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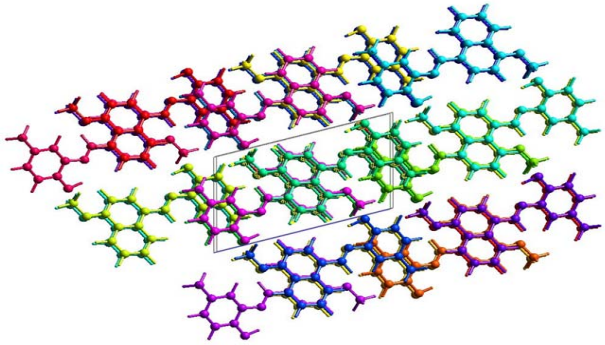
Supporting information for article:

The synthesis and crystal structure of (*E*)-2-{[(4-methoxynaphthalen-1-yl)methylidene]amino}-4-methylphenol: Hirshfeld surface analysis, DFT calculations and anticorrosion studies

Ahmed Abderrahim Yahiaoui, Nadir Ghichi, Douniazed Hannachi, Bilel Mezhoud, Amel Djedouani, Khairedine Kraim, Aurélien Crochet and Helen Stoeckli-Evans



Crystal | Atoms | Surface | Energies

R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x, y, z	13.75	HF/3-21G	1.1	-0.6	-6.9	0.0	-5.5
1	-x, -y, -z	10.60	HF/3-21G	0.9	-0.3	-4.3	0.4	-2.8
1	-x, -y, -z	12.92	HF/3-21G	-0.9	-0.0	-0.9	0.0	-1.7
2	x, y, z	8.00	HF/3-21G	-10.3	-2.7	-22.2	8.8	-25.2
2	x, y, z	13.73	HF/3-21G	0.3	-0.8	-15.1	0.0	-13.8
1	-x, -y, -z	8.05	HF/3-21G	-10.6	-5.8	-65.7	30.5	-49.1
1	-x, -y, -z	11.24	HF/3-21G	-7.7	-2.0	-25.7	13.7	-21.3
1	-x, -y, -z	4.98	HF/3-21G	0.9	-5.5	-80.7	33.4	-48.3
2	x, y, z	7.77	HF/3-21G	2.8	-0.2	-3.3	0.0	-0.3
2	x, y, z	12.48	HF/3-21G	-0.3	-0.2	-2.3	0.0	-2.6
1	-x, -y, -z	12.05	HF/3-21G	-0.7	-3.8	-9.6	0.0	-11.8
1	-x, -y, -z	6.99	HF/3-21G	-17.1	-5.8	-32.4	20.0	-34.2
2	x, y, z	11.47	HF/3-21G	0.2	-0.1	-1.0	0.0	-0.7
1	-x, -y, -z	14.62	HF/3-21G	1.2	-0.1	-0.9	0.0	0.4
2	x, y, z	12.79	HF/3-21G	-1.0	-0.1	-0.9	0.0	-1.8
1	-x, -y, -z	12.94	HF/3-21G	-1.3	-0.5	-7.1	0.0	-8.0
1	-x, -y, -z	7.52	HF/3-21G	4.7	-3.8	-51.7	20.3	-27.9
1	-x, -y, -z	8.57	HF/3-21G	-4.9	-0.8	-4.3	0.0	-9.4
1	-x, -y, -z	16.16	HF/3-21G	4.9	-0.5	-2.3	0.0	2.6

Figure S1 . The colour-coded interaction mappings within a radius of 6 Å of a central reference molecule (left) and the various contributions to the total energy (E_{tot}) for **I** (right).

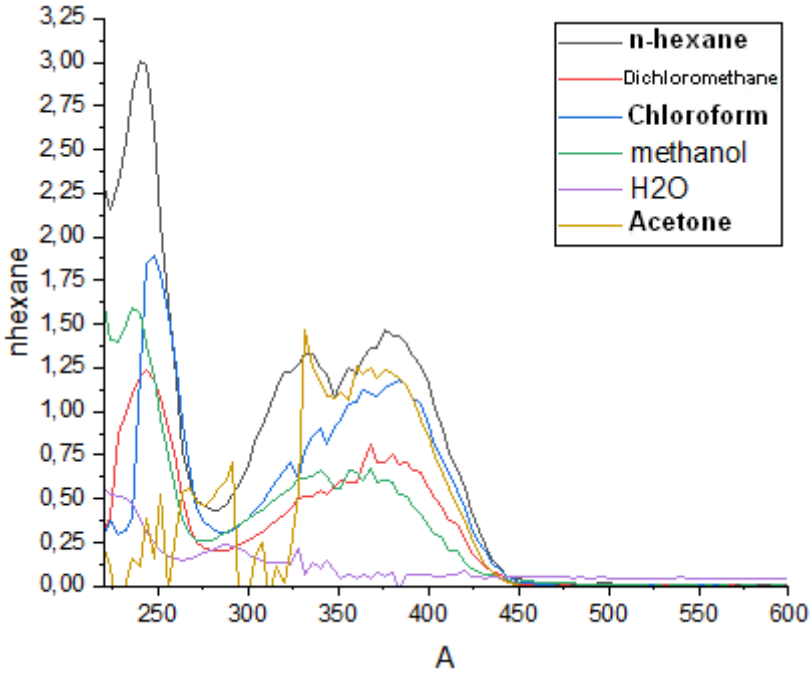


Figure S2.

Experiemntal UV-vis spectra of **I**.

