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Supplementary material

PROPERTIS OF *N*-(SUBSTITUTED PHENYL)-2-CHLOROACETAMIDES: LSER AND LFER

Borko M. Matijević[a,*], Đenđi Đ. Vaštag[a], Suzana Lj. Apostolov[a], Miloš K. Milčić[b], Aleksandar D. Marinković[c], Slobodan D. Petrović[c]

[a] *University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia*

[b] *Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia*

[c] *Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia*

Table S1 Melting point and yield of *N*-(substituted phenyl) chloroacetamides

Comp	Substituent	m.p. ºC	Lit. m.p. ºC	Yield %	Reference
1	H	136-137	136-139	86	Hernandez-Nunez et al., 2009
2	4-CH_3	160-162	162	89	Tai-Bao et al., 2009
3	4-OCH_3	117-119	117-119	84	Rahaim et al., 2006
4	4-Cl	166-168	168-170	65	Ki Sun et al., 2003
5	4-Br	178-180	178-180	88	Hauser, 1962
6	4-F	128-130	130-131	83	Harte and Gunnlaugsson, 2006
7	4-I	192-195	191-194	72	Jacobs and Heidelberger, 1917
8	4-CH_3CO	144-145	144-145	64	Tricerri and Guzzon, 1955
9	4-OH	144-146	-	76	-
10	4-CN	180-183	184-186	56	Hernandez-Nunez et al., 2009
11	3-CN	165-170	168-170	61	Soyer et al., 2004
12	3-Br	110-113	-	83	-

Table S2 Characterization of investigated *N*-(substituted phenyl)-2-chloroacetamides

R	IR (KBr) ν_{max} (cm^{-1})
H	3267 (N-H); 3207, 3145, 3098 (C-H aromatic ring); 2947 (C-H); 1671 (C=O); 1618 (C=C); 1557 (N-H deformation); 1498, (C-H bending); 1443 (C-H bending); 1344 (C-H); 1251 (C-N); 749 (N-H).
4-CH_3	3273 (N-H); 3204, 3135, 3090 (C-H aromatic ring); 2954 (C-H); 1673 (C=O); 1616 (C=C); 1554 (N-H); 1402 (C-H); 1343 (C-H); 1251 (C-N); 818 (N-H).
4-OCH_3	3295 (N-H); 3139, 3073 (C-H aromatic ring); 2957 (C-H); 2909 2835 (C-H); 1663 (C=O); 1612 (C=C); 1547 (N-H); 1510 (N-H); 1465 (C-H); 1413 (C-H); 1247 (C-N); 830 (N-H).
4-Cl	3264(N-H); 3199, 3131, 3082 (C-H aromatic ring); 3005, 2952(C-H); 1669 (C=O); 1614 (C=C); 1551 (N-H); 1490 (C-H); 1400 (C-H); 1248 (C-N); 825 (N-H).
4-Br	3263 (N-H); 3194 (C-H); 3125, 3077 (C-H aromatic ring); 3000 2953 (C-H); 1669 (C=O); 1549 (N-H); 1488 (C-H); 1395 (C-H); 1248 (C-N); 822 (N-H).
4-F	3275, 3221 (N-H); 3165 (C-H aromatic ring); 2947 (C-H); 1668 (C=O); 1508 (N-H); 1406 (C-H); 1292; 1212 (C-N); 832 (N-H).
4-I	3309, 3270 (N-H); 3194, 3077 (C-H aromatic ring); 2936 (C-H); 2953 (C-H); 1672 (C=O); 1610 (N-H); 1543 (C-H); 1392-1089 (CH); 1245 (C-N); 817 (N-H).
4-$COCH_3$	3325, 3286 (N-H); 3196, 3109 (C-H aromatic ring); 2922, 2857 (C-H); 1707 (C=O); 1655 (C=C); 1599 (N-H); 1539 (C-H); 1283 (C-O); 1252 (C-N); 834 (N-H).
4-OH	3296 (O-H); 3144 (N-H); 3098 (C-H); 1677 (C=O); 1508 (N-H); 1313 (C-H); 1211 (C-N); 820 (N-H).
4-CN	3265 (N-H); 3192, 3119 (C-H); 2946 (C-H); 2226 (C≡N); 1681 (C=O); 1603 (C=C); 1539 (N-H); 1408, 1345 (C-H); 1256 (C-N); 839 (N-H).
3-CN	3265 (N-H); 3096 (C-H); 2964 C-H); 2232 (C≡N); 1678 (C=O); 1610 (C=C); 1561 (N-H); 1485 (C-H); 1293 (C-N); 1089 (C-H); 799 (N-H).
3-Br	3268 (N-H); 3193, 3127 (C-H); 2945 (C-H); 1679 (C=O); 1594 (N-H); 1424 (C-H); 1249 (C-N); 779 (N-H).

