Supporting Information

Comparison of Global Reactivity Descriptors Calculated Using Various Density Functionals: A QSAR Perspective

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Table S1. Bond Lengths and Bond Angles of The Optimized Chlorobenzenes Using Various Methods With 6-31++G** Basis Set

parameters	B3LYP	MPWB1K	MPW1B95	BB1K	SVWN5	BLYP	M05	M05-2X	Observed value[a]
$r(C_1\text{-}C_2)$	1.39548	1.3825	1.38739	1.38361	1.39007	1.40573	1.39405	1.39034	1.391
$r(C_1\text{-}C_6)$	1.39559	1.38239	1.38729	1.38351	1.39009	1.40574	1.39395	1.39024	
$r(C_2\text{-}C_3)$	1.39753	1.38451	1.38922	1.38554	1.3907	1.40797	1.39425	1.39303	1.394
$r(C_3\text{-}C_4)$	1.39747	1.38439	1.38913	1.38541	1.39136	1.40769	1.3944	1.39315	1.400
$r(C_4\text{-}C_5)$	1.39756	1.3843	1.38905	1.38532	1.39137	1.4077	1.39432	1.39306	
$r(C_5\text{-}C_6)$	1.39743	1.38461	1.38932	1.38563	1.39069	1.40796	1.39434	1.39312	
$r(C_1\text{-}Cl_7)$	1.75934	1.73021	1.73778	1.7319	1.73235	1.78124	1.74225	1.74536	1.739
$r(C_2\text{-}H_8)$	1.08481	1.07807	1.08171	1.07871	1.09479	1.09147	1.08442	1.0821	1.078
$r(C_3\text{-}H_9)$	1.08606	1.07908	1.08275	1.07977	1.09555	1.09327	1.08574	1.08281	1.087
$r(C_4\text{-}H_{10})$	1.0858	1.07885	1.08249	1.07954	1.095	1.0927	1.0854	1.08265	1.080
$r(C_5\text{-}H_{11})$	1.08606	1.07908	1.08275	1.07977	1.09555	1.09327	1.08574	1.0828	
$r(C_6\text{-}H_{12})$	1.08481	1.07807	1.08171	1.07871	1.09479	1.09147	1.08442	1.0821	
$\angle C_1C_2C_3$	119.020	119.024	119.017	119.025	119.018	118.859	119.023	118.938	119.05
$\angle C_2C_3C_4$	120.473	120.452	119.017	120.456	120.496	120.526	120.519	120.422	120.24
$\angle C_3C_4C_5$	119.707	119.739	119.725	119.736	119.698	119.707	119.695	119.793	119.79
$\angle C_4C_5C_6$	120.473	120.452	120.467	120.456	120.496	120.526	120.518	120.422	
$\angle C_5C_6C_1$	119.020	119.024	119.017	119.025	119.019	118.859	119.023	118.938	
$\angle C_6C_1C_2$	121.308	121.310	121.307	121.303	121.273	121.523	121.222	121.488	121.65
$\angle C_2C_1Cl_7$	119.342	119.340	119.342	119.344	119.364	119.239	119.385	119.252	
$\angle C_3C_2H_8$	120.887	121.004	120.991	120.993	121.223	120.966	120.893	121.124	
$\angle C_4C_3H_9$	120.187	120.168	120.177	120.170	120.199	120.233	120.171	120.180	
$\angle C_5C_4H_{10}$	120.149	120.133	120.140	120.135	120.150	120.145	120.155	120.106	
$\angle C_6C_5H_{11}$	119.333	119.372	119.348	119.367	119.307	119.242	119.303	119.392	
$\angle C_1C_6H_{12}$	120.101	119.980	120.000	119.989	119.756	120.173	120.092	119.946	

[a] Reference 37

Table S2. Bond Lengths and Bond Angles of The Optimized 1,3,5-C3B using Various Methods With 6-31++G** Basis Set

parameters	B3LYP	MPWB1K	MPW1B95	BB1K	SVWN5	BLYP	M05	M05-2X	Observed value[a]
$r(C_1\text{-}C_2)$	1.395	1.382	1.387	1.383	1.390	1.406	1.393	1.390	1.394
$r(C_1\text{-}C_6)$	1.395	1.382	1.387	1.383	1.390	1.406	1.393	1.390	
$r(C_2\text{-}C_3)$	1.395	1.382	1.387	1.383	1.390	1.406	1.394	1.390	
$r(C_3\text{-}C_4)$	1.395	1.382	1.387	1.383	1.389	1.406	1.393	1.390	
$r(C_4\text{-}C_5)$	1.395	1.382	1.387	1.383	1.390	1.406	1.394	1.390	
$r(C_5\text{-}C_6)$	1.395	1.382	1.386	1.383	1.390	1.406	1.393	1.390	
$r(C_1\text{-}Cl_7)$	1.753	1.723	1.731	1.725	1.726	1.772	1.735	1.738	1.728
$r(C_2\text{-}H_8)$	1.083	1.076	1.080	1.077	1.094	1.089	1.083	1.081	1.081
$r(C_3\text{-}Cl_9)$	1.753	1.723	1.730	1.725	1.726	1.772	1.735	1.739	
$r(C_4\text{-}H_{10})$	1.083	1.076	1.080	1.077	1.094	1.089	1.082	1.081	
$r(C_5\text{-}Cl_{11})$	1.753	1.723	1.731	1.725	1.726	1.772	1.735	1.737	
$r(C_6\text{-}H_{12})$	1.083	1.076	1.080	1.077	1.094	1.090	1.083	1.081	
$\angle C_1C_2C_3$	118.021	118.154	118.087	118.103	118.063	117.885	118.107	117.901	
$\angle C_2C_3C_4$	121.972	121.846	121.913	121.899	121.955	122.113	121.893	122.109	
$\angle C_3C_4C_5$	118.034	118.145	118.077	118.100	118.031	117.886	118.101	117.918	
$\angle C_4C_5C_6$	121.967	121.861	121.931	121.899	121.964	122.119	121.900	122.050	
$\angle C_5C_6C_1$	118.029	118.138	118.072	118.103	118.049	117.876	118.098	117.933	
$\angle C_6C_1C_2$	121.978	121.857	121.920	121.896	121.938	122.121	121.901	122.088	122.36
$\angle C_2C_1Cl_7$	119.014	119.055	119.063	119.059	119.023	118.937	119.055	118.914	
$\angle C_3C_2H_8$	120.989	120.907	120.975	120.928	120.947	121.060	120.926	121.018	
$\angle C_4C_3Cl_9$	119.011	119.066	119.080	119.052	119.032	118.951	119.068	119.107	
$\angle C_5C_4H_{10}$	120.989	120.916	120.967	120.928	120.978	121.054	120.934	121.043	
$\angle C_6C_5Cl_{11}$	119.008	119.046	119.074	119.050	119.007	118.942	119.029	118.985	
$\angle C_1C_6H_{12}$	120.984	120.921	120.980	120.926	120.968	121.058	120.941	121.037	