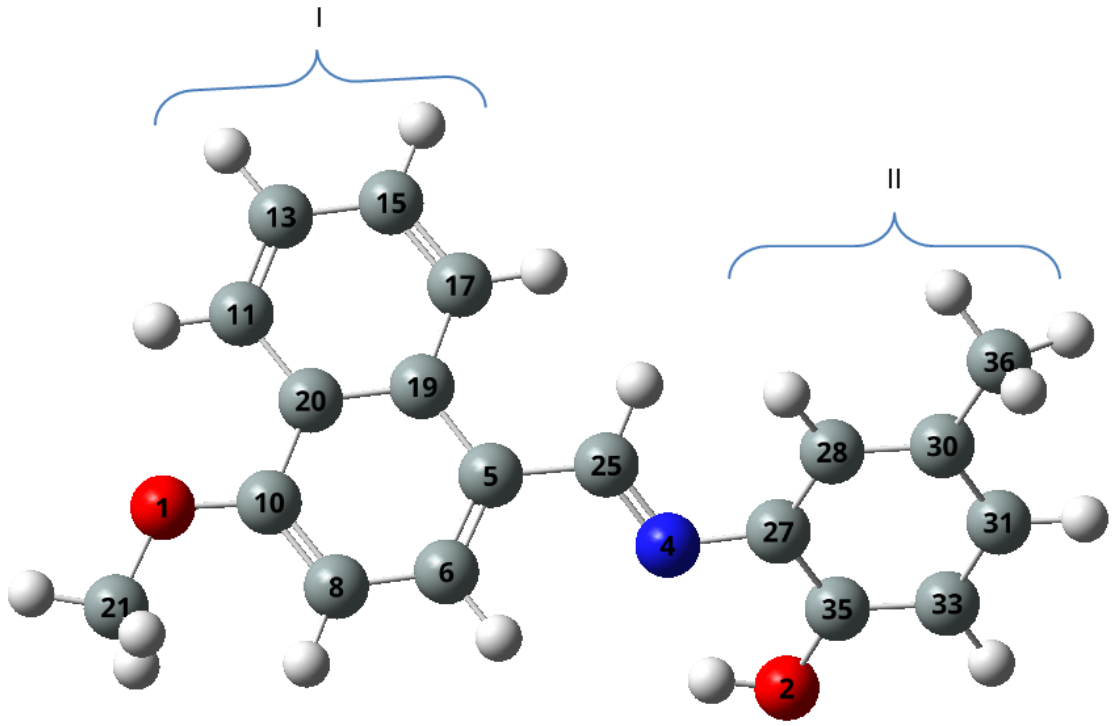


Figure S3. GEOM-I-II OF compound **I**.

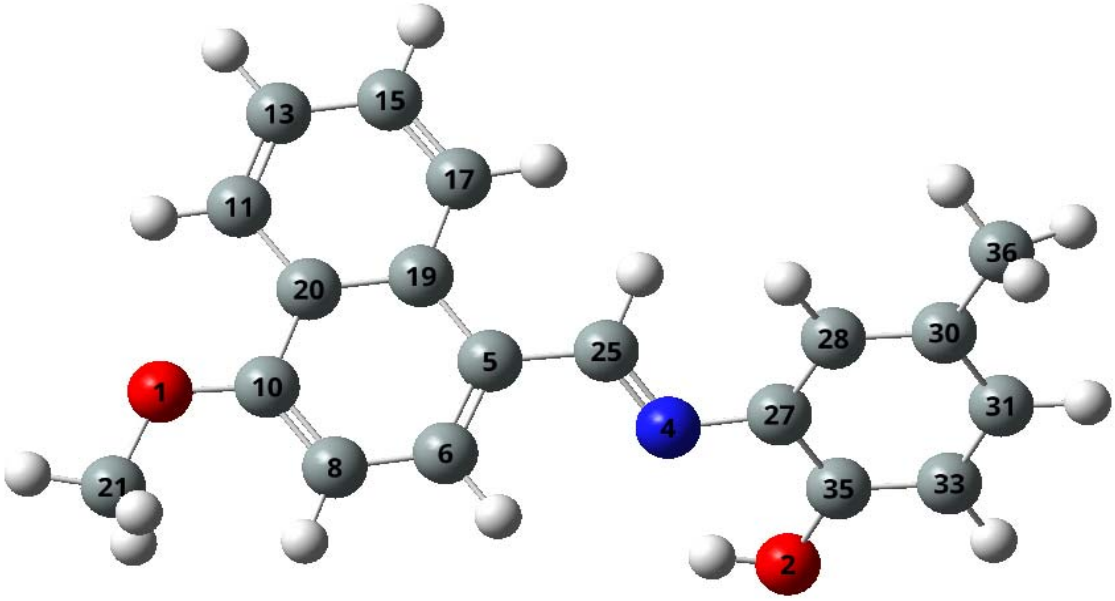


Figure S4. Geometry-final of **I.**

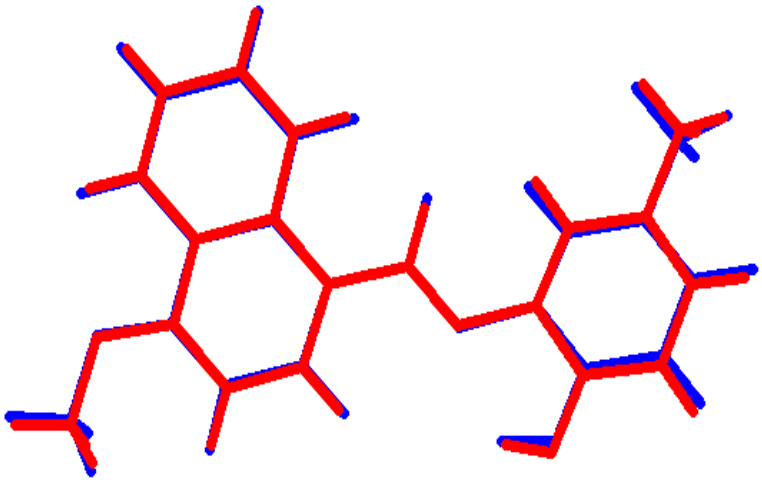


Figure S5. Overlap of the crystallographic structure and the optimized geometry of **I** in water.