^{1}H and ^{13}C NMR spectral data:

N-phenylchloroacetamide (**1**). ^{1}H NMR ($CDCl_3$): δ 4.272 (2H, s, Cl-CH_2), 7.057-7.130 (1H, t, J_{HH} = 7.4 Hz, Ar-4H), 7.302-7.380 (2H, t, J_{HH} = 7.8 Hz, Ar-H), 7.597-7.636 (2H, d, J_{HH} = 7.8 Hz, Ar-H), 10.321 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 43.833 (Cl-CH_2), 119.651 (C_2,C_5), 124.130 (C_4) 129.119 (C_3,C_5), 138.751 (C_1), 164.934 (C=O).

N-(4-methylphenyl)chloroacetamide (**2**). ^{1}H NMR ($CDCl_3$): δ 2.255 (2H, s, CH_3), 4.421 (1H, s, Cl-CH_2), 7.111-7.153 (2H, d, J_{HH} = 8.2 Hz, Ar-H), 7.473-7.515 (2H, d, J_{HH} = 8.2 Hz, Ar-H), 10.222 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 20.655 (CH_3), 43.797 (Cl-CH_2), 119.614 (C_2,C_6), 129.483 (C_3,C_5), 133.088 (C_1), 136.238 (C_4), 164.643 (C=O).

N-(4-metoxylphenyl)chloroacetamide (**3**). ^{1}H NMR ($CDCl_3$): δ 3.729 (2H, s, OCH_3), 4.229 (1H, s, Cl-CH_2), 6.886-6.948 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7.481-7.560 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 10.177 (1H, s, NH).). ^{13}C NMR ($CDCl_3$): δ 43.742 (Cl-CH_2), 55.359 (OCH_3), 114.189 (C_3,C_5), 121.217 (C_2,C_6), 131.814 (C_1), 155.885(C_4), 164.424 (C=O).

N-(4-chlorophenyl)chloroacetamide (**4**). ^{1}H NMR ($CDCl_3$): δ 4.280 (1H, s, Cl-CH_2), 7.358-7.431 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7.613-7.686 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 10.445 (1H, s, NH), ^{13}C NMR ($CDCl_3$): δ 43.741 (Cl-CH_2), 121.162 (C_2,C_6), 129.010 (C_3,C_5), 137.677 (C_1), 165.061 (C=O).

N-(4-bromophenyl)chloroacetamide (**5**). ^{1}H NMR ($CDCl_3$): δ 4.274 (1H, s, Cl-CH_2), 7.495-7.616 (4H, m, Ar-H), 10.447 (1H, s, N-H). ^{13}C NMR ($CDCl_3$): δ 43.742 (Cl-CH_2), 115.736 (C_4), 121.526 (C_2,C_6), 131.923 (C_3,C_5), 138.095 (C_1), 165.061 (C=O).

N-(4-fluorophenyl)chloroacetamide (**6**). ^{1}H NMR ($CDCl_3$): δ 4.369 (1H, s, Cl-CH_2), 7.122-7.226 (2H, t, J_{HH} = 9.0 Hz, Ar-H)), 7,588-7,675 (2H, m, Ar-H), 10,337 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 43.688 (Cl-CH_2), 115.463-115.900 (C_3,C_5), 121.381 (C_2,C_6), 135.073 (C_1), 160.983 (C_4), 164.861 (C=O).

N-(4-iodophenyl)chloroacetamide (**7**). ^{1}H NMR ($CDCl_3$): δ 4.263 (1H, s, Cl-CH_2), 7.425-7.4709 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7,658-7,701 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 10.416 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 43.760 (Cl-CH_2), 87.732 (C_4), 121.745 (C_2,C_6), 137.750-138.551 (C_3,C_5), 165.043 (C=O).

N-(4-acetylphenyl)chloroacetamide (**8**). ^{1}H NMR ($CDCl_3$): δ 2.544 (3H, s, CH_3), 4.328 (1H, s, Cl-CH_2), 7,723-7,768 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7.945-7.990 (2H, d, J_{HH} = 9.0 Hz, Ar-H),

10.646 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 26.645 (CH_3), 43.833 (Cl-CH_2), 118.868 (C_2,C_6), 129.793 (C_3,C_5), 132.451 (C_4), 143.030 (C_1), 165.462 (C=O), 196.798 ($COCH_3$).

N-(4-hydroxyphenyl)chloroacetamide (**9**). ^{1}H NMR ($CDCl_3$): δ 4.280 (2H, s, Cl-CH_2), 4.684 (1H, s, OH), 7.139-7.184 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7.625-7.686 (2H, d, J_{HH} = 8.8 Hz, Ar-H). ^{13}C NMR ($CDCl_3$): δ 43.706 (Cl-CH_2), 120.671(C_3,C_5), 122.091 (C_2,C_6), 136.7489 (C_1), 146.180 (C_4), 164.989-166.791 (C=O).

N-(4-cyanophenyl)chloroacetamide (**10**). ^{1}H NMR ($CDCl_3$): δ 4.319 (2H, s, Cl-CH_2), 7.552-7.619 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 7.782-7.877 (2H, d, J_{HH} = 9.0 Hz, Ar-H), 10.745 (1H, s, 2-H). ^{13}C NMR ($CDCl_3$): δ 43.669 (Cl-CH_2), 111.985 (C_3), 118.668 (CN), 122.309 (C_2), 124.203 (C_6), 127.662 (C_4), 130.321-130.594 (C_5), 139.516 (C_1), 165.589 (C=O).