[a] Reference 38

Table S3. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With 6-31G* Basis Set

System	B3LYP		MPWB1K		MPW1B95		BB1K		SVWN5		BLYP		M05		M05-2X	
	I	A	I	A	I	A	I	A	I	A	I	A	I	A	I	A
CB	6.70	0.34	5.74	0.98	5.75	1.01	5.73	0.97	6.51	1.74	5.67	0.96	6.95	0.08	8.17	-0.75
1,2-C2B	6.85	0.66	5.83	1.25	5.84	1.28	5.82	1.24	6.60	2.01	5.80	1.25	7.05	0.42	8.28	-0.43
1,3-C2B	6.92	0.72	5.92	1.31	5.92	1.35	5.90	1.30	6.68	2.08	5.88	1.32	7.15	0.47	8.37	-0.35
1,4-C2B	6.75	0.74	5.72	1.35	5.74	1.38	5.72	1.34	6.49	2.12	5.71	1.35	6.95	0.49	8.17	-0.33
1,2,3-C3B	7.09	0.94	6.06	1.48	6.06	1.51	6.04	1.47	6.82	2.25	6.03	1.50	7.30	0.71	8.54	-0.12
1,2,4-C3B	6.92	1.02	5.87	1.58	5.88	1.61	5.86	1.57	6.64	2.35	5.88	1.60	7.12	0.78	8.33	-0.04
1,3,5-C3B	7.25	1.05	6.20	1.59	6.21	1.62	6.19	1.58	6.98	2.36	6.19	1.62	7.47	0.82	8.71	0.00
1,2,3,4-C4B	7.05	1.23	5.98	1.72	5.99	1.76	5.97	1.72	6.75	2.50	6.00	1.80	7.24	1.00	8.46	0.18
1,2,3,5-C4B	7.12	1.28	6.04	1.79	6.06	1.82	6.03	1.78	6.81	2.56	6.07	1.82	7.30	1.04	8.53	0.24
1,2,4,5-C4B	7.02	1.29	5.94	1.81	5.96	1.84	5.93	1.80	6.70	2.58	5.98	1.84	7.19	1.05	8.41	0.24
1,2,3,4,5-C5B	7.16	1.48	6.07	1.93	6.08	1.97	-	-	6.83	2.71	6.11	2.17	7.33	1.25	8.56	0.45
1,2,3,4,5,6-C6B	7.30	1.73	6.18	2.21	0.00	0.00	6.17	2.20	6.96	2.95	6.24	2.53	7.47	1.44	8.70	0.63
benzene	6.70	-0.10	5.85	0.57	5.84	0.60	5.84	0.57	6.62	1.33	5.67	0.53	7.00	-0.36	8.22	-1.21

Table S4. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With 6-31G** Basis Set

System	B3LYP		MPWB1K		MPW1B95		BB1K		SVWN5		BLYP		M05		M05-2X	
	I	A	I	A	I	A	I	A	I	A	I	A	I	A	I	A
CB	6.71	0.36	5.75	1.00	5.76	1.03	5.74	1.00	6.52	1.77	5.68	0.98	6.95	0.10	8.16	-0.75
1,2-C2B	6.85	0.68	5.84	1.27	5.85	1.30	5.83	1.26	6.60	2.04	5.80	1.27	7.06	0.43	8.28	-0.42
1,3-C2B	6.93	0.74	5.92	1.33	5.93	1.36	5.91	1.32	6.69	2.10	5.89	1.34	7.15	0.49	8.36	-0.35
1,4-C2B	6.75	0.76	5.73	1.37	5.74	1.40	5.72	1.36	6.49	2.14	5.72	1.37	6.95	0.50	8.16	-0.33
1,2,3-C3B	7.10	0.95	6.06	1.49	6.07	1.52	6.05	1.48	6.82	2.26	6.04	1.51	7.30	0.72	8.54	-0.12
1,2,4-C3B	6.93	1.04	5.88	1.60	5.89	1.63	5.87	1.59	6.64	2.37	5.89	1.61	7.12	0.79	8.33	-0.04
1,3,5-C3B	7.25	1.06	6.21	1.59	6.21	1.63	6.20	1.59	6.98	2.38	6.19	1.63	7.48	0.83	8.70	0.00
1,2,3,4-C4B	7.05	1.24	5.98	1.73	6.00	1.77	5.97	1.73	6.75	2.51	6.00	1.80	7.24	1.00	8.46	0.18
1,2,3,5-C4B	7.12	1.29	6.04	1.79	6.06	1.83	6.03	1.79	6.81	2.57	6.07	1.83	7.30	1.05	8.53	0.24
1,2,4,5-C4B	7.02	1.30	5.94	1.82	5.96	1.86	5.93	1.81	6.70	2.60	5.98	1.86	7.19	1.05	8.41	0.24
1,2,3,4,5-C5B	7.16	1.48	6.07	1.94	6.08	1.98	6.06	1.93	6.83	2.72	6.11	2.17	7.33	1.25	8.56	0.45
1,2,3,4,5,6-C6B	7.30	1.73	6.18	2.20	-	-	6.17	2.20	6.96	2.95	6.24	2.53	-	-	8.70	0.63
benzene	6.72	-0.07	5.87	0.60	5.86	0.63	5.86	0.59	6.64	1.37	5.69	0.56	7.02	-0.34	8.21	-1.20