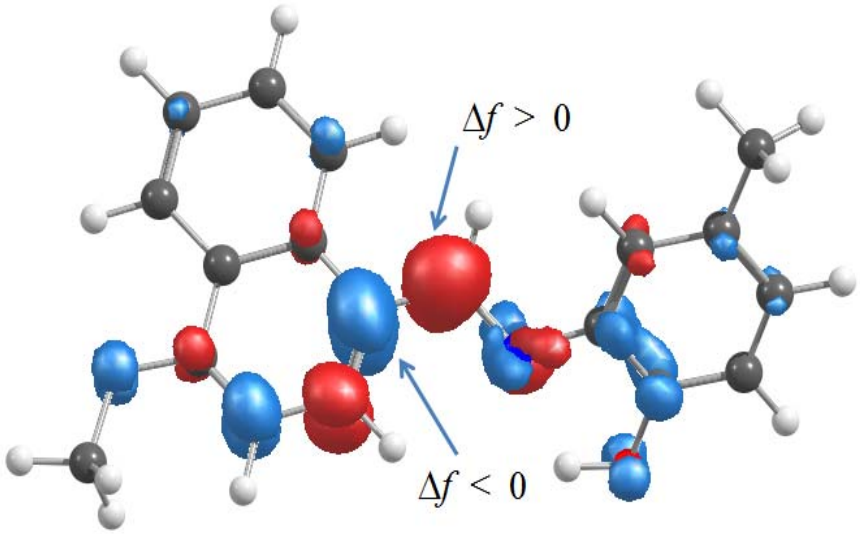


Figure S6. Dual descriptor Δf(r) of compound **I**.

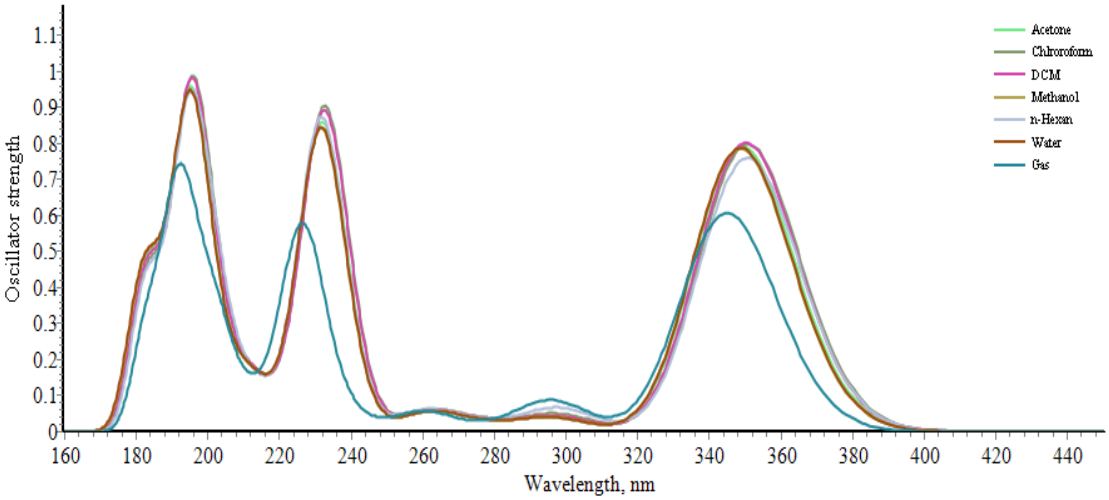


Figure S7. Simulated UV-vis spectra of **I**.

