5.211	5.949	5.759	5.485
	6.330	6.146	5.958	6.438	6.260	6.079	6.564	6.426	6.287
	6.582	6.511	6.472	6.613	6.535	6.487	6.665	6.598	6.538

TABLE 1. /Continued/

E_{exp}	Point			Sphere			Mataga-Nishimoto		
eV	B=-1.0	B=-1.5	B=-2.0	B=-1.0	B=-1.5	B=-2.0	B=-1.0	B=-1.5	B=-2.0
				1,4- dichlorobenzene					
	0.164	0.361	0.622	0.161	0.355	0.612	0.143	0.316	0.547
4.541	4.727	4.537	4.284	4.755	4.596	4.375	4.795	4.684	4.524
5.510	5.680	5.626	5.305	5.894	5.652	5.341	5.959	5.790	5.549
	6.372	6.208	6.093	6.482	6.317	6.185	6.602	6.475	6.348
	6.576	6.505	6.467	6.585	6.512	6.472	6.633	6.559	6.508
				Bromobenzene					
	0.101	0.225	0.394	0.093	0.208	0.367	0.079	0.176	0.311
4.678	4.812	4.726	4.604	4.815	4.732	4.615	4.837	4.781	4.700
5.821	5.828	5.638	5.458	5.924	5.768	5.600	6.006	5.917	5.801
6.457	6.547	6.413	6.294	6.566	6.436	6.317	6.660	6.578	6.485
6.457	6.470	6.456	6.450	6.568	6.515	6.487	6.662	6.604	6.558
				1,2- dibromobenzene					
	0.179	0.397	0.688	0.177	0.391	0.679	0.152	0.338	0.591
4.558	4.721	4.551	4.345	4.748	4.600	4.418	4.793	4.690	4.556
5.648	5.677	5.318	4.949	5.785	5.468	5.121	5.930	5.729	5.462
	6.829	6.005	5.852	6.341	6.156	5.987	6.538	6.388	6.244
	6.500	6.472	6.458	6.568	6.509	6.479	6.654	6.588	6.538
				1,3- dibromobenzene					
	0.178	0.391	0.673	0.176	0.386	0.664	0.151	0.334	0.579
	4.721	4.552	4.349	4.748	4.601	4.420	4.793	4.690	4.556
	5.663	5.279	4.873	5.770	5.422	5.032	5.925	5.704	5.401
	6.165	5.974	5.770	6.340	6.141	5.933	6.537	6.388	6.236
	6.494	6.459	6.441	6.557	6.489	6.456	6.651	6.577	6.519
				1,4- dibromobenzene					
	0.178	0.389	0.668	0.175	0.384	0.659	0.151	0.332	0.575
4.508	4.687	4.459	4.171	4.730	4.543	4.293	4.786	4.663	4.487
5.414	5.794	5.477	5.115	5.813	5.509	5.153	5.936	5.738	5.467
	6.200	6.071	5.989	6.384	6.219	6.102	6.578	6.438	6.306
	6.523	6.468	6.443	6.534	6.475	6.448	6.615	6.540	6.492
				Iodobenzene					
	0.111	0.246	0.430	0.105	0.233	0.408	0.088	0.196	0.346
4.805	4.784	4.666	4.508	4.789	4.676	4.524	4.823	4.749	4.645
5.438	5.596	5.406	5.239	5.754	5.556	5.377	5.966	5.837	5.687
6.391	6.314	6.191	6.098	6.360	6.230	6.129	6.607	6.492	6.378
6.391	6.329	6.382	6.406	6.412	6.426	6.432	6.615	6.553	6.514
				1,2- diiodobenzene					
	0.198	0.436	0.753	0.196	0.431	0.743	0.169	0.375	0.652
4.787	4.659	4.446	4.205	4.693	4.502	4.280	4.766	4.637	4.472
5.209	5.398	5.026	4.655	5.553	5.181	4.811	5.850	5.575	5.253
	5.864	5.738	5.615	6.044	5.878	5.729	6.435	6.259	6.093
	6.488	6.474	6.466	6.414	6.430	6.433	6.606	6.538	6.499

TABLE 1. /Continued/

$E_{exp.}$ (eV)	Point			Sphere			Mataga-Nishimoto		
	B=-1.0	B=-1.5	B=-2.0	B=-1.0	B=-1.5	B=-2.0	B=-1.0	B=-1.5	B=-2.0
				1,3- diiodobenzene					
	0.197	0.430	0.735	0.194	0.424	0.726	0.168	0.370	0.639
4.769	4.659	4.449	4.212	4.693	4.504	4.284	4.766	4.637	4.473
5.438	5.382	4.980	4.568	5.530	5.124	4.709	5.839	5.535	5.170
	5.841	5.660	5.455	6.027	5.818	5.600	6.435	6.253	6.062
	6.466	6.340	6.395	6.413	6.418	6.416	6.598	6.520	6.476
				1,4- diiodobenzene					
	0.196	0.428	0.729	0.194	0.422	0.720	0.168	0.368	0.634
4.626	4.605	4.320	3.989	4.659	4.410	4.103	4.755	4.594	4.373
5.102	5.600	5.221	4.827	5.634	5.262	4.870	5.861	5.590	5.257
	5.899	5.867	5.848	6.087	5.992	5.933	6.479	6.314	6.183
	6.433	6.420	6.415	6.447	6.427	6.419	6.563	6.495	6.461