Table S5. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With 6-31+G* Basis Set

System	B3LYP		MPWB1K		MPW1B95		BB1K		SVWN5		BLYP		M05		M05-2X	
	I	A	I	A	I	A	I	A	I	A	I	A	I	A	I	A
CB	6.94	0.77	6.01	1.38	6.01	1.41	5.97	1.32	6.75	2.10	5.96	1.39	7.14	0.46	8.35	-0.33
1,2-C2B	7.06	1.06	6.08	1.62	6.08	1.65	6.04	1.57	6.81	2.35	6.07	1.65	7.23	0.76	8.44	-0.03
1,3-C2B	7.13	1.11	6.15	1.68	6.16	1.71	6.11	1.62	6.90	2.41	6.14	1.71	7.32	0.81	8.52	0.02
1,4-C2B	6.95	1.13	5.95	1.71	5.97	1.74	5.92	1.66	6.69	2.44	5.97	1.74	7.12	0.82	8.32	0.05
1,2,3-C3B	7.29	1.29	6.28	1.81	6.29	1.84	6.24	1.76	7.02	2.54	6.28	1.85	7.46	1.01	8.68	0.21
1,2,4-C3B	7.11	1.38	6.09	1.92	6.10	1.95	6.05	1.87	6.83	2.66	6.12	1.96	7.26	1.08	8.47	0.31
1,3,5-C3B	7.43	1.38	6.42	1.91	6.43	1.94	6.38	1.86	7.17	2.65	6.42	1.96	7.62	1.11	8.84	0.32
1,2,3,4-C4B	7.22	1.51	6.18	2.01	6.20	2.04	6.15	1.96	6.93	2.75	6.22	2.11	7.37	1.23	8.59	0.45
1,2,3,5-C4B	7.29	1.59	6.24	2.09	6.26	2.13	6.21	2.04	6.98	2.83	6.29	2.15	7.44	1.32	8.66	0.54
1,2,4,5-C4B	7.19	1.63	6.14	2.14	6.16	2.17	6.11	2.08	6.88	2.87	6.20	2.19	7.33	1.34	8.53	0.57
1,2,3,4,5-C5B	7.32	1.74	6.26	2.21	6.27	2.24	6.22	2.16	7.00	2.95	6.32	2.45	7.46	1.48	8.67	0.70
1,2,3,4,5,6-C6B	7.45	2.00	6.36	2.47	6.38	2.54	6.33	2.41	7.11	3.16	6.44	2.80	7.58	1.61	8.81	0.82
benzene	6.99	0.39	6.17	1.01	6.16	1.04	6.13	0.96	6.91	1.73	6.02	1.01	7.25	0.08	8.43	-0.73

Table S6. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With 6-31+G** Basis Set

System	B3LYP		MPWB1K		MPW1B95		BB1K		SVWN5		BLYP		M05		M05-2X	
	I	A	I	A	I	A	I	A	I	A	I	A	I	A	I	A
CB	6.95	0.80	6.02	1.40	6.02	1.43	5.98	1.35	6.76	2.13	5.97	1.41	7.15	0.49	8.34	-0.32
1,2-C2B	7.07	1.08	6.08	1.64	6.09	1.67	6.04	1.59	6.82	2.37	6.07	1.67	7.23	0.78	8.44	-0.03
1,3-C2B	7.13	1.13	6.16	1.70	6.17	1.73	6.12	1.64	6.90	2.43	6.15	1.73	7.32	0.83	8.51	0.03
1,4-C2B	6.95	1.16	5.96	1.74	5.97	1.77	5.92	1.68	6.70	2.47	5.97	1.76	7.12	0.84	8.31	0.05
1,2,3-C3B	7.29	1.30	6.29	1.82	6.29	1.85	6.25	1.77	7.02	2.55	6.29	1.87	7.46	1.03	8.68	0.21
1,2,4-C3B	7.11	1.40	6.09	1.94	6.10	1.97	6.05	1.89	6.83	2.68	6.12	1.98	7.27	1.10	8.46	0.31
1,3,5-C3B	7.43	1.39	6.42	1.92	6.43	1.96	6.38	1.87	7.17	2.66	6.43	1.97	7.62	1.12	8.84	0.32
1,2,3,4-C4B	7.23	1.52	6.18	2.02	6.20	2.06	6.15	1.97	6.93	2.77	6.23	2.11	7.37	1.24	8.58	0.45
1,2,3,5-C4B	7.29	1.60	6.24	2.10	6.26	2.14	6.21	2.05	6.98	2.84	6.29	2.16	7.44	1.33	8.65	0.54
1,2,4,5-C4B	7.19	1.64	6.14	2.15	6.16	2.19	6.11	2.10	6.88	2.89	6.20	2.20	7.33	1.35	8.53	0.58
1,2,3,4,5-C5B	7.32	1.75	6.26	2.21	6.27	2.25	6.22	2.17	7.00	2.96	6.32	2.44	7.46	1.48	8.67	0.70
1,2,3,4,5,6-C6B	7.45	2.00	6.36	2.46	6.38	2.53	6.33	2.41	7.11	3.16	6.44	2.80	7.58	1.61	8.80	0.82
benzene	7.01	0.42	6.19	1.05	6.18	1.07	5.98	1.35	6.94	1.77	6.04	1.04	7.26	0.11	8.43	-0.72