N-(3-cyanophenyl)chloroacetamide (**11**). ^{1}H NMR ($CDCl_3$): δ 4.339 (1H, s, Cl-CH_2), 7.552-7.619 (2H, d, J_{HH} = 5.6 Hz, Ar-H), 7.782-7.813 (1H, m, Ar-H), 8.094 (1H, s, Ar-H), 10.745 (1H, s, NH). ^{13}C NMR ($CDCl_3$): δ 43.669 (Cl-CH_2), 111.985 (C_3), 118.668 (CN), 122.309 (C_2), 124.203 (C_6), 127.662 (C_4), 130.321-130.594 (C_5), 139.516 (C_1), 165.589 (C=O).

N-(3-bromophenyl)chloroacetamide (**12**). ^{1}H NMR ($CDCl_3$): δ 4.286 (3H, s, Cl-CH_2), 7.285-7.358 (2H, m, Ar-H), 7.470-7.571 (1H, m, Ar-H), 7.962 (1H, s, Ar-H), 10.489 (1H, s, N-H). ^{13}C NMR ($CDCl_3$): δ 43.688 (Cl-CH_2), 118.376 (C_2), 121.836 (C5), 121.927 (C_6), 126.697 (C_4), 131.067 (C_3), 140.262 (C_1), 165.243 (C=O).

Table S3 Kamlet-Taft solvatochromic parameters of solvents

solvent	π^*	α	β
Methanol	0.60	0.93	0.62
Ethanol	0.54	0.83	0.77
1-propanol	0.52	0.78	0.83
2-propanol	0.48	0.76	0.95
1-butanol	0.47	0.84	0.84
2-butanol	0.40	0.79	0.84
2-metil-2-propanol	0.41	0.68	1.01
Water	1.09	1.17	0.18
Dioxane	0.55	0.00	0.37
acetonitrile	0.75	0.19	0.31
Chloroform	0.58	0.44	0.00
Hexane	-0.04	0.00	0.00
Heptanes	-0.08	0.00	0.00
Methyl acetate	0.60	0.00	0.42
ethylacetate	0.55	0.00	0.45
ethylenglicole	0.92	0.90	0.52
DMSO	1.00	0.00	0.76
Acetic acid	0.64	1.12	0.45

Table S4 Percentage contribution of solvatochromic parameters

substituent	*P*s(%)	*P*a(%)	*P*b(%)
H	86.64	0.00	13.36
4-CH_3	67.74	18.43	13.84
4-OCH_3	72.80	7.11	20.10
4-Cl	74.80	0.00	25.20
4-Br	82.29	4.37	13.34
4-F	88.49	11.51	0.00
4-I	73.54	7.96	18.50
4-$COCH_3$	36.44	16.82	46.75
4-OH	74.09	0.00	25.91
4-CN	57.13	5.08	37.79
3-CN	91.91	8.09	0.00
3-Br	70.97	13.98	15.05

Table S5 Values of Hammett sigma constants, $\sigma_{m,p}$

Substituent	$\sigma_{m,p}$
H	0.00
4-CH_3	-0.17
4-OCH_3	-0.27
4-Cl	0.23
4-Br	0.23
4-F	0.06
4-I	0.18
4-$COCH_3$	0.50
4-OH	-0.37
4-CN	0.66
3-CN	0.56
3-Br	0.39

Table S6 Selected interatomic distances and torsion angle (in gas phase) of *trans* isomers in *N*-(substituted phenyl)-2-chloroacetamides obtained by the use of DFT method

Compound	Interatomic distances			Torsion angle[a]
	C1-N	N-(C=O)	C=O	
H	1.415	1.359	1.219	-0.003
4-CH_3	1.416	1.358	1.220	-0.383
4-OCH_3	1.417	1.356	1.221	0.026
4-Cl	1.413	1.360	1.219	0.041
4-Br	1.413	1.360	1.219	-0.046
4-F	1.415	1.359	1.219	0.033
4-I	1.412	1.361	1.218	-0.034
4-$COCH_3$	1.409	1.363	1.217	-0.006
4-OH	1.417	1.356	1.220	0.104
4-CN	1.407	1.365	1.217	-0.082
3-CN	1.410	1.363	1.217	-0.010
3-Br	1.412	1.361	1.218	-0.001

[a] torsion angle (C=O)-NH-C1-C2

Table S7. Results of electronic transitions, absorption wavelength, oscillator strength, CI expansion coefficient and % of single particle excitation contribution obtained by TD-DFT calculations in water