TABLE 2. Wave functions of fluoro-, chloro- and bromobenzenes calculated by MIM method

$E_{calc.}$ (eV)	Wave function						
	Ψ_G	$\Psi_{B_{2U}}$	$\Psi_{B_{1U}}$	$\Psi_{E_{1U}}$	$\Psi_{E_{1U'}}$	$\Psi_T{}^1{}_{D_1}$	$\Psi_T{}^2{}_{D_1}$
	Fluorobenzene /B=-1.5 eV; Mataga-Nishimoto/						
-0.161	.991		-.013		-.012		.130
4.804		.991		-.039		.124	
5.956	.039		.969		.150		-.192
6.630		.061		.983		- 174	
6.632	.031		-.185		.968		-.167
10.061		-.115		.180		.977	
9.662	-.121		.164		.201		.958
	Chlorobenzene /B=-2.0 eV; Mataga-Nishimoto/						
-0.298	.983		-.023		-.021		.179
4.720		.978		-.078		.193	
5.834	.077		.925		.249		-.276
6.522		.127		.959		-.254	
6.573	.047		-.310		.931		-.188
9.572		-.165		.273		.948	
9.562	-.158		.217		.268		.925
	Bromobenzene /B=-2.0 eV; Mataga-Nishimoto/						
-0.311	.982		-.024		-.022		.187
4.700		.973		-. 087		.216	
5.801	.087		.909		.268		-.308
6.485		.149		.944		-.293	
6.558	.050		-.344		.916		-.202
9.135		-.179		.317		.931	
9.228	-.161		.236		.299		.911

TABLE 3. MIM wave function of iodobenzene

$E_{calc.}$ (eV)	Wave function					
	Ψ_G	$\Psi_{B_{2U}}$	$\Psi_{B_{1U}}$	$\Psi_{E_{1U}}$	$\Psi_{E_{1U'}}$	$\Psi_{T^1D_1}$ $\Psi_{T^2D_1}$
	Iodobenzene /β=-1.0eV; Point/					
-0.111	.991		-.009		-.008	.134
4.784		.972		-.048	.230	
5.596	.107		.620		.261	-.732
7.112		-.123		.732	.670	
6.970	-.056		.220		.847	.481
6.314		-.201		-.680	.706	
6.329	-.060		.753		-.463	.464
	Iodobenzene /β=-1.0 eV; Sphere/					
-0.105	.992		-.008		-.008	.127
4.789		.975		-.046	.219	
5.754	.085		.756		.249	-.599
6.360		.184		.722	-.667	
7.076	-.071		.252		.743	.616
7.159		-.128		.691	.712	
6.412	-.063		.604		-.621	.495
	Iodobenzene /β=-1.5 eV;Mataga-Nishimato/					
-0.196	.987		-.015		-.014	.158
4.749		.976		-.065	.210	
5.837	.074		.901		.240	-.353
6.492		.140		.919	-.369	
6.553	.051		-.349		.896	-.271
8.162		-.169		.389	.905	
8.181	-.132		.257		.374	.881

TABLE 4. MIM wave functions of the ortho-disubstituted fluoro-, chloro- and bromobenzenes

$E_{calc.}$	Wave function								
(eV)	Ψ_G	$\Psi_{B_{2U}}$	$\Psi_{B_{1U}}$	$\Psi_{E_{1U}}$	$\Psi_{E_{1U'}}$	$\Psi_{T^1D_1}$	$\Psi_{T^2D_1}$	$\Psi_{T^1D_2}$	$\Psi_{T^2D_2}$
1,2- difluorobenzene /β=-1.5 eV; Mataga-Nishimoto/									
-0.299	.985	.012	-.018	-.000	-.016	.001	.121	.105	-.059
4.725	-.023	.984	.007	-.022	.005	.135	-.007	.050	-.104
5.824	.050	-.007	.913	.158	.253	-.029	-.161	-.167	-.142
6.458	.004	.028	-.312	.808	.424	-.170	-.019	-.104	-.171
6.625	.031	.024	-.174	-.490	.837	.108	-.113	-.056	.013
9.422	-.010	-.134	-.064	.059	-.079	.801	.165	-.346	-.424
10.435	-.155	-.052	.165	.036	.194	.046	.732	.591	-.146
9.940	-.025	-.101	-.050	-.012	-.061	.082	-.583	.607	-.518
9.605	.034	-.015	.072	.277	.089	.539	-.210	.329	.683
1,2- dichlorobenzene /β=-2.0 eV; Mataga-Nishimoto/									
-0.562	.971	.022	-.031	-.001	-.028	.002	.167	.146	-.080
4.585	-.040	.966	.017	-.039	.012	.192	-.019	.069	-.144
5.536	.091	-.012	.801	.254	.361	-.066	-.218	-.233	-.222
6.290	-.022	.062	-.429	.816	.204	-.240	.051	-.074	-.197
6.555	.049	-.036	-.329	-.347	.856	.111	-.133	-.069	.002
9.045	-.015	-.108	-.050	.033	-.064	.611	.452	-.577	-.266
10.266	-.191	-.060	.232	.086	.275	.084	.678	.597	-.014
9.373	.007	-.183	-.041	.243	-.052	.671	-.488	.445	-.128
9.448	.092	.109	.088	.283	.109	.241	.045	-.148	.893
1,2- dibromobenzene /β=-2.0 eV; Mataga-Nishimoto/									
-0.591	.968	.023	-.033	-.001	-.030	.002	.176	.153	-.084
4.556	-.043	.960	.019	-.042	.014	.210	-.024	.076	-.156
5.462	.100	-.014	.770	.267	.372	-.076	-.238	-.254	-.246
6.244	-.032	.072	-.439	.807	.148	-.271	.075	-.068	-.212
6.538	.052	-.038	-.370	-.307	.852	.114	-.143	-.075	-.002
8.968	-.034	-.245	-.083	.144	-.108	.625	-.375	.371	-.481
9.877	-.190	-.059	.255	.111	.308	.098	.654	.592	.037
8.613	.012	.076	.035	-.021	.047	-.518	-.533	.639	.173
9.088	.104	.045	.053	.386	.068	.443	-.186	-.008	.775