Table S7. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With 6-311++G** Basis Set

System	B3LYP		SVWN5		BLYP		M05		M05-2X	
	I	A	I	A	I	A	I	A	I	A
CB	7.01	0.86	6.83	2.21	6.03	1.48	7.18	0.52	8.41	-0.25
1,2-C2B	7.11	1.13	6.89	2.45	6.12	1.73	7.26	0.80	8.50	0.04
1,3-C2B	7.18	1.19	6.97	2.51	6.20	1.79	7.34	0.85	8.57	0.10
1,4-C2B	7.00	1.22	6.76	2.55	6.02	1.83	7.14	0.87	8.37	0.13
1,2,3-C3B	7.33	1.35	7.09	2.62	6.34	1.92	7.48	1.03	8.73	0.28
1,2,4-C3B	7.15	1.46	6.89	2.75	6.17	2.04	7.28	1.12	8.52	0.39
1,3,5-C3B	7.48	1.44	7.23	2.73	6.48	2.03	7.64	1.13	8.89	0.38
1,2,3,4-C4B	7.26	1.57	6.98	2.83	6.27	2.14	7.38	1.25	8.63	0.52
1,2,3,5-C4B	7.33	1.65	7.04	2.91	6.33	2.21	7.45	1.33	8.70	0.60
1,2,4,5-C4B	7.22	1.70	6.93	2.96	6.24	2.26	7.33	1.36	8.58	0.64
1,2,3,4,5-C5B	7.35	1.80	7.04	3.02	6.36	2.45	7.46	1.48	8.71	0.76
1,2,3,4,5,6-C6B	7.48	1.99	7.16	3.15	6.47	2.80	7.58	1.60		
benzene	7.08	0.48	7.03	1.85	6.11	1.10	7.31	0.14	8.51	-0.65

Table S8. Ionization Potential and Electron Affinity of Chlorinated Benzenes in eV, Calculated Using Various Methods With AUG-CC-PVDZ And AUG-CC-PVTZ Basis Set

System	B3LYP AUG-CC-PVDZ		MPWB1K AUG-CC-PVDZ		B3LYP AUG-CC-PVTZ	
	I	A	I	A	I	A
CB	6.98	0.90	6.05	1.48	6.99	0.86
1,2-C2B	7.09	1.17	6.11	1.72	7.08	1.13
1,3-C2B	7.15	1.22	6.18	1.78	7.15	1.18
1,4-C2B	6.97	1.25	5.98	1.82	6.96	1.21
1,2,3-C3B	7.31	1.37	6.31	1.89		
1,2,4-C3B	7.12	1.49	6.11	2.02	7.10	1.44
1,3,5-C3B	7.45	1.47	6.44	1.99	7.44	1.44
1,2,3,4-C4B	7.23	1.60	6.20	2.09	7.21	1.55
1,2,3,5-C4B	7.29	1.68			7.27	1.64
1,2,4,5-C4B	7.19	1.73	6.16	2.23	7.17	1.68
1,2,3,4,5-C5B	7.32	1.82				
1,2,3,4,5,6-C6B	7.44	2.01			7.40	1.90
benzene	7.06	0.51	6.24	1.12	7.09	0.48

Table S9. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from B3LYP, MPW1B95, MPWB1K and BB1K Methods With 6-31G* Basis Set Using Koopmans' Theorem

system	B3LYP			MPW1B95			MPWB1K			BB1K		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.36	-3.52	0.98	4.74	-3.38	1.20	4.77	-3.36	1.19	4.76	-3.35	1.18
1,2-C2B	6.19	-3.75	1.14	4.56	-3.56	1.39	4.59	-3.54	1.37	4.58	-3.53	1.36
1,3-C2B	6.20	-3.82	1.18	4.58	-3.63	1.44	4.60	-3.61	1.42	4.60	-3.60	1.41
1,4-C2B	6.00	-3.74	1.17	4.36	-3.56	1.45	4.38	-3.53	1.43	4.38	-3.53	1.42
1,2,3-C3B	6.15	-4.02	1.31	4.55	-3.79	1.58	4.58	-3.77	1.55	4.57	-3.76	1.54
1,2,4-C3B	5.90	-3.97	1.34	4.27	-3.75	1.65	4.29	-3.73	1.62	4.29	-3.72	1.61
1,3,5-C3B	6.19	-4.15	1.39	4.59	-3.92	1.67	4.62	-3.89	1.64	4.61	-3.88	1.63
1,2,3,4-C4B	5.82	-4.14	1.47	4.23	-3.88	1.78	4.26	-3.85	1.74	4.25	-3.84	1.74
1,2,3,5-C4B	5.84	-4.20	1.51	4.23	-3.94	1.83	4.26	-3.91	1.80	4.26	-3.91	1.79
1,2,4,5-C4B	5.73	-4.16	1.51	4.11	-3.90	1.85	4.13	-3.88	1.82	4.13	-3.87	1.81
1,2,3,4,5-C5B	5.69	-4.32	1.64	4.11	-4.03	1.97	4.13	-4.00	1.94			
1,2,3,4,5,6-C6B	5.56	-4.52	1.83				3.98	-4.19	2.21	3.98	-4.18	2.20
benzene	6.80	-3.30	0.80	5.24	-3.22	0.99	5.28	-3.21	0.98	5.27	-3.20	0.97