Compound No.	Excited State No.	Energy (nm)	Oscillator strength	Excitation	CI expansion coefficient*	% of single particle excitation contribution*
1	1	239.07	0.0102	HOMO-1→LUMO	0.36900	27.2
				HOMO→LUMO+1	0.58280	67.9
	2	230.07	0.4593	HOMO-1→LUMO+1	-0.14862	4.4
				HOMO→LUMO	0.67889	92.2
2	1	244.91	0.0171	HOMO-1→LUMO	-0.31856	20.3
				HOMO→LUMO+1	0.61371	75.3
	2	234.35	0.5311	HOMO-1→LUMO+2	0.14481	4.2
				HOMO→LUMO	0.67877	92.1
3	1	256.96	0.0520	HOMO-1→LUMO	-0.18307	6.7
				HOMO-1→LUMO+1	-0.11727	2.7
				HOMO→LUMO	-0.41682	34.7
				HOMO→LUMO+1	0.51346	52.7
	2	239.14	0.5501	HOMO-1→LUMO	-0.10839	2.3
				HOMO→LUMO	0.53696	57.7
				HOMO→LUMO+1	0.41487	34.4
4	1	246.43	0.0147	HOMO-1→LUMO	-0.31338	19.6
				HOMO→LUMO+1	0.62072	77.1
	2	236.36	0.5737	HOMO-1→LUMO+1	0.13404	3.6
				HOMO→LUMO	0.68169	92.9
5	1	246.73	0.0119	HOMO-1→LUMO	0.31563	19.9
				HOMO→LUMO+1	0.61890	76.6
	2	238.27	0.6307	HOMO-1→LUMO+1	-0.12661	3.2
				HOMO→LUMO	0.68112	92.8
6	1	245.14	0.0315	HOMO-1→LUMO	0.27820	15.5
				HOMO→LUMO+1	0.63185	79.8
	2	228.92	0.4395	HOMO-1→LUMO+1	-0.15206	4.6
				HOMO→LUMO	0.67384	90.8
7	1	271.90	0.0009	HOMO-3→LUMO+1	0.23329	10.9
				HOMO→LUMO+1	0.65221	85.1
	2	247.52	0.0008	HOMO-2→LUMO	0.31521	19.9
				HOMO→LUMO+2	0.61280	75.1
	3	240.91	0.6976	HOMO-3→LUMO	-0.11813	2.8
				HOMO-2→LUMO+2	0.11710	2.7
					0.67592	91.4

				HOMO→LUMO		
8	1	300.21	0.0001	HOMO-2→LUMO	0.63541	10.7
				HOMO-2→LUMO+5	0.23381	10.9
	2	264.41	0.6897	HOMO→LUMO	0.69040	95.3
9	1	256.38	0.0493	HOMO-1→LUMO	0.20246	8.2
				HOMO→LUMO	-0.29690	17.6
				HOMO→LUMO+1	0.58897	69.4
	2	236.94	0.5112	HOMO-1→LUMO+1	-0.13002	3.4
				HOMO→LUMO	0.60603	73.5
				HOMO→LUMO+1	0.30813	19.0
10	1	252.05	0.7534	HOMO-1→LUMO+1	0.10821	2.3
				HOMO→LUMO	0.68815	94.7
	2	245.89	0.0005	HOMO-1→LUMO	-0.47735	45.6
				HOMO→LUMO+2	0.50887	51.8
11	1	260.27	0.0738	HOMO-1→LUMO	-0.19031	7.2
				HOMO-1→LUMO+1	-0.20207	8.2
				HOMO→LUMO	0.60817	74.0
				HOMO→LUMO+1	-0.19477	7.6
	2	233.33	0.2233	HOMO-1→LUMO	0.33026	21.8
				HOMO→LUMO	0.54657	59.7
				HOMO→LUMO+1	0.27245	14.8
12	1	244.50	0.0211	HOMO-1→LUMO	-0.34398	23.7
				HOMO-1→LUMO+1	0.10656	2.3
				HOMO→LUMO	0.16632	5.5
				HOMO→LUMO+1	0.55715	62.1
	2	231.45	0.3830	HOMO-1→LUMO	0.18885	7.1
				HOMO-1→LUMO+1	0.16346	5.3
				HOMO→LUMO	0.63979	81.9
				HOMO→LUMO+1	-0.11182	2.5

* only single particle excitation with CI expansion coefficient larger than 0.1 are shown

Table S8 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-phenylchloroacetamide (**1**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0537	0.0552	0.0015
2	1.3999	1.3502	-0.0497
3	-1.1854	-1.0715	0.1139
4	-1.1603	-1.1305	0.0298
5	-0.7864	-0.7871	-0.0007
6	0.1014	0.098	-0.0034
7	0.1006	0.0964	-0.0042
8	0.43	0.4266	-0.0034
9	-0.0468	-0.1291	-0.0823
10	-0.0148	0.0774	0.0922
11	-0.0391	-0.1088	-0.0697
12	0.0019	-0.0031	-0.005
13	0.3123	0.364	0.0517
14	-0.0009	-0.0449	-0.044
15	0.0435	0.0381	-0.0054
16	0.0187	0.0147	-0.004
17	0.0474	0.0418	-0.0056
18	0.0875	0.0837	-0.0038
19 (H)	0.0222	0.0131	-0.0091