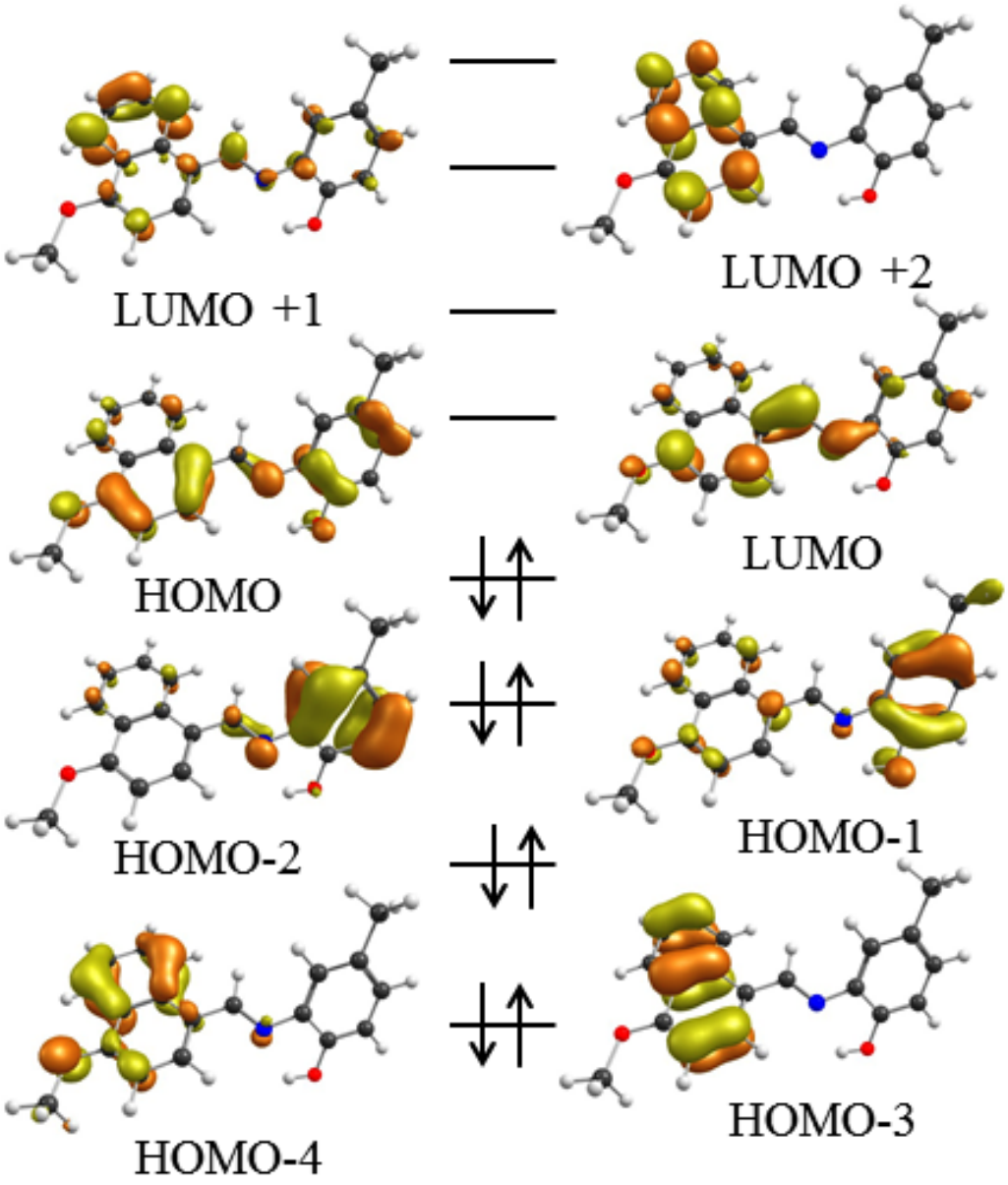


Fig S8. Diagram-TDDFT

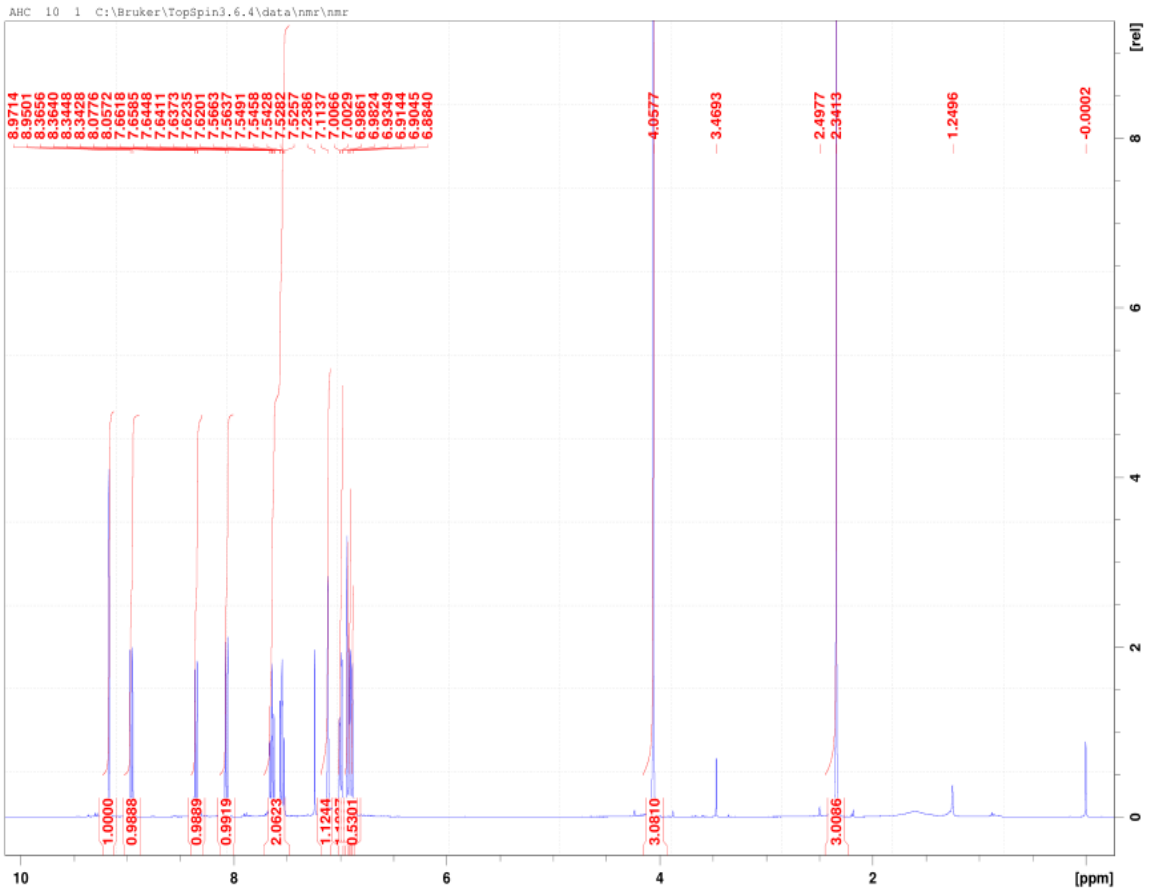


Fig. S9 ^{1}H NMR spectrum of **I**

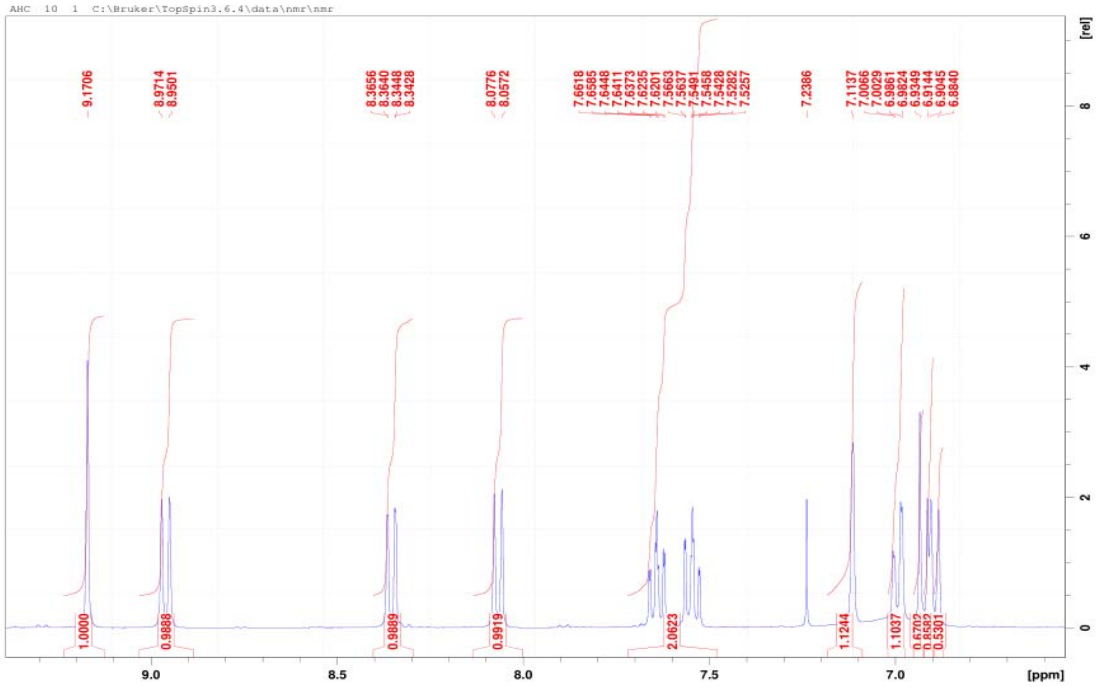


Fig. S10 ^{1}H NMR spectrum of **I** zoom

Table S1 . Local reactivity descriptors were calculated for the corrosion inhibitor in gas and solvent.