Table S10. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from SVWN5, BLYP, M05 and M05-2X Methods With 6-31G* Basis Set Using Koopmans' Theorem

system	SVWN5			BLYP			M05			M05-2X		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	4.76	-4.12	1.79	4.71	-3.31	1.16	6.86	-3.51	0.90	8.92	-3.71	0.77
1,2-C2B	4.58	-4.31	2.02	4.55	-3.52	1.36	6.64	-3.74	1.05	8.71	-3.93	0.89
1,3-C2B	4.60	-4.38	2.09	4.56	-3.60	1.42	6.67	-3.81	1.09	8.72	-4.01	0.92
1,4-C2B	4.37	-4.30	2.12	4.37	-3.53	1.43	6.47	-3.72	1.07	8.50	-3.92	0.90
1,2,3-C3B	4.57	-4.53	2.25	4.53	-3.77	1.57	6.59	-4.01	1.22	8.66	-4.21	1.03
1,2,4-C3B	4.28	-4.49	2.36	4.29	-3.74	1.63	6.34	-3.95	1.23	8.37	-4.14	1.03
1,3,5-C3B	4.61	-4.67	2.36	4.57	-3.90	1.67	6.65	-4.15	1.29	8.71	-4.35	1.09
1,2,3,4-C4B	4.25	-4.62	2.52	4.20	-3.90	1.81	6.24	-4.12	1.36	8.28	-4.32	1.13
1,2,3,5-C4B	4.25	-4.68	2.58	4.24	-3.95	1.83	6.26	-4.17	1.39	8.29	-4.38	1.16
1,2,4,5-C4B	4.12	-4.64	2.62	4.14	-3.91	1.85	6.14	-4.12	1.38	8.17	-4.33	1.15
1,2,3,4,5-C5B	4.12	-4.77	2.77	3.94	-4.14	2.17	6.09	-4.29	1.51	8.11	-4.50	1.25
1,2,3,4,5,6-C6B	4.00	-4.95	3.07	3.70	-4.39	2.60	6.03	-4.45	1.64	8.07	-4.67	1.35
benzene	5.29	-3.98	1.50	5.14	-3.10	0.93	7.37	-3.32	0.75	9.42	-3.51	0.65

Table S11. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from B3LYP, MPW1B95, MPWB1K and BB1K Methods With 6-31G** Basis Set Using Koopmans' Theorem

system	B3LYP			MPW1B95			MPWB1K			BB1K		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.35	-3.54	0.99	4.72	-3.40	1.22	4.75	-3.38	1.20	4.75	-3.37	1.20
1,2-C2B	6.18	-3.76	1.15	4.55	-3.57	1.40	4.57	-3.55	1.38	4.57	-3.54	1.37
1,3-C2B	6.18	-3.83	1.19	4.56	-3.65	1.46	4.59	-3.63	1.43	4.59	-3.62	1.43
1,4-C2B	5.99	-3.76	1.18	4.34	-3.57	1.47	4.36	-3.55	1.44	4.36	-3.54	1.44
1,2,3-C3B	6.14	-4.03	1.32	4.54	-3.80	1.59	4.57	-3.77	1.56	4.57	-3.77	1.55
1,2,4-C3B	5.89	-3.98	1.35	4.26	-3.76	1.66	4.28	-3.74	1.63	4.28	-3.73	1.62
1,3,5-C3B	6.19	-4.16	1.40	4.58	-3.92	1.68	4.61	-3.90	1.65	4.61	-3.89	1.64
1,2,3,4-C4B	5.82	-4.14	1.48	4.22	-3.88	1.79	4.25	-3.86	1.75	4.25	-3.85	1.75
1,2,3,5-C4B	5.83	-4.21	1.52	4.23	-3.94	1.84	4.25	-3.92	1.81	4.25	-3.91	1.80
1,2,4,5-C4B	5.72	-4.16	1.51	4.10	-3.91	1.86	4.12	-3.88	1.83	4.12	-3.87	1.82
1,2,3,4,5-C5B	5.68	-4.32	1.64	4.10	-4.03	1.98	4.13	-4.00	1.94	4.12	-4.00	1.94
1,2,3,4,5,6-C6B	5.56	-4.52	1.83				3.98	-4.19	2.21	3.98	-4.18	2.20
benzene	6.79	-3.32	0.81	5.23	-3.25	1.01	5.27	-3.24	1.00	5.27	-3.23	0.99