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

Table S9 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-methylphenyl)chloroacetamide (**2**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0794	0.0805	0.0011
2	1.4033	1.3748	-0.0285
3	-1.2129	-1.1086	0.1043
4	-1.1	-1.0632	0.0368
5	0.0318	0.0312	-0.0006
6	0.0971	0.0946	-0.0025
7	0.0982	0.0959	-0.0023
8	0.4372	0.4357	-0.0015
9	0.0162	-0.0751	-0.0913
10	-0.0531	0.0652	0.1183
11	-0.0546	-0.1464	-0.0918
12	-0.0398	-0.088	-0.0482
13	0.382	0.4728	0.0908
14	0.0148	-0.0508	-0.0656
15	0.0219	0.0142	-0.0077
16	0.0294	0.0207	-0.0087
17	0.1002	0.097	-0.0032
18	0.0172	0.0069	-0.0103
19 (C)	0.0239	0.0166	-0.0073
20 (H)	0.018	0.0194	0.0014
21 (H)	0.0151	0.0159	0.0008
22 (H)	0.0246	0.0385	0.0139

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S10 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-methoxyphenyl)chloroacetamide (**3**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0598	0.0599	1E-04
2	1.4219	1.4149	-0.007
3	-1.193	-1.0967	0.0963
4	-1.0978	-1.0618	0.036
5	0.1408	0.1402	-0.0006
6	0.0922	0.0916	-0.0006
7	0.0934	0.0928	-0.0006
8	0.4263	0.4247	-0.0016
9	-0.0525	-0.1216	-0.0691
10	0.4957	0.6121	0.1164
11	-0.0136	-0.1704	-0.1568
12	0.0179	-0.1385	-0.1564
13	0.3713	0.5211	0.1498
14	-0.0079	-0.1266	-0.1187
15	0.0307	0.0253	-0.0054
16	0.0602	0.0532	-0.007
17	0.1084	0.1065	-0.0019
18	0.0259	0.018	-0.0079
19 (O)	-1.0488	-0.9208	0.128
20 (C)	0.4468	0.4383	-0.0085
21 (H)	0.0665	0.0664	-1E-04
22 (H)	0.0304	0.0383	0.0079
23 (H)	0.0285	0.0372	0.0087

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S11 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-chlorophenyl)chloroacetamide (**4**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0605	0.0604	-0.0001
2	1.4044	1.3913	-0.0131
3	-1.1453	-1.0303	0.115
4	-1.1225	-1.081	0.0415
5	-0.0813	-0.0817	-0.0004
6	0.1077	0.1068	-0.0009
7	0.096	0.0953	-0.0007
8	0.4303	0.4281	-0.0022
9	-0.0199	-0.1448	-0.1249
10	0.0152	0.1393	0.1241
11	-0.0581	-0.1782	-0.1201
12	0.0314	-0.052	-0.0834
13	0.3421	0.438	0.0959
14	0.0232	-0.0859	-0.1091
15	0.0624	0.0572	-0.0052
16	0.0642	0.0585	-0.0057
17	0.1069	0.105	-0.0019
18	0.0322	0.0239	-0.0083
19 (Cl)	-0.4528	-0.3534	0.0994

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

Table S12 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-bromophenyl)chloroacetamide (**5**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0615	0.0623	0.0008
2	1.4114	1.3973	-0.0141
3	-1.2264	-1.1206	0.1058
4	-1.1557	-1.1173	0.0384
5	-0.4253	-0.4257	-0.0004
6	0.0926	0.0917	-0.0009
7	0.0959	0.0952	-0.0007
8	0.4465	0.4448	-0.0017
9	0.0254	-0.1076	-0.133
10	-0.1515	-0.0387	0.1128
11	0.0342	-0.0858	-0.12
12	-0.0192	-0.1097	-0.0905
13	0.3229	0.4177	0.0948
14	-0.0742	-0.1973	-0.1231
15	0.0842	0.0789	-0.0053
16	0.0641	0.0584	-0.0057
17	0.1062	0.1025	-0.0037
18	0.0305	0.0233	-0.0072
19 (Br)	1.2415	1.3942	0.1527

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

Table S13 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-fluorophenyl)chloroacetamide (**6**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0664	0.0662	-0.0002
2	1.4173	1.4049	-0.0124
3	-1.1526	-1.0123	0.1403
4	-1.0957	-1.0412	0.0545
5	0.0237	0.0234	-0.0003
6	0.1016	0.1009	-0.0007
7	0.0954	0.0948	-0.0006
8	0.4075	0.4042	-0.0033
9	-0.0135	-0.141	-0.1275
10	0.4581	0.5958	0.1377
11	0.0436	-0.0786	-0.1222
12	0.0291	-0.057	-0.0861
13	0.3375	0.455	0.1175
14	-0.0381	-0.1444	-0.1063
15	0.0669	0.06	-0.0069
16	0.0545	0.0481	-0.0064
17	0.1076	0.1059	-0.0017
18	0.0366	0.026	-0.0106
19 (F)	-0.5968	-0.5625	0.0343