TABLE 5. MIM wave functions of the meta-disubstituted fluoro-, chloro- and bromobenzenes

$E_{calc.}$ (eV)	Wave function								
	ψ_G	$\psi_{B_{2U}}$	$\psi_{B_{1U}}$	$\psi_{E_{1U}}$	$\psi_{E_{1U}'}$	$\psi_{T}^{1}{}_{D_1}$	$\psi_{T}^{2}{}_{D_1}$	$\psi_{T}^{1}{}_{D_3}$	$\psi_{T}^{2}{}_{D_3}$
1,3- difluorobenzene /β=-1.5 eV; Mataga-Nishimoto/									
-0.296	.986	.012	-.006	.000	-.005	.001	.119	-.103	-.060
4.726	-.023	.984	-.001	-.022	-.001	.135	-.005	-.051	-.103
5.810	.017	-.003	.909	-.154	.262	.027	-.171	-.184	.133
6.458	-.002	.029	.315	.806	-.427	-.169	.019	.105	-.170
6.618	.009	.020	-.184	.495	.831	-.110	-.118	-.065	-.023
9.427	.020	-.143	.063	.057	.079	.801	-.139	.290	-.470
10.267	-.137	-.034	.142	-.034	.168	-.000	.915	-.103	-.287
10.136	.092	.097	.118	-.047	.141	-.103	.176	.891	.332
9.589	-.008	-.003	-.056	.274	-.069	.537	.233	-.220	.725
1,3- dichlorobenzene /β=-2.0 eV. Mataga-Nishimoto/									
-0.551	.972	.022	-.011	.000	-.010	.002	.165	-.141	-.084
4.585	-.042	.967	.007	-.042	.005	.193	-.017	-.075	-.139
5.485	.031	-.024	.794	-.231	.375	.050	-.244	-.272	.195
6.287	.003	.057	.402	.830	-.186	-.246	-.059	.067	-.208
6.538	.013	.022	-.367	.327	.847	-.107	-.140	-.090	-.020
9.112	.052	-.195	.059	.017	.076	.678	-.311	.294	-.554
10.007	-.137	-.028	.239	-.121	.287	-.066	.804	.179	-.380
9.752	.173	.149	.104	-.134	.127	-.258	.869	.169	.228
9.321	.013	.000	.035	.341	.043	.599	.345	.120	.624
1,3 dibromobenzene /β=-2.0 EV; Mataga-Nishimoto/									
-0.579	.970	.023	-.011	.000	-.010	.002	.173	-.147	-.088
4.556	-.045	.960	.010	-.046	.007	.210	-.021	-.084	-.150
5.401	.035	-.032	.764	-.237	.386	.055	-.268	-.299	.212
6.236	.005	.065	.398	.825	-.126	-.279	-.087	.056	-.231
6.519	.013	.021	-.417	.277	.840	-.108	-.149	-.100	-.019
8.725	.062	-.209	.048	-.006	.064	.626	-.376	.281	-.578
9.631	-.115	-.017	.269	-.166	.331	-.104	.728	.283	-.395
9.321	.196	.168	.070	-.166	.088	-.317	-.306	.805	.225
8.945	.033	.004	.071	.361	.092	.600	.322	.247	.575

TABLE 6. MIM wave functions of the para-disubstituted fluoro-chloro- and bromobenzenes