Table S12. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from SVWN5, BLYP, M05 and M05-2X Methods With 6-31G** Basis Set Using Koopmans' Theorem

system	SVWN5			BLYP			M05			M05-2X		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	4.75	-4.14	1.81	4.70	-3.33	1.18	6.85	-3.53	0.91	8.91	-3.71	0.77
1,2-C2B	4.57	-4.32	2.04	4.54	-3.54	1.38	6.63	-3.74	1.06	8.70	-3.93	0.89
1,3-C2B	4.59	-4.40	2.11	4.55	-3.61	1.43	6.67	-3.82	1.09	8.71	-4.00	0.92
1,4-C2B	4.35	-4.32	2.14	4.35	-3.54	1.44	6.46	-3.73	1.07	8.49	-3.91	0.90
1,2,3-C3B	4.56	-4.54	2.26	4.53	-3.78	1.58	6.58	-4.01	1.22	8.65	-4.21	1.02
1,2,4-C3B	4.27	-4.50	2.37	4.27	-3.75	1.64	6.33	-3.95	1.23	8.36	-4.14	1.03
1,3,5-C3B	4.61	-4.68	2.38	4.56	-3.91	1.67	6.64	-4.16	1.30	8.70	-4.35	1.09
1,2,3,4-C4B	4.24	-4.63	2.53	4.20	-3.90	1.81	6.24	-4.12	1.36	8.27	-4.32	1.13
1,2,3,5-C4B	4.24	-4.69	2.59	4.24	-3.95	1.84	6.25	-4.18	1.40	8.29	-4.38	1.16
1,2,4,5-C4B	4.11	-4.65	2.63	4.12	-3.92	1.86	6.14	-4.12	1.38	8.16	-4.33	1.15
1,2,3,4,5-C5B	4.11	-4.78	2.77	3.94	-4.14	2.17	6.08	-4.29	1.52	8.11	-4.50	1.25
1,2,3,4,5,6-C6B	4.00	-4.95	3.07	3.70	-4.39	2.60				8.07	-4.67	1.35
benzene	5.28	-4.00	1.52	5.13	-3.12	0.95	7.36	-3.34	0.76	9.41	-3.51	0.65

Table S13. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from B3LYP, MPW1B95, MPWB1K and BB1K Methods With 6-31+G* Basis Set Using Koopmans' Theorem

system	B3LYP			MPW1B95			MPWB1K			BB1K		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.17	-3.86	1.21	4.61	-3.71	1.49	4.63	-3.69	1.47	4.65	-3.64	1.43
1,2-C2B	6.00	-4.06	1.37	4.43	-3.87	1.69	4.46	-3.85	1.66	4.47	-3.80	1.62
1,3-C2B	6.02	-4.12	1.41	4.45	-3.93	1.74	4.47	-3.91	1.71	4.49	-3.87	1.66
1,4-C2B	5.82	-4.04	1.40	4.22	-3.86	1.76	4.24	-3.83	1.73	4.26	-3.79	1.69
1,2,3-C3B	6.00	-4.29	1.53	4.45	-4.06	1.86	4.47	-4.04	1.83	4.48	-4.00	1.78
1,2,4-C3B	5.73	-4.25	1.57	4.15	-4.03	1.96	4.16	-4.00	1.92	4.18	-3.96	1.87
1,3,5-C3B	6.05	-4.41	1.61	4.48	-4.18	1.95	4.51	-4.16	1.92	4.52	-4.12	1.88
1,2,3,4-C4B	5.71	-4.37	1.67	4.15	-4.12	2.04	4.17	-4.09	2.01	4.18	-4.05	1.97
1,2,3,5-C4B	5.70	-4.44	1.73	4.13	-4.19	2.13	4.15	-4.17	2.09	4.17	-4.12	2.04
1,2,4,5-C4B	5.56	-4.41	1.75	3.99	-4.16	2.17	4.00	-4.14	2.14	4.02	-4.09	2.08
1,2,3,4,5-C5B	5.58	-4.53	1.84	4.03	-4.26	2.25	4.05	-4.23	2.21	4.06	-4.19	2.16
1,2,3,4,5,6-C6B	5.45	-4.72	2.05	3.84	-4.46	2.59	3.90	-4.41	2.50	3.92	-4.37	2.44
benzene	6.60	-3.69	1.03	5.12	-3.60	1.27	5.16	-3.59	1.25	5.17	-3.54	1.21

Table S14. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from SVWN5, BLYP, M05 and M05-2X Methods With 6-31+G* Basis Set Using Koopmans' Theorem

system	SVWN5			BLYP			M05			M05-2X		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	4.64	-4.43	2.11	4.57	-3.68	1.48	6.68	-3.80	1.08	8.67	-4.01	0.93
1,2-C2B	4.47	-4.58	2.35	4.42	-3.86	1.68	6.47	-3.99	1.23	8.48	-4.20	1.04
1,3-C2B	4.48	-4.65	2.42	4.43	-3.92	1.74	6.50	-4.06	1.27	8.50	-4.27	1.07
1,4-C2B	4.25	-4.57	2.46	4.23	-3.85	1.75	6.30	-3.97	1.25	8.27	-4.18	1.06
1,2,3-C3B	4.48	-4.78	2.55	4.43	-4.07	1.87	6.44	-4.24	1.39	8.47	-4.45	1.17
1,2,4-C3B	4.17	-4.74	2.70	4.16	-4.04	1.96	6.18	-4.17	1.41	8.16	-4.39	1.18
1,3,5-C3B	4.52	-4.91	2.67	4.47	-4.19	1.97	6.51	-4.37	1.47	8.52	-4.58	1.23
1,2,3,4-C4B	4.17	-4.84	2.81	4.11	-4.17	2.11	6.14	-4.30	1.51	8.14	-4.52	1.25
1,2,3,5-C4B	4.15	-4.91	2.90	4.14	-4.22	2.15	6.12	-4.38	1.56	8.12	-4.60	1.30
1,2,4,5-C4B	4.01	-4.88	2.97	4.01	-4.19	2.19	5.99	-4.33	1.57	7.96	-4.55	1.30
1,2,3,4,5-C5B	4.04	-4.98	3.06	3.87	-4.38	2.48	5.98	-4.47	1.67	7.97	-4.69	1.38
1,2,3,4,5,6-C6B	3.95	-5.14	3.34	3.64	-4.62	2.93	5.97	-4.60	1.77	7.99	-4.81	1.45
benzene	5.18	-4.32	1.80	5.01	-3.52	1.23	7.16	-3.67	0.94	9.16	-3.85	0.81