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

Table S14 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-iodophenyl)chloroacetamide (**7**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0413	0.0411	-0.0002
2	1.3943	1.4031	0.0088
3	-1.143	-1.0736	0.0694
4	-1.0589	-1.0291	0.0298
5	-1.1526	-1.1537	-0.0011
6	0.1042	0.1048	0.0006
7	0.1045	0.1053	0.0008
8	0.4232	0.4208	-0.0024
9	0.0484	0.0933	0.0449
10	-0.2933	-0.4522	-0.1589
11	0.1066	0.1457	0.0391
12	-0.0611	-0.0276	0.0335
13	0.3184	0.4409	0.1225
14	-0.0739	-0.0456	0.0283
15	0.0707	0.0418	-0.0289
16	0.0518	0.0161	-0.0357
17	0.1175	0.1077	-0.0098
18	0.0361	0.0195	-0.0166
19 (I)	0.5782	0.4569	-0.1213

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

Table S15 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-acetylphenyl)chloroacetamide (**8**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0111	0.0124	0.0013
2	1.3802	1.3448	-0.0354
3	-1.2496	-1.2446	0.005
4	-1.089	-1.1023	-0.0133
5	-1.47	-1.4702	-0.0002
6	0.112	0.1095	-0.0025
7	0.108	0.1056	-0.0024
8	0.4427	0.4427	0
9	-0.0515	-0.131	-0.0795
10	-0.0252	0.07	0.0952
11	-0.0791	-0.1163	-0.0372
12	0.0162	0.0094	-0.0068
13	0.3942	0.2697	-0.1245
14	0.0118	0.0087	-0.0031
15	0.0794	0.0773	-0.0021
16	0.0414	0.041	-0.0004
17	0.1137	0.1167	0.003
18	0.0261	0.0275	0.0014
19 (C)	0.9637	0.4426	-0.5211
20 (O)	-1.0615	-0.477	0.5845
21 (C)	-0.0563	0.1069	0.1632
22 (H)	0.0409	0.0399	-0.001
23 (H)	0.0283	0.0178	-0.0105
24 (H)	0.0333	0.0189	-0.0144

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S16 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-hydroxyphenyl)chloroacetamide (**9**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.07	0.0696	-0.0004
2	1.3981	1.3974	-0.0007
3	-1.2141	-1.1066	0.1075
4	-1.1435	-1.0963	0.0472
5	-1.3085	-1.309	-0.0005
6	0.094	0.0941	1E-04
7	0.0916	0.0919	0.0003
8	0.4227	0.4203	-0.0024
9	0.0442	-0.0786	-0.1228
10	0.4692	0.6017	0.1325
11	-0.0365	-0.1625	-0.126
12	-0.0583	-0.1964	-0.1381
13	0.3796	0.5356	0.156
14	-0.0245	-0.159	-0.1345
15	0.0132	0.0048	-0.0084
16	0.1123	0.1111	-0.0012
17	0.0278	0.0186	-0.0092
18	0.0609	0.0546	-0.0063
19 (O)	-1.111	-1.0019	0.1091
20 (H)	0.5958	0.5936	-0.0022

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S17 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(4-cyanophenyl)chloroacetamide (**10**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0684	0.0713	0.0029
2	1.4143	1.2623	-0.152
3	-1.1858	-0.9922	0.1936
4	-1.079	-1.0389	0.0401
5	0.1692	0.1683	-0.0009
6	0.1009	0.0901	-0.0108
7	0.1001	0.0874	-0.0127
8	0.4304	0.4286	-0.0018
9	-0.0046	-0.1298	-0.1252
10	0.0726	0.1115	0.0389
11	-0.0125	0.0023	0.0148
12	0.0098	0.1373	0.1275
13	0.3909	0.3358	-0.0551
14	0.0202	-0.0004	-0.0206
15	0.0649	0.0627	-0.0022
16	0.0628	0.061	-0.0018
17	0.123	0.1228	-0.0002
18	0.0308	0.0265	-0.0043
19 (C)	0.7609	0.7037	-0.0572
20 (N)	-1.0108	-0.9835	0.0273

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S18 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(3-cyanophenyl)chloroacetamide (**11**)

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.1118	0.1123	0.0005
2	1.3831	1.3679	-0.0152
3	-1.1744	-0.998	0.1764
4	-1.0971	-1.026	0.0711
5	-0.3645	-0.3643	0.0002
6	0.1038	0.1031	-0.0007
7	0.1011	0.1003	-0.0008
8	0.434	0.4318	-0.0022
9	0.103	-0.0211	-0.1241
10	-0.013	0.0982	0.1112
11	0.0204	-0.0111	-0.0315
12	-0.0192	-0.0137	0.0055
13	0.3762	0.4614	0.0852
14	-0.018	-0.151	-0.133
15	0.0383	0.0342	-0.0041
16	0.1275	0.1251	-0.0024
17	0.0328	0.0263	-0.0065
18	0.0535	0.0497	-0.0038
19 (C)	0.8079	0.7479	-0.06
20 (N)	-1.0386	-1.1044	-0.0658

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atoms are labeled with their chemical symbols.