Acetone	f^{-}_{k}	f^{+}_{k}	f^{0}	Δf	ω^{-}	ω^{+}	$\Delta\omega$
1-O	0.0579	0.0245	0.0412	-0.0334	0.0049	0.0021	-0.0028
2- O	0.0424	0.0204	0.0314	-0.0220	0.0036	0.0017	-0.0019
3-H	0.0062	0.0003	0.0032	-0.0059	0.0005	0.0000	-0.0005
4-N	0.0821	0.1364	0.1092	0.0544	0.0069	0.0115	0.0046
5-C	0.1284	0.0114	0.0699	-0.1170	0.0108	0.0010	-0.0099
6-C	0.0390	0.1502	0.0946	0.1113	0.0033	0.0127	0.0094
7- H	0.0177	0.0193	0.0185	0.0016	0.0015	0.0016	0.0001
8-C	0.0494	-0.0238	0.0128	-0.0255	0.0042	-0.0020	-0.0062
9-H	0.0189	0.0178	0.0183	-0.0011	0.0016	0.0015	-0.0001
10-C	0.0871	0.1207	0.1039	0.0336	0.0074	0.0102	0.0028
11-C	0.0368	0.0405	0.0387	0.0037	0.0031	0.0034	0.0003
12-H	0.0106	0.0097	0.0102	-0.0009	0.0009	0.0008	-0.0001
13-C	0.0395	0.0211	0.0303	-0.0184	0.0033	0.0018	-0.0016
14-H	0.0121	0.0107	0.0114	-0.0014	0.0010	0.0009	-0.0001
15-C	0.0270	0.0375	0.0322	0.0105	0.0023	0.0032	0.0009
16-H	0.0120	0.0111	0.0116	-0.0010	0.0010	0.0009	-0.0001
17-C	0.0511	0.0102	0.0306	-0.0409	0.0043	0.0009	-0.0035
18-H	0.0096	0.0072	0.0084	-0.0024	0.0008	0.0006	-0.0002
19-C	-0.0323	0.0276	0.0024	-0.0047	-0.0027	0.0023	0.0051
20-C	0.0158	-0.0246	0.0044	0.0089	0.0013	-0.0021	-0.0034
21-C	-0.0091	-0.0048	0.0069	-0.0043	-0.0008	-0.0004	0.0004
22-H	0.0117	0.0089	0.0103	-0.0028	0.0010	0.0008	-0.0002
23-H	0.0126	0.0089	0.0108	-0.0037	0.0011	0.0008	-0.0003

24-H	0.0124	0.0088	0.0106	-0.0036	0.0010	0.0007	-0.0003
25-C	-0.0180	0.1530	0.0675	0.1350	-0.0015	0.0129	0.0145
26-H	0.0205	0.0255	0.0230	0.0051	0.0017	0.0022	0.0004
27-C	0.0258	-0.0239	0.0010	-0.0019	0.0022	-0.0020	-0.0042
28-C	0.0144	0.0551	0.0347	0.0407	0.0012	0.0047	0.0034
29-H	0.0116	0.0086	0.0101	-0.0030	0.0010	0.0007	-0.0003
30-C	0.0326	0.0002	0.0164	-0.0324	0.0028	0.0000	-0.0027
31-C	0.0682	0.0576	0.0629	-0.0107	0.0058	0.0049	-0.0009
32-H	0.0123	0.0102	0.0112	-0.0020	0.0010	0.0009	-0.0002
33-C	-0.0006	0.0134	0.0064	0.0128	0.0000	0.0011	0.0012
34-H	0.0141	0.0106	0.0123	-0.0034	0.0012	0.0009	-0.0003
35-C	0.0594	0.0258	0.0426	-0.0336	0.0050	0.0022	-0.0028
36-C	-0.0056	-0.0011	0.0034	-0.0045	-0.0005	-0.0001	0.0004
37-H	0.0112	0.0057	0.0084	-0.0054	0.0009	0.0005	-0.0005
38-H	0.0075	0.0043	0.0059	-0.0032	0.0006	0.0004	-0.0003
39-H	0.0078	0.0050	0.0064	-0.0028	0.0007	0.0004	-0.0002

Chloroform	f_k	f'_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0484	0.0248	0.0366	-0.0236	0.0035	0.0018	-0.0017
2- O	0.0589	0.0219	0.0404	-0.0370	0.0043	0.0016	-0.0027
3-H	0.0087	-0.0013	0.0037		0.0006	-0.0001	-0.0007
4-N	0.0652	0.1324	0.0988	-0.0073	0.0048	0.0097	0.0049
5-C	0.0938	0.0123	0.0530	0.0672	0.0069	0.0009	-0.0060
6-C	0.0408	0.1446	0.0927		0.0030	0.0106	0.0076
7- H	0.0141	0.0184	0.0162	-0.0816	0.0010	0.0013	0.0003
8-C	0.0341	-0.0245	0.0048	0.1039	0.0025	-0.0018	-0.0043
9-H	0.0176	0.0193	0.0185		0.0013	0.0014	0.0001
10-C	0.0775	0.1229	0.1002	0.0043	0.0057	0.0090	0.0033
11-C	0.0292	0.0434	0.0363	-0.0096	0.0021	0.0032	0.0010
12-H	0.0101	0.0114	0.0107		0.0007	0.0008	0.0001
13-C	0.0331	0.0236	0.0283	0.0016	0.0024	0.0017	-0.0007
14-H	0.0123	0.0134	0.0128	0.0454	0.0009	0.0010	0.0001
15-C	0.0264	0.0406	0.0335		0.0019	0.0030	0.0010
16-H	0.0119	0.0132	0.0125	0.0142	0.0009	0.0010	0.0001
17-C	0.0382	0.0098	0.0240	0.0012	0.0028	0.0007	-0.0021
18-H	0.0072	0.0069	0.0071		0.0005	0.0005	0.0000
19-C	-0.0271	0.0246	0.0013	-0.0094	-0.0020	0.0018	0.0038
20-C	0.0139	-0.0260	0.0060	0.0011	0.0010	-0.0019	-0.0029
21-C	-0.0083	-0.0054	0.0068		-0.0006	-0.0004	0.0002
22-H	0.0121	0.0113	0.0117	0.0142	0.0009	0.0008	-0.0001
23-H	0.0111	0.0095	0.0103	0.0014	0.0008	0.0007	-0.0001
24-H	0.0107	0.0092	0.0100		0.0008	0.0007	-0.0001
25-C	-0.0009	0.1425	0.0708	-0.0284	-0.0001	0.0104	0.0105
26-H	0.0208	0.0250	0.0229	-0.0003	0.0015	0.0018	0.0003
27-C	0.0480	-0.0269	0.0105		0.0035	-0.0020	-0.0055
28-C	0.0039	0.0530	0.0284	-0.0026	0.0003	0.0039	0.0036
29-H	0.0148	0.0075	0.0112	0.0121	0.0011	0.0005	-0.0005
30-C	0.0556	0.0018	0.0287		0.0041	0.0001	-0.0039
31-C	0.0783	0.0595	0.0689	-0.0029	0.0057	0.0043	-0.0014
32-H	0.0168	0.0124	0.0146	-0.0008	0.0012	0.0009	-0.0003
33-C	0.0005	0.0152	0.0079		0.0000	0.0011	0.0011
34-H	0.0190	0.0126	0.0158	-0.0016	0.0014	0.0009	-0.0005