Table S15. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from B3LYP, MPW1B95, MPWB1K and BB1K Methods With 6-31+G** Basis Set Using Koopmans' Theorem

system	B3LYP			MPW1B95			MPWB1K			BB1K		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.15	-3.88	1.22	4.59	-3.73	1.51	4.62	-3.71	1.49	4.63	-3.66	1.45
1,2-C2B	5.99	-4.07	1.39	4.42	-3.88	1.71	4.44	-3.86	1.68	4.46	-3.82	1.63
1,3-C2B	6.00	-4.13	1.42	4.44	-3.95	1.76	4.46	-3.93	1.73	4.48	-3.88	1.68
1,4-C2B	5.80	-4.05	1.42	4.20	-3.87	1.78	4.22	-3.85	1.76	4.24	-3.80	1.71
1,2,3-C3B	5.99	-4.29	1.54	4.44	-4.07	1.87	4.46	-4.05	1.84	4.48	-4.01	1.80
1,2,4-C3B	5.71	-4.26	1.59	4.13	-4.04	1.97	4.15	-4.02	1.94	4.17	-3.97	1.89
1,3,5-C3B	6.04	-4.41	1.61	4.47	-4.19	1.96	4.50	-4.17	1.93	4.52	-4.13	1.89
1,2,3,4-C4B	5.70	-4.37	1.68	4.14	-4.13	2.06	4.17	-4.10	2.02	4.17	-4.06	1.98
1,2,3,5-C4B	5.69	-4.45	1.74	4.12	-4.20	2.14	4.14	-4.17	2.10	4.16	-4.13	2.05
1,2,4,5-C4B	5.55	-4.42	1.76	3.97	-4.17	2.19	3.99	-4.15	2.16	4.01	-4.10	2.10
1,2,3,4,5-C5B	5.57	-4.54	1.85	4.02	-4.26	2.26	4.04	-4.23	2.22	4.05	-4.20	2.17
1,2,3,4,5,6-C6B	5.45	-4.72	2.05	3.85	-4.46	2.58	3.90	-4.41	2.50	3.92	-4.37	2.44
benzene	6.59	-3.72	1.05	5.11	-3.63	1.29	5.15	-3.62	1.27	4.63	-3.66	1.45

Table S16. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated From SVWN5, BLYP, M05 and M05-2X Methods With 6-31+G** Basis Set Using Koopmans' Theorem

system	SVWN5			BLYP			M05			M05-2X		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	4.63	-4.45	2.14	4.56	-3.69	1.50	6.66	-3.82	1.09	8.66	-4.01	0.93
1,2-C2B	4.45	-4.60	2.37	4.41	-3.87	1.70	6.46	-4.00	1.24	8.47	-4.20	1.04
1,3-C2B	4.47	-4.67	2.44	4.42	-3.94	1.75	6.49	-4.08	1.28	8.49	-4.27	1.07
1,4-C2B	4.23	-4.58	2.49	4.21	-3.87	1.77	6.28	-3.98	1.26	8.26	-4.18	1.06
1,2,3-C3B	4.47	-4.79	2.56	4.42	-4.08	1.88	6.43	-4.24	1.40	8.46	-4.45	1.17
1,2,4-C3B	4.15	-4.75	2.72	4.15	-4.05	1.98	6.16	-4.18	1.42	8.15	-4.39	1.18
1,3,5-C3B	4.51	-4.92	2.68	4.46	-4.20	1.98	6.50	-4.37	1.47	8.52	-4.58	1.23
1,2,3,4-C4B	4.16	-4.85	2.82	4.12	-4.17	2.11	6.13	-4.31	1.51	8.13	-4.52	1.25
1,2,3,5-C4B	4.14	-4.91	2.92	4.13	-4.23	2.16	6.11	-4.38	1.57	8.11	-4.60	1.30
1,2,4,5-C4B	3.99	-4.88	2.99	4.00	-4.20	2.21	5.98	-4.34	1.58	7.95	-4.55	1.30
1,2,3,4,5-C5B	4.04	-4.98	3.07	3.87	-4.38	2.48	5.98	-4.47	1.67	7.97	-4.69	1.38
1,2,3,4,5,6-C6B	3.95	-5.14	3.34	3.64	-4.62	2.93	5.97	-4.59	1.77	7.99	-4.81	1.45
benzene	5.17	-4.35	1.83	5.00	-3.54	1.25	7.15	-3.68	0.95	9.15	-3.85	0.81