Table S19 Difference in atomic charges (Δ_{Charge}) between excited and ground state of appropriate atom in *N*-(3-bromophenyl)chloroacetamide

Atom Number*	Charge (Ground state)	Charge (Excited state)	Δ_{Charge}
1	0.0542	0.055	0.0008
2	1.4306	1.3314	-0.0992
3	-1.1611	-1.0863	0.0748
4	-1.0792	-1.0842	-0.005
5	0.106	0.1056	-0.0004
6	0.1039	0.0964	-0.0075
7	0.1065	0.0988	-0.0077
8	0.4342	0.4334	-0.0008
9	-0.0537	-0.0468	0.0069
10	0.0003	0.0462	0.0459
11	0.0266	-0.1037	-0.1303
12	0.0272	-0.0579	-0.0851
13	0.365	0.3324	-0.0326
14	-0.0471	0.0466	0.0937
15	0.0294	0.0248	-0.0046
16	0.1286	0.1269	-0.0017
17	0.0212	0.0164	-0.0048
18	0.0449	0.0403	-0.0046
19 (Br)	-0.475	-0.3127	0.1623

* First 18 atoms are numbered by atom numbering scheme shown in Fig. S2. The substituent atom is labeled with its chemical symbol.

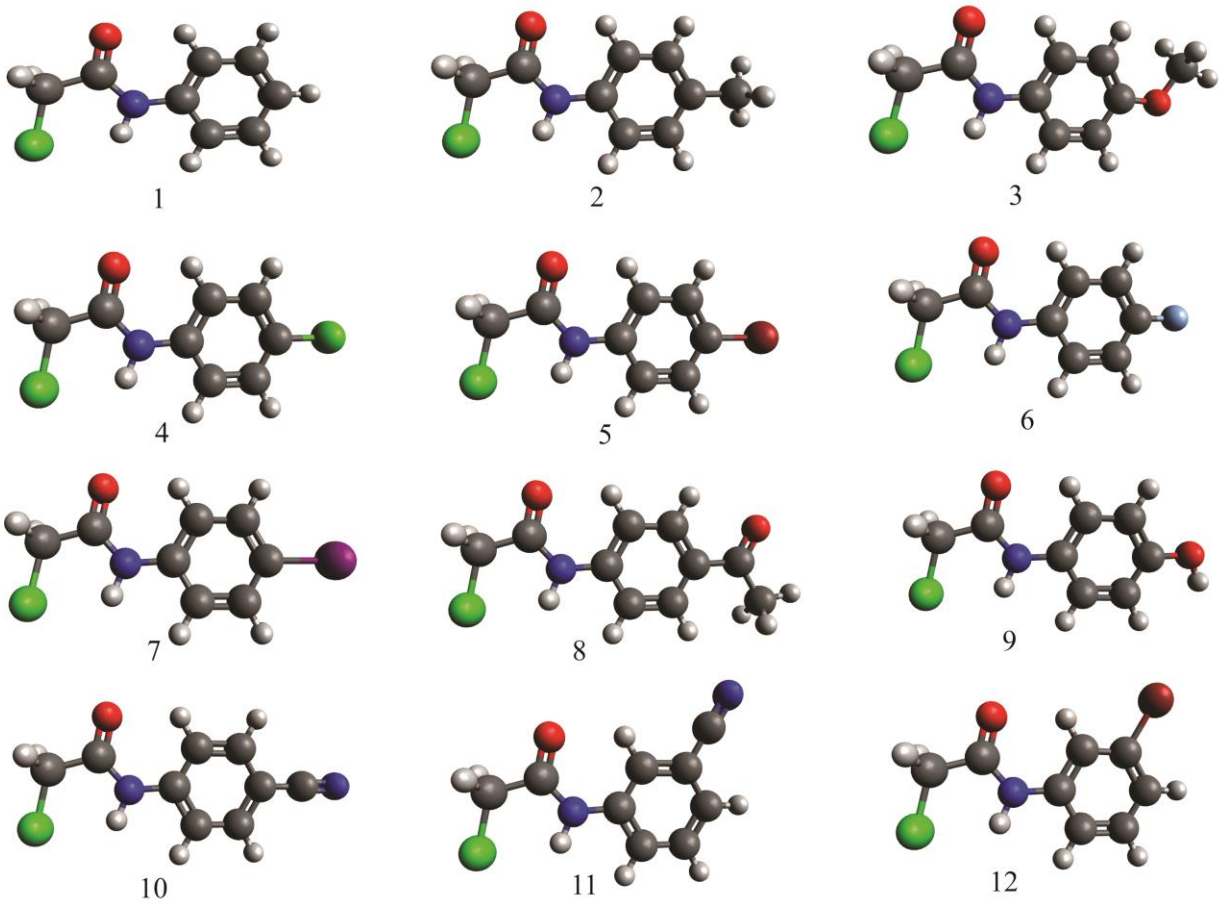

Figure S1 Optimized geometries of investigated molecules.