35-C	0.0732	0.0245	0.0489	-0.0015	0.0054	0.0018	-0.0036
36-C	-0.0097	-0.0020	0.0058	0.1416	-0.0007	-0.0001	0.0006
37-H	0.0171	0.0074	0.0123		0.0013	0.0005	-0.0007
38-H	0.0107	0.0045	0.0076	0.0042	0.0008	0.0003	-0.0005
39-H	0.0121	0.0069	0.0095	-0.0210	0.0009	0.0005	-0.0004
				0.0491			
				-0.0073			
				-0.0538			
				-0.0188			
				-0.0045			
				0.0146			
				-0.0065			
				-0.0487			
				-0.0077			
				-0.0097			
				-0.0063			
				-0.0051			

DCM	f'_k	f''_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0532	0.0247	0.0389	-0.0285	0.0042	0.0020	-0.0023
2- O	0.0501	0.0210	0.0355	-0.0291	0.0040	0.0017	-0.0023
3-H	0.0073	-0.0004	0.0035	-0.0070	0.0006	0.0000	-0.0006
4-N	0.0750	0.1348	0.1049	0.0598	0.0060	0.0107	0.0048
5-C	0.1119	0.0118	0.0618	-0.1001	0.0089	0.0009	-0.0080
6-C	0.0402	0.1480	0.0941	0.1078	0.0032	0.0118	0.0086
7- H	0.0161	0.0189	0.0175	0.0029	0.0013	0.0015	0.0002
8-C	0.0418	-0.0241	0.0088	-0.0177	0.0033	-0.0019	-0.0053
9-H	0.0182	0.0184	0.0183	0.0002	0.0014	0.0015	0.0000
10-C	0.0825	0.1216	0.1020	0.0392	0.0066	0.0097	0.0031
11-C	0.0329	0.0417	0.0373	0.0088	0.0026	0.0033	0.0007
12-H	0.0103	0.0104	0.0103	0.0001	0.0008	0.0008	0.0000
13-C	0.0361	0.0222	0.0291	-0.0140	0.0029	0.0018	-0.0011
14-H	0.0120	0.0118	0.0119	-0.0002	0.0010	0.0009	0.0000
15-C	0.0266	0.0388	0.0327	0.0122	0.0021	0.0031	0.0010
16-H	0.0118	0.0119	0.0119	0.0001	0.0009	0.0010	0.0000
17-C	0.0448	0.0100	0.0274	-0.0349	0.0036	0.0008	-0.0028
18-H	0.0086	0.0071	0.0078	-0.0015	0.0007	0.0006	-0.0001
19-C	-0.0297	0.0264	0.0017	-0.0033	-0.0024	0.0021	0.0045
20-C	0.0149	-0.0251	0.0051	0.0102	0.0012	-0.0020	-0.0032
21-C	-0.0086	-0.0050	0.0068	-0.0036	-0.0007	-0.0004	0.0003
22-H	0.0117	0.0099	0.0108	-0.0019	0.0009	0.0008	-0.0001
23-H	0.0118	0.0091	0.0105	-0.0027	0.0009	0.0007	-0.0002
24-H	0.0115	0.0089	0.0102	-0.0026	0.0009	0.0007	-0.0002
25-C	-0.0100	0.1487	0.0694	0.1387	-0.0008	0.0119	0.0126
26-H	0.0207	0.0253	0.0230	0.0046	0.0017	0.0020	0.0004