$E_{calc.}$ (eV)	Wave function								
	ψ_G	$\psi_{B_{2U}}$	$\psi_{B_{1U}}$	$\psi_{E_{1U}}$	$\psi_{E_{1U'}}$	$\psi_{T}^{1}{}_{D_1}$	$\psi_{T}^{2}{}_{D_1}$	$\psi_{T}^{1}{}_{D_4}$	$\psi_{T}^{2}{}_{D_4}$
	1,4-difluorobenzene /β=-1.5 eV; Mataga-Nishimoto/								
-.295	.986	.000	.000	.000	.000	.000	.119	.000	.119
4.703	.000	.976	.000	-.086	.000	.142	.000	-.142	.000
5.843	.000	.000	.936	.000	.245	.000	-.179	.000	.179
6.506	.000	.137	.000	.957	.000	-.181	.000	.181	.000
6.581	.000	.000	-.293	.000	.941	.000	-.121	.000	.121
9.685	.000	-.171	.000	.278	.000	.669	.000	-.669	.000
10.268	.000	.000	.197	.000	.234	.000	.673	.000	-.673
9.274	.000	.000	.000	.000	.000	.707	.000	.707	.000
10.171	-.168	.000	.000	.000	.000	.000	.697	.000	.697
	1,4- dichlorobenzene /β=-2.0 eV; Mataga-Nishimoto/								
-0.547	.973	.000	.000	.000	.000	.000	.163	.000	.163
4.524	.000	.944	.000	-.152	.000	.207	.000	-.207	.000
5.549	.000	.000	.843	.000	.375	.000	-.273	.000	.273
6.348	.000	.244	.000	.919	.000	-.220	.000	.220	.000
6.508	.000	.000	-.465	.000	.868	.000	-.123	.000	.123
9.604	.000	-.221	.000	.365	.000	.640	.000	.640	.000
9.954	.000	.000	.270	.000	.325	.000	.641	.000	-.641
8.856	.000	.000	.000	.000	.000	.707	.000	.707	.000
9.742	-.231	.000	.000	.000	.000	.000	.688	.000	.688
	1,4- dibromobenzene /β=-2.0 eV; Mataga-Nishimoto/								
-0.575	.970	.000	.000	.000	.000	.000	.171	.000	.171
4.487	.000	.934	.000	-.164	.000	.226	.000	- .226	.000
5.467	.000	.000	.814	.000	.391	.000	-.304	.000	.304
6.306	.000	.273	.000	.901	.000	-.238	.000	.238	.000
6.492	.000	.000	-.502	.000	.846	.000	-.127	.000	.127
9.286	.000	-.232	.000	.402	.000	.626	.000	-.626	.000
9.556	.000	.000	.294	.000	.362	.000	.626	.000	-.626
8.460	.000	.000	.000	.000	.000	.707	.000	.707	.000
9.275	-.242	.000	.000	.000	.000	.000	.686	.000	.686

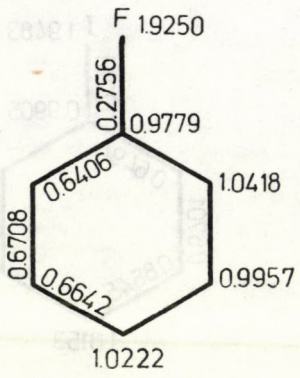
TABLE 7. MIM wave functions of the ortho-diiodobenzene

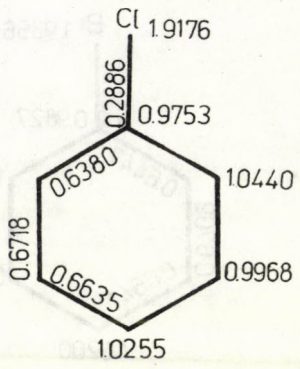
$E_{calc.}$ (eV)	Wave function								
	ψ_G	$\psi_{B_{2U}}$	$\psi_{B_{1U}}$	$\psi_{E_{1U}}$	$\psi_{E_{1U}'}$	$\psi_T{}^1{}_{D_1}$	$\psi_T{}^2{}_{D_1}$	$\psi_T{}^1{}_{D_2}$	$\psi_T{}^2{}_{D_2}$
1,2- diiodobenzene /β=-1.0 eV; Point/									
-0.198	.985	.008	-.012	-.000	-.011	.001	.120	.104	-.059
4.659	-.025	.929	.018	-.031	.012	.299	-.017	.064	-.203
5.398	.052	-.026	.528	.272	.268	-.213	-.237	-.433	-.533
7.027	.047	-.012	-.039	.845	-.129	.330	-.244	-.002	.310
6.488	.064	.025	-.418	-.079	.687	-.082	-.562	.114	.085
5.864	.058	-.206	.427	-.388	.105	.713	-.233	-.101	.194
7.398	-.098	-.037	.297	.216	.594	.072	.550	.434	.069
6.697	-.072	-.219	.016	.036	-.233	.143	-.287	.685	-.565
6.222	.035	.209	.523	-.080	-.147	-.464	-.339	.343	.454
1,2- diiodobenzene /β=-1.0 eV; Sphere/									
-0.196	.986	.008	-.012	-.000	-.011	.001	.118	.103	-.058
4.693	-.025	.949	.011	-.026	.007	.244	-.014	.077	-.179
5.553	.062	-.018	.653	.238	.289	-.136	-.294	-.390	-.415
7.114	.057	-.016	-.053	.768	-.147	.404	-.301	-.015	.358
6.414	.017	-.145	-.518	-.041	.538	.461	.020	-.346	-.295
6.044	.049	-.117	.425	-.530	.021	.605	-.220	.024	.328
7.475	-.096	-.035	.294	.244	.557	.099	.542	.462	.127
6.560	.060	.099	-.187	-.101	.506	-.343	-.630	.321	.261
6.801	.071	.230	.017	-.039	.197	-.229	.264	-.628	.620
1,2- diiodobenzene /β=-1.5 eV; Mataga-Nishimoto/									
-0.375	.977	.015	-.022	-.000	-.020	.001	.150	.130	-.073
4.637	-.034	.961	.012	-.032	.008	.208	-.017	.078	-.158
5.575	.082	-.011	.777	.234	.336	-.075	-.263	-.280	-.263
6.259	-.027	.066	-.422	.772	.160	-.332	.084	-.089	-.263
6.538	.050	-.040	-.366	-.297	.841	.154	-.184	-.101	-.007
8.116	.091	.008	.012	.478	.018	.518	-.282	-.000	.644
8.698	-.152	-.050	.274	.147	.366	.106	.633	.569	.091
7.697	.017	.092	.041	-.029	.069	-.538	-.527	.608	.218
7.977	.053	.244	.083	-.096	.127	-.498	.331	-.432	.601