Table S17. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated From B3LYP, SVWN5, BLYP and M05 Methods With 6-311++G** Basis Set Using Koopmans' Theorem

system	B3LYP			SVWM			BLYP			MO5		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.14	-3.94	1.26	4.62	-4.52	2.21	4.55	-3.75	1.55	6.66	-3.85	1.11
1,2-C2B	5.98	-4.12	1.42	4.44	-4.67	2.45	4.39	-3.93	1.75	6.46	-4.03	1.26
1,3-C2B	5.99	-4.19	1.46	4.46	-4.74	2.52	4.41	-3.99	1.81	6.49	-4.10	1.29
1,4-C2B	5.78	-4.11	1.46	4.20	-4.66	2.58	4.20	-3.93	1.84	6.26	-4.00	1.28
1,2,3-C3B	5.99	-4.34	1.57	4.47	-4.85	2.63	4.42	-4.13	1.93	6.44	-4.26	1.41
1,2,4-C3B	5.69	-4.30	1.63	4.13	-4.82	2.81	4.13	-4.10	2.04	6.16	-4.20	1.43
1,3,5-C3B	6.03	-4.46	1.65	4.50	-4.98	2.76	4.45	-4.25	2.03	6.51	-4.39	1.48
1,2,3,4-C4B	5.69	-4.42	1.72	4.15	-4.91	2.90	4.13	-4.20	2.14	6.13	-4.32	1.52
1,2,3,5-C4B	5.68	-4.49	1.78	4.13	-4.97	3.00	4.12	-4.27	2.22	6.11	-4.39	1.58
1,2,4,5-C4B	5.53	-4.46	1.80	3.97	-4.94	3.08	3.98	-4.25	2.27	5.97	-4.35	1.58
1,2,3,4,5-C5B	5.56	-4.58	1.88	4.02	-5.03	3.15	3.91	-4.40	2.48	5.98	-4.47	1.67
1,2,3,4,5,6-C6B	5.48	-4.74	2.04	4.00	-5.15	3.32	3.67	-4.64	2.93	5.98	-4.59	1.76
benzene	6.60	-3.78	1.08	5.18	-4.44	1.90	5.01	-3.61	1.30	7.17	-3.73	0.97

Table S18. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from M05-2X Method With 6-311++G** Basis Set Using Koopmans' Theorem

system	M05-2X		
	η(eV)	μ(eV)	ω(eV)
CB	8.65	-4.08	0.96
1,2-C2B	8.45	-4.27	1.08
1,3-C2B	8.47	-4.34	1.11
1,4-C2B	8.24	-4.25	1.10
1,2,3-C3B	8.46	-4.51	1.20
1,2,4-C3B	8.13	-4.45	1.22
1,3,5-C3B	8.51	-4.64	1.26
1,2,3,4-C4B	8.11	-4.57	1.29
1,2,3,5-C4B	8.10	-4.65	1.34
1,2,4,5-C4B	7.93	-4.61	1.34
1,2,3,4,5-C5B	7.95	-4.74	1.41
1,2,3,4,5,6-C6B benzene	9.16	-3.93	0.84

Table S19. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from Various Methods Using Koopmans' Theorem

system	B3LYP AUG-CC-PVDZ			MPWB1K AUG-CC-PVDZ			B3LYP AUG-CC-PVTZ		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	6.09	-3.94	1.27	4.57	-3.77	1.55	6.13	-3.92	1.25
1,2-C2B	5.92	-4.13	1.44	4.39	-3.92	1.75	5.95	-4.10	1.41
1,3-C2B	5.93	-4.19	1.48	4.41	-3.98	1.80	5.97	-4.16	1.45
1,4-C2B	5.71	-4.11	1.48	4.16	-3.90	1.83	5.75	-4.09	1.45
1,2,3-C3B	5.93	-4.34	1.59	4.42	-4.10	1.90			
1,2,4-C3B	5.63	-4.30	1.64	4.08	-4.07	2.02	5.66	-4.27	1.61
1,3,5-C3B	5.98	-4.46	1.66	4.45	-4.22	2.00	6.00	-4.44	1.64
1,2,3,4-C4B	5.63	-4.41	1.73	4.11	-4.15	2.09	5.65	-4.38	1.70
1,2,3,5-C4B	5.61	-4.49	1.79				5.64	-4.45	1.76
1,2,4,5-C4B	5.46	-4.46	1.82	3.92	-4.20	2.24	5.49	-4.42	1.78
1,2,3,4,5-C5B	5.50	-4.57	1.90						
1,2,3,4,5,6-C6B	5.43	-4.73	2.06				5.50	-4.65	1.97
benzene	6.54	-3.78	1.09	5.12	-3.68	1.32	6.61	-3.78	1.08

Table S20. Global Reactivity Descriptors, Hardness (η), Chemical Potential (μ) and Electrophilicity (ω), Calculated from Various Methods Using ΔSCF Method

system	B3LYP 6-31G*			M05-2X 6-31++G**		
	η(eV)	μ(eV)	ω(eV)	η(eV)	μ(eV)	ω(eV)
CB	10.22	-3.57	0.62	10.10	-3.96	0.78
1,2-C2B	8.83	-4.28	1.04	9.06	-4.54	1.14
1,3-C2B	8.91	-4.29	1.03	9.73	-4.26	0.93
1,4-C2B	9.48	-3.82	0.77	9.50	-4.17	0.92
1,2,3-C3B	8.69	-4.52	1.17	8.95	-4.77	1.27
1,2,4-C3B	8.49	-4.40	1.14	8.77	-4.65	1.24
1,3,5-C3B	8.84	-4.57	1.18	9.67	-4.55	1.07
1,2,3,4-C4B	8.29	-4.58	1.27	8.60	-4.82	1.35
1,2,3,5-C4B	8.34	-4.61	1.27	8.96	-4.69	1.23
1,2,4,5-C4B	8.59	-4.36	1.11	9.03	-4.56	1.15
1,2,3,4,5-C5B	8.06	-4.73	1.39	8.43	-4.97	1.47
1,2,3,4,5,6-C6B	8.09	-4.82	1.43	8.43	-5.08	1.53
benzene	10.96	-3.38	0.52	10.63	-3.83	0.69