27-C	0.0364	-0.0251	0.0056	-0.0113	0.0029	-0.0020	-0.0049
28-C	0.0099	0.0542	0.0320	0.0443	0.0008	0.0043	0.0035
29-H	0.0131	0.0082	0.0106	-0.0050	0.0010	0.0006	-0.0004
30-C	0.0429	0.0009	0.0219	-0.0420	0.0034	0.0001	-0.0034
31-C	0.0740	0.0584	0.0662	-0.0156	0.0059	0.0047	-0.0012
32-H	0.0144	0.0111	0.0127	-0.0033	0.0011	0.0009	-0.0003
33-C	-0.0002	0.0141	0.0070	0.0139	0.0000	0.0011	0.0011
34-H	0.0164	0.0114	0.0139	-0.0050	0.0013	0.0009	-0.0004
35-C	0.0664	0.0253	0.0458	-0.0411	0.0053	0.0020	-0.0033
36-C	-0.0074	-0.0015	0.0044	-0.0059	-0.0006	-0.0001	0.0005
37-H	0.0138	0.0064	0.0101	-0.0074	0.0011	0.0005	-0.0006
38-H	0.0089	0.0044	0.0066	-0.0046	0.0007	0.0003	-0.0004
39-H	0.0097	0.0058	0.0077	-0.0039	0.0008	0.0005	-0.0003
Methanol	f'_k	f''_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0594	0.0244	0.0419	-0.0350	0.0051	0.0021	-0.0030
2- O	0.0401	0.0202	0.0301	-0.0199	0.0034	0.0017	-0.0017
3-H	0.0059	0.0005	0.0032	-0.0054	0.0005	0.0000	-0.0005
4-N	0.0840	0.1369	0.1104	0.0529	0.0072	0.0118	0.0046
5-C	0.1344	0.0102	0.0723	-0.1242	0.0116	0.0009	-0.0107
6-C	0.0386	0.1508	0.0947	0.1122	0.0033	0.0130	0.0097
7- H	0.0182	0.0195	0.0188	0.0013	0.0016	0.0017	0.0001
8-C	0.0519	-0.0238	0.0140	-0.0280	0.0045	-0.0020	-0.0065
9-H	0.0191	0.0177	0.0184	-0.0014	0.0016	0.0015	-0.0001
10-C	0.0885	0.1203	0.1044	0.0318	0.0076	0.0103	0.0027
11-C	0.0384	0.0398	0.0391	0.0014	0.0033	0.0034	0.0001
12-H	0.0108	0.0095	0.0101	-0.0013	0.0009	0.0008	-0.0001
13-C	0.0399	0.0214	0.0307	-0.0185	0.0034	0.0018	-0.0016
14-H	0.0122	0.0103	0.0112	-0.0018	0.0010	0.0009	-0.0002
15-C	0.0337	0.0305	0.0321	-0.0033	0.0029	0.0026	-0.0003
16-H	0.0121	0.0109	0.0115	-0.0012	0.0010	0.0009	-0.0001
17-C	0.0378	0.0254	0.0316	-0.0124	0.0032	0.0022	-0.0011
18-H	0.0113	0.0059	0.0086	-0.0053	0.0010	0.0005	-0.0005
19-C	-0.0281	0.0230	0.0026	-0.0052	-0.0024	0.0020	0.0044
20-C	0.0168	-0.0252	0.0042	0.0084	0.0014	-0.0022	-0.0036
21-C	-0.0092	-0.0047	0.0069	-0.0045	-0.0008	-0.0004	0.0004
22-H	0.0117	0.0087	0.0102	-0.0031	0.0010	0.0007	-0.0003
23-H	0.0129	0.0089	0.0109	-0.0040	0.0011	0.0008	-0.0003
24-H	0.0126	0.0087	0.0107	-0.0039	0.0011	0.0007	-0.0003
25-C	-0.0199	0.1540	0.0670	0.1340	-0.0017	0.0132	0.0150
26-H	0.0204	0.0256	0.0230	0.0051	0.0018	0.0022	0.0004
27-C	0.0228	-0.0235	0.0004	0.0008	0.0020	-0.0020	-0.0040
28-C	0.0156	0.0554	0.0355	0.0397	0.0013	0.0048	0.0034
29-H	0.0112	0.0088	0.0100	-0.0024	0.0010	0.0008	-0.0002
30-C	0.0297	0.0000	0.0149	-0.0297	0.0026	0.0000	-0.0026
31-C	0.0663	0.0574	0.0618	-0.0089	0.0057	0.0049	-0.0008
32-H	0.0116	0.0100	0.0108	-0.0017	0.0010	0.0009	-0.0001
33-C	-0.0006	0.0132	0.0063	0.0125	-0.0001	0.0011	0.0012
34-H	0.0134	0.0104	0.0119	-0.0030	0.0011	0.0009	-0.0003
35-C	0.0573	0.0260	0.0416	-0.0312	0.0049	0.0022	-0.0027
36-C	-0.0051	-0.0010	0.0031	-0.0041	-0.0004	-0.0001	0.0004
37-H	0.0104	0.0055	0.0080	-0.0049	0.0009	0.0005	-0.0004