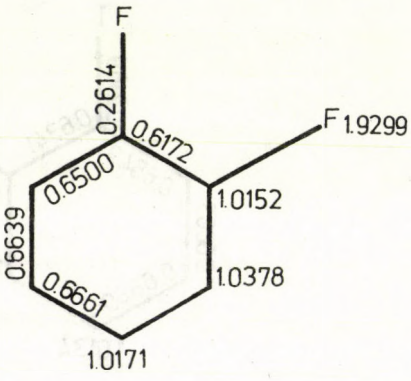
TABLE 8. MIM wave functions of meta-diiodobenzene

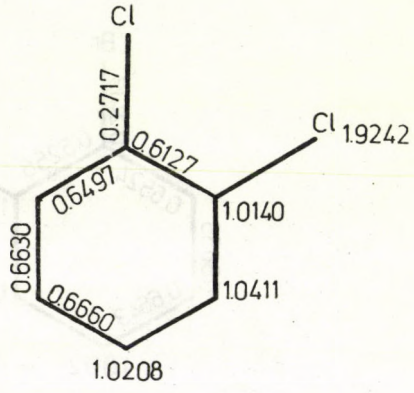
$E_{calc.}$ (eV)	Wave function								
	ψ_G	$\psi_{B_{2U}}$	$\psi_{B_{1U}}$	$\psi_{E_{1U}}$	$\psi_{E_{1U'}}$	$\psi_{T^1_{D_1}}$	$\psi_{T^2_{D_1}}$	$\psi_{T^1_{D_3}}$	$\psi_{T^2_{D_3}}$
-	1.3- diiodobenzene /β=-1.0 eV; Point/								
-0.197	.986	.008	-.004	.000	-.004	.001	.119	-.103	-.060
4.659	-.026	.930	-.010	-.031	-.007	.300	-.008	-.066	-.200
5.382	.017	.012	.537	-.257	.276	.187	-.263	-.464	.500
7.016	-.033	-.038	.061	.828	.204	.337	.319	-.085	.212
6.466	.029	-.102	-.474	.044	.676	.119	-.464	-.126	-.245
5.841	-.006	-.178	-.395	-.397	-.104	.701	.266	.109	.262
7.342	-.035	.020	.298	-.271	.624	.087	.539	.350	-.162
6.821	.151	.174	.009	.104	.080	-.033	-.379	.739	.490
6.224	-.036	.248	-.487	-.064	.139	-.497	.308	-.259	.517
	1,3- diiodobenzene /β=-1.0 eV; Sphere/								
-0.194	.986	.008	-.004	.000	-.004	.001	.117	-.101	-.059
4.693	-.026	.949	-.003	-.026	-.002	.245	-.010	-.079	-.177
5.530	.021	-.001	.653	-.220	.296	.113	-.320	-.426	.375
7.098	-.042	-.051	.081	.743	.229	.418	.393	-.096	.218
6.413	-.011	.127	-.559	.036	.577	-.410	-.058	-.315	.259
6.027	-.007	-.099	-.374	-.535	-.027	.603	.238	-.004	.377
7.422	-.034	.018	.294	-.304	.578	-.119	.524	.379	-.231
6.913	.146	.170	.018	.128	.088	-.029	-.338	.734	.521
6.556	-.047	.202	.164	-.058	-.431	-.454	.530	-.105	.493
	1,3- diiodobenzene /β=-1.5 eV; Mataga-Nishimoto/								
-0.370	.978	.015	-.007	.000	-.007	.001	.148	-.127	-.075
4.637	-.035	.961	.004	-.034	.003	.208	-.015	-.083	-.154
5.535	.028	-.019	.769	-.213	.347	.059	-.289	-.321	.230
6.253	.004	.060	.388	.785	-.141	-.340	-.096	.077	-.281
6.520	.013	.023	-.408	.269	.828	-.145	-.191	-.131	-.019
7.763	.058	-.206	.049	.005	.080	.633	-.393	.288	-.555
8.552	-.071	.005	.287	-.211	.392	-.133	.655	.386	-.345
8.214	.177	.169	.018	-.210	.025	-.354	-.441	.719	.240
8.017	.047	.030	.078	.420	.118	.522	.266	.320	.595

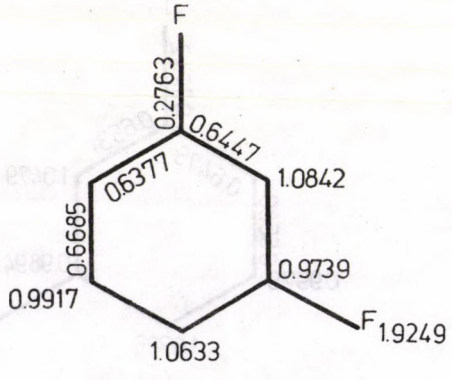
Table 9. *PPP charge densities and bond orders of mono- and disubstituted fluoro- and chlorobenzenes*