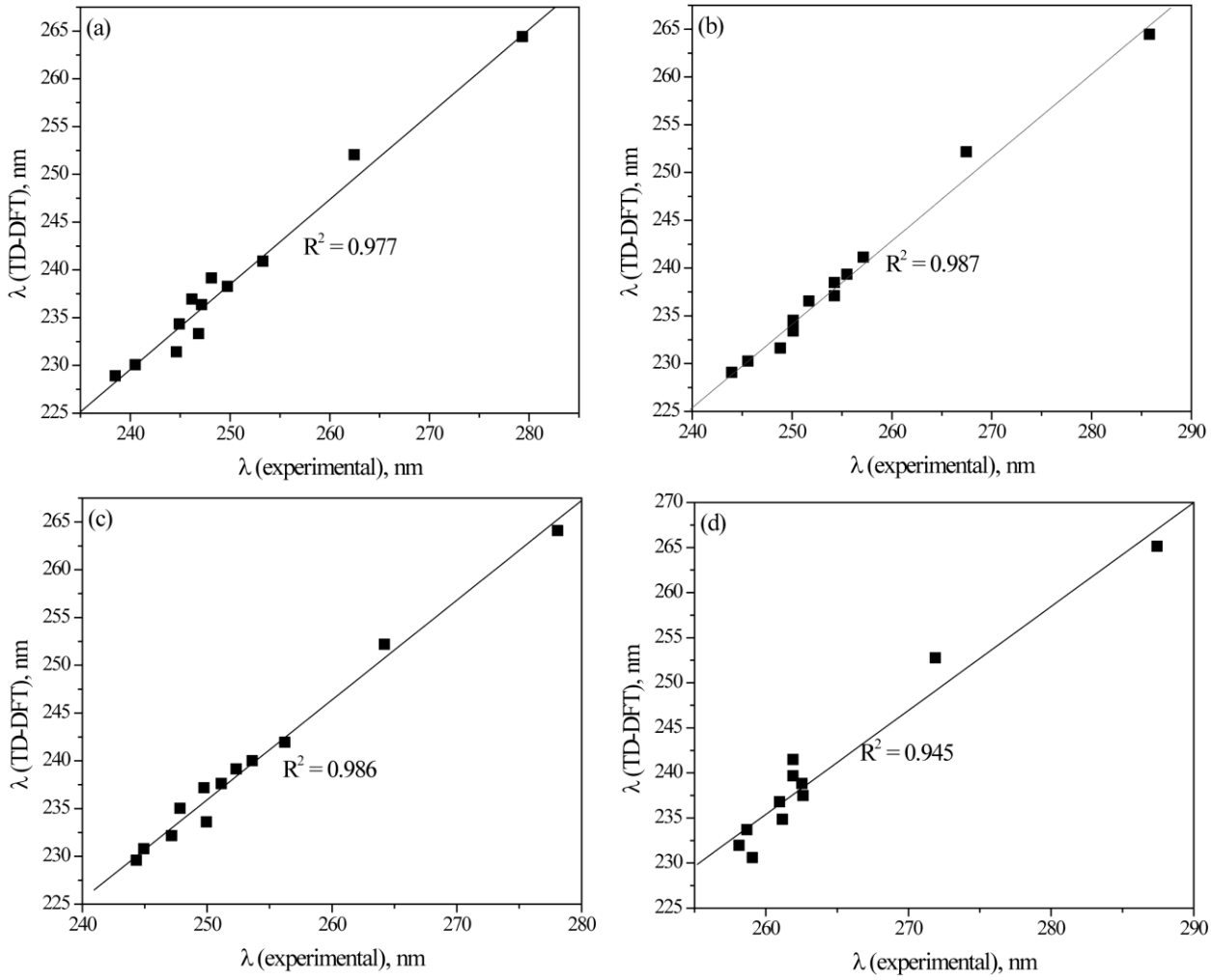

Figure S2 Experimental versus TD-DFT calculated λ (nm) values for compounds **1**-**12** in water (a), ethanol (b), chloroform (c) and DMSO (d).

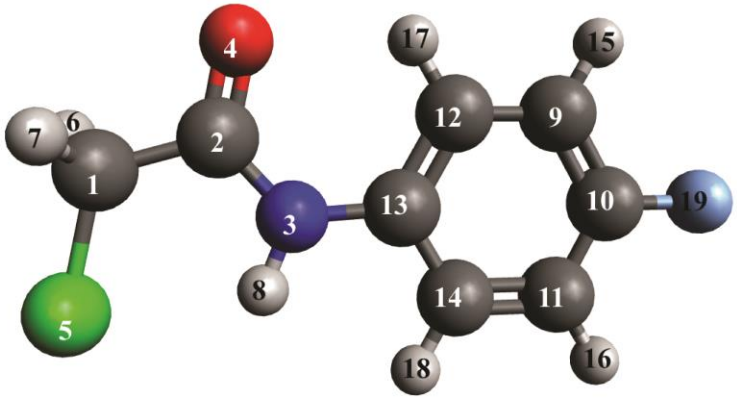

Figure S3 Atom numbering scheme used in Bader's analysis

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