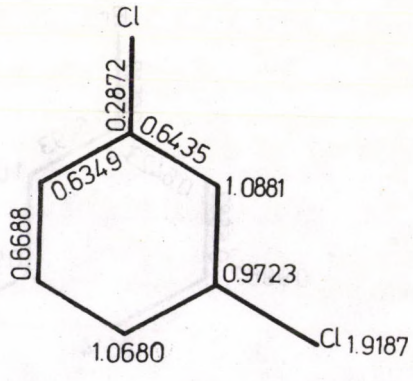


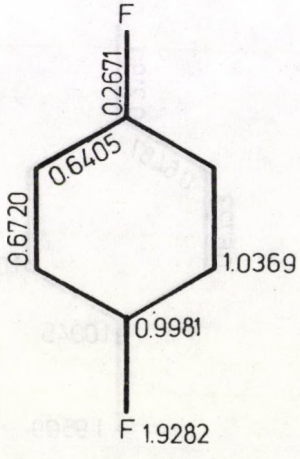












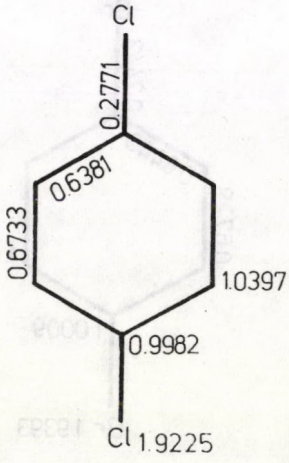
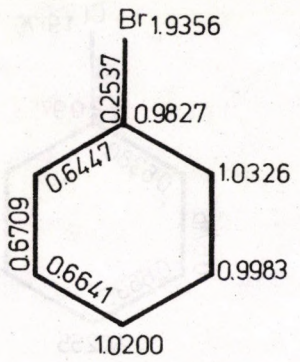
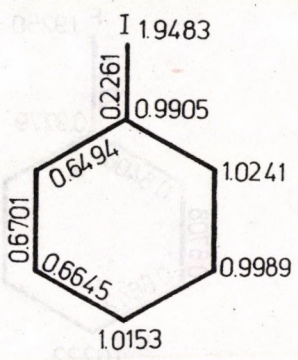
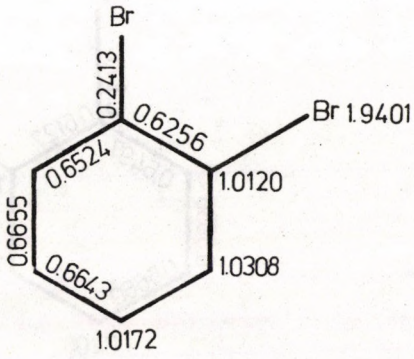
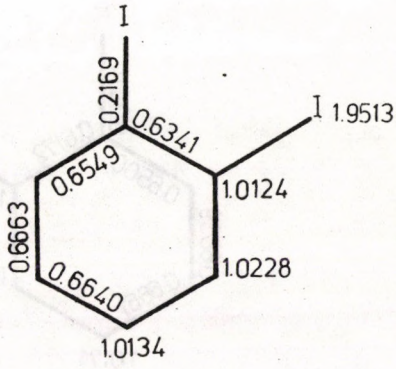


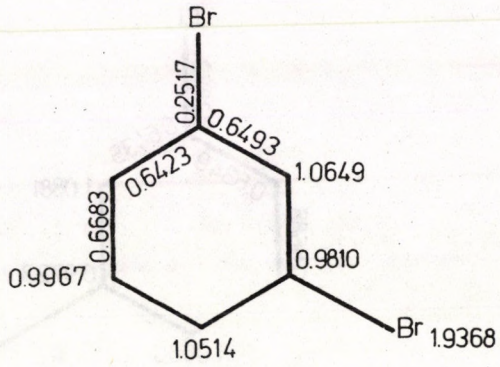
Table 10. *PPP charge densities and bond orders of mono- and disubstituted bromo- and iodobenzenes*

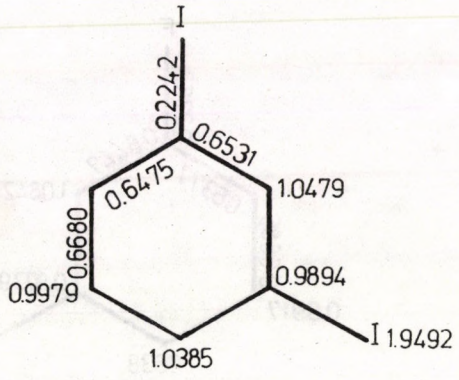


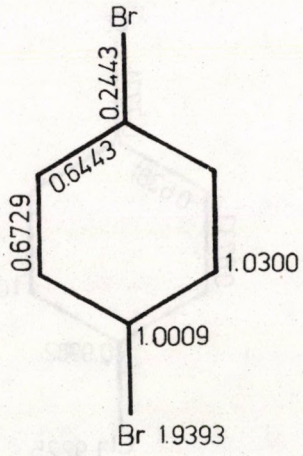


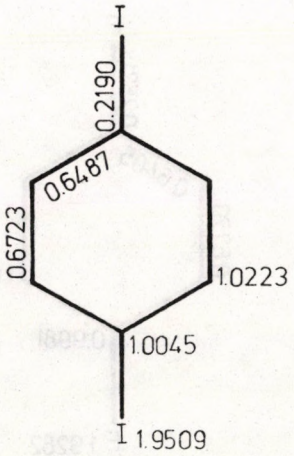












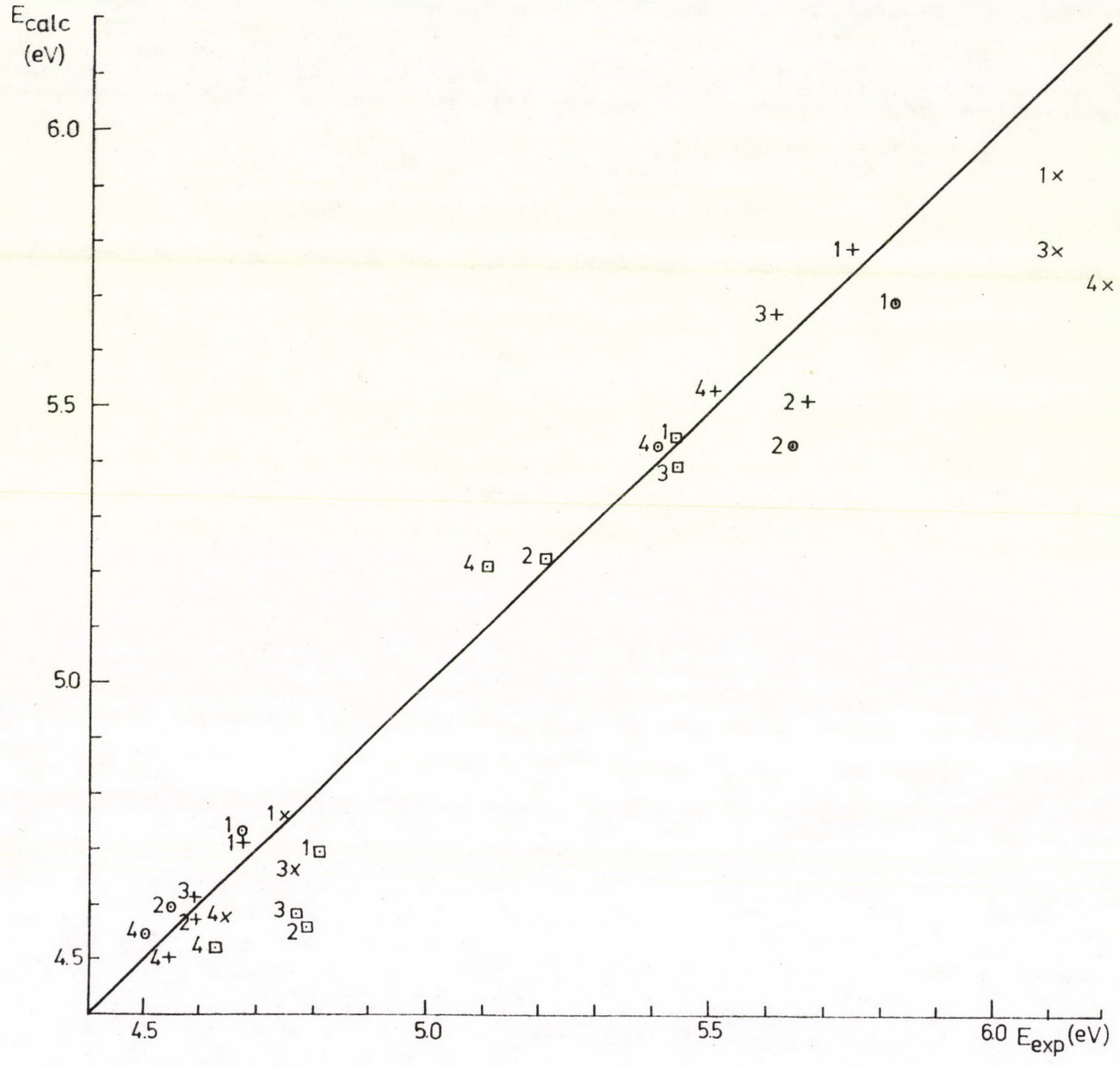
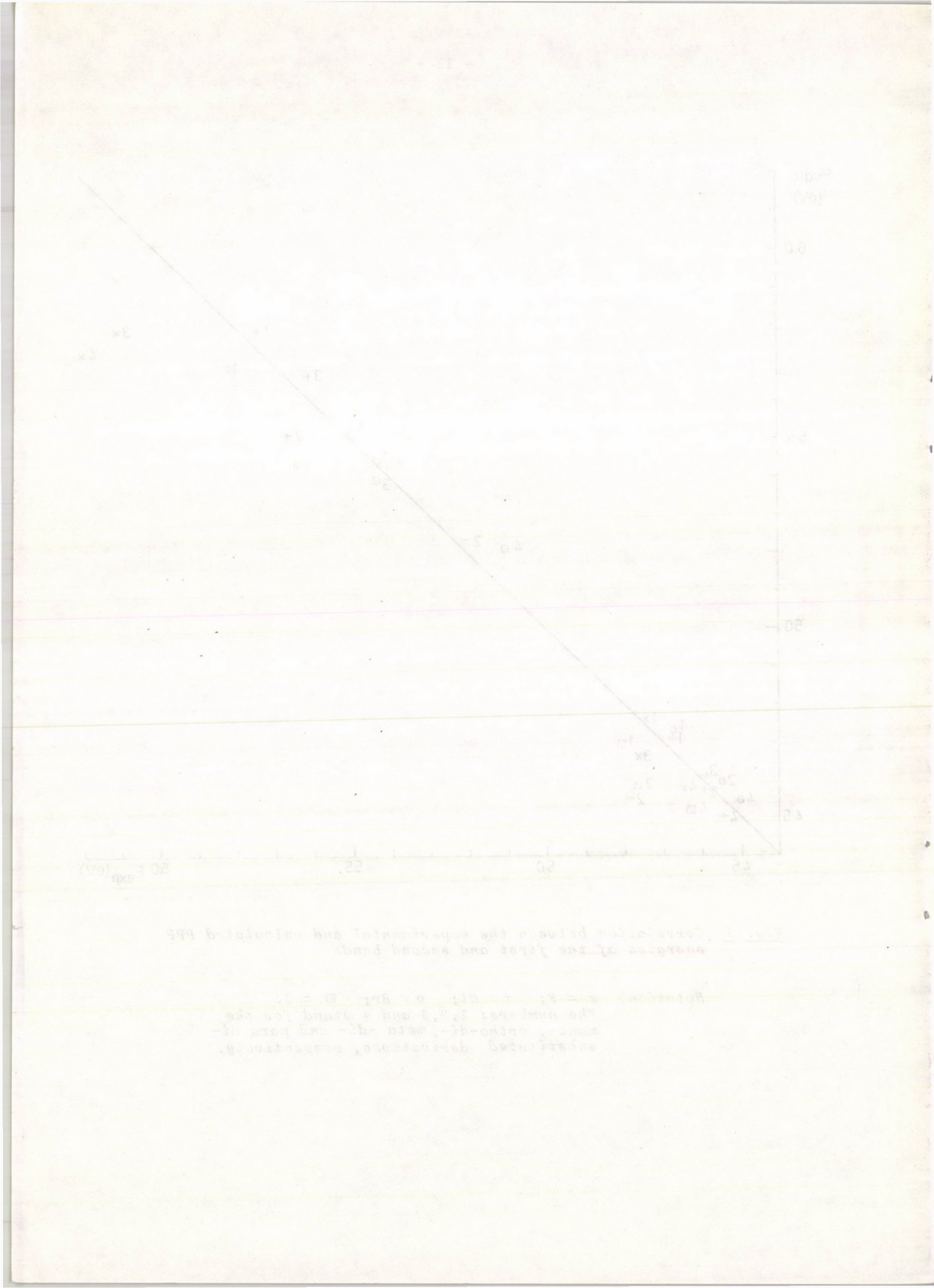
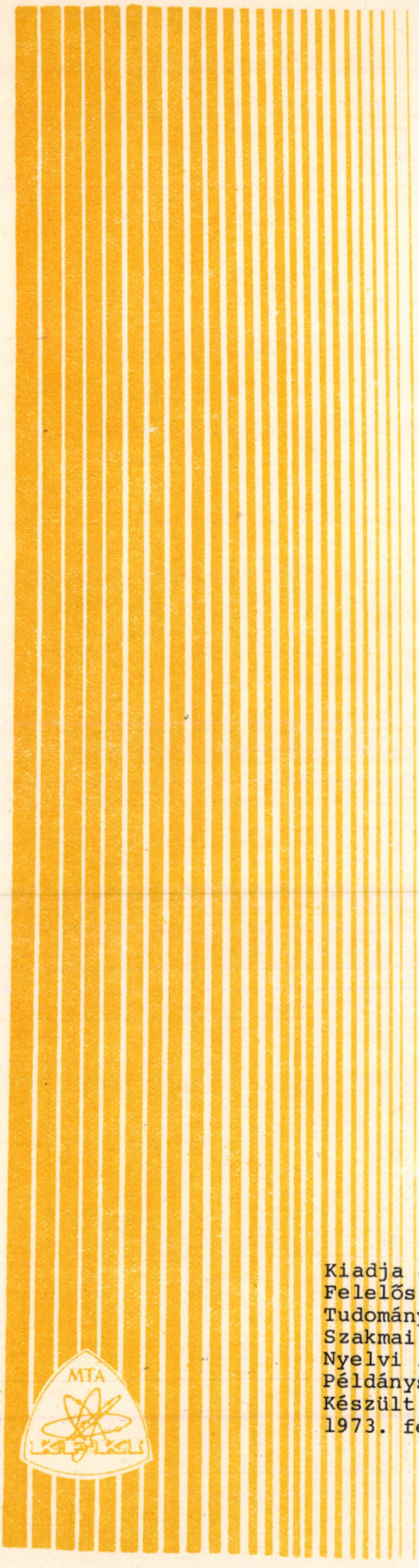


Fig. 1 *Correlation between the experimental and calculated PPP energies of the first and second bands*

Notation: *x = F; + = Cl; ⊙ = Br; ⊡ = I. The numbers: 1, 2, 3 and 4 stand for the mono-, ortho-di-, meta -di- and para-di- substituted derivatives, respectively.*





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Szakmai lektor: Kapuy Ede
Nyelvi lektor: Kovács Jenőné
Példányszám: 375 Törzsszám: 73-7745
Készült a KFKI sokszorosító üzemében, Budapest, 1973. február hó