38-H	0.0071	0.0043	0.0057	-0.0028	0.0006	0.0004	-0.0002
39-H	0.0073	0.0048	0.0060	-0.0025	0.0006	0.0004	-0.0002
n-Hexane	f_k	f'_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0447	0.0248	0.0347	-0.0199	0.0026	0.0014	-0.0011
2- O	0.0697	0.0248	0.0472	-0.0449	0.0040	0.0014	-0.0026
3-H	0.0099	-0.0038	0.0030	-0.0061	0.0006	-0.0002	-0.0008
4-N	0.0485	0.1266	0.0876	0.0781	0.0028	0.0073	0.0045
5-C	0.0730	0.0133	0.0432	-0.0597	0.0042	0.0008	-0.0034
6-C	0.0393	0.1354	0.0874	0.0962	0.0023	0.0078	0.0056
7- H	0.0112	0.0171	0.0142	0.0059	0.0006	0.0010	0.0003
8-C	0.0259	-0.0253	0.0003	-0.0006	0.0015	-0.0015	-0.0030
9-H	0.0185	0.0217	0.0201	0.0033	0.0011	0.0013	0.0002
10-C	0.0733	0.1256	0.0995	0.0523	0.0042	0.0073	0.0030
11-C	0.0265	0.0475	0.0370	0.0210	0.0015	0.0027	0.0012
12-H	0.0112	0.0139	0.0126	0.0026	0.0006	0.0008	0.0002
13-C	0.0321	0.0269	0.0295	-0.0051	0.0019	0.0016	-0.0003
14-H	0.0150	0.0176	0.0163	0.0027	0.0009	0.0010	0.0002
15-C	0.0277	0.0448	0.0363	0.0171	0.0016	0.0026	0.0010
16-H	0.0138	0.0168	0.0153	0.0030	0.0008	0.0010	0.0002
17-C	0.0305	0.0096	0.0201	-0.0210	0.0018	0.0006	-0.0012
18-H	0.0051	0.0066	0.0058	0.0014	0.0003	0.0004	0.0001
19-C	-0.0261	0.0199	0.0031	-0.0061	-0.0015	0.0012	0.0027
20-C	0.0118	-0.0282	0.0082	0.0165	0.0007	-0.0016	-0.0023
21-C	-0.0089	-0.0065	0.0077	-0.0024	-0.0005	-0.0004	0.0001
22-H	0.0148	0.0154	0.0151	0.0006	0.0009	0.0009	0.0000
23-H	0.0109	0.0105	0.0107	-0.0004	0.0006	0.0006	0.0000
24-H	0.0103	0.0101	0.0102	-0.0002	0.0006	0.0006	0.0000
25-C	0.0084	0.1262	0.0673	0.1178	0.0005	0.0073	0.0068
26-H	0.0206	0.0240	0.0223	0.0034	0.0012	0.0014	0.0002
27-C	0.0588	-0.0318	0.0135	-0.0270	0.0034	-0.0018	-0.0052
28-C	-0.0060	0.0500	0.0220	0.0440	-0.0003	0.0029	0.0032
29-H	0.0170	0.0058	0.0114	-0.0112	0.0010	0.0003	-0.0006
30-C	0.0724	0.0045	0.0384	-0.0680	0.0042	0.0003	-0.0039
31-C	0.0780	0.0623	0.0701	-0.0157	0.0045	0.0036	-0.0009
32-H	0.0210	0.0158	0.0184	-0.0053	0.0012	0.0009	-0.0003
33-C	0.0020	0.0179	0.0100	0.0159	0.0001	0.0010	0.0009
34-H	0.0233	0.0158	0.0196	-0.0075	0.0013	0.0009	-0.0004
35-C	0.0771	0.0226	0.0498	-0.0545	0.0045	0.0013	-0.0031
36-C	-0.0138	-0.0035	0.0087	-0.0103	-0.0008	-0.0002	0.0006
37-H	0.0225	0.0104	0.0164	-0.0122	0.0013	0.0006	-0.0007
38-H	0.0137	0.0050	0.0093	-0.0087	0.0008	0.0003	-0.0005
39-H	0.0163	0.0100	0.0132	-0.0063	0.0009	0.0006	-0.0004
Water	f_k	f'_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0609	0.0244	0.0426	-0.0365	0.0053	0.0021	-0.0032
2- O	0.0379	0.0200	0.0290	-0.0179	0.0033	0.0018	-0.0016
3-H	0.0056	0.0007	0.0031	-0.0049	0.0005	0.0001	-0.0004
4-N	0.0856	0.1374	0.1115	0.0518	0.0075	0.0120	0.0045
5-C	0.1392	0.0101	0.0746	-0.1292	0.0122	0.0009	-0.0113
6-C	0.0380	0.1514	0.0947	0.1134	0.0033	0.0133	0.0099
7- H	0.0186	0.0196	0.0191	0.0010	0.0016	0.0017	0.0001
8-C	0.0542	-0.0237	0.0153	-0.0305	0.0047	-0.0021	-0.0068

9-H	0.0193	0.0175	0.0184	-0.0018	0.0017	0.0015	-0.0002
10-C	0.0898	0.1199	0.1049	0.0301	0.0079	0.0105	0.0026
11-C	0.0396	0.0394	0.0395	-0.0002	0.0035	0.0035	0.0000
12-H	0.0109	0.0093	0.0101	-0.0016	0.0010	0.0008	-0.0001
13-C	0.0410	0.0211	0.0310	-0.0199	0.0036	0.0018	-0.0017
14-H	0.0122	0.0100	0.0111	-0.0021	0.0011	0.0009	-0.0002
15-C	0.0338	0.0301	0.0319	-0.0037	0.0030	0.0026	-0.0003
16-H	0.0121	0.0106	0.0114	-0.0015	0.0011	0.0009	-0.0001
17-C	0.0396	0.0254	0.0325	-0.0142	0.0035	0.0022	-0.0012
18-H	0.0116	0.0060	0.0088	-0.0056	0.0010	0.0005	-0.0005
19-C	-0.0289	0.0233	0.0028	-0.0056	-0.0025	0.0020	0.0046
20-C	0.0170	-0.0250	0.0040	0.0080	0.0015	-0.0022	-0.0037
21-C	-0.0093	-0.0046	0.0070	-0.0047	-0.0008	-0.0004	0.0004
22-H	0.0117	0.0084	0.0101	-0.0034	0.0010	0.0007	-0.0003
23-H	0.0131	0.0088	0.0110	-0.0043	0.0011	0.0008	-0.0004
24-H	0.0129	0.0086	0.0108	-0.0042	0.0011	0.0008	-0.0004
25-C	-0.0221	0.1553	0.0666	0.1332	-0.0019	0.0136	0.0155
26-H	0.0203	0.0256	0.0230	0.0053	0.0018	0.0022	0.0005
27-C	0.0199	-0.0232	0.0017	0.0033	0.0017	-0.0020	-0.0038
28-C	0.0167	0.0556	0.0362	0.0389	0.0015	0.0049	0.0034
29-H	0.0108	0.0089	0.0099	-0.0019	0.0009	0.0008	-0.0002
30-C	0.0270	-0.0002	0.0134	-0.0269	0.0024	0.0000	-0.0024
31-C	0.0642	0.0571	0.0607	-0.0071	0.0056	0.0050	-0.0006
32-H	0.0110	0.0097	0.0104	-0.0013	0.0010	0.0009	-0.0001
33-C	-0.0007	0.0129	0.0061	0.0122	-0.0001	0.0011	0.0012
34-H	0.0127	0.0102	0.0114	-0.0025	0.0011	0.0009	-0.0002
35-C	0.0552	0.0262	0.0407	-0.0290	0.0048	0.0023	-0.0025
36-C	-0.0047	-0.0009	0.0028	-0.0037	-0.0004	-0.0001	0.0003
37-H	0.0097	0.0053	0.0075	-0.0043	0.0008	0.0005	-0.0004
38-H	0.0067	0.0043	0.0055	-0.0024	0.0006	0.0004	-0.0002
39-H	0.0068	0.0046	0.0057	-0.0022	0.0006	0.0004	-0.0002
Gas	f'_k	f''_k	f^0	Δf	ω^-	ω^+	$\Delta\omega$
1-O	0.0443	0.0239	0.0341	-0.0204	0.0020	0.0011	-0.0009
2- O	0.0754	0.0285	0.0520	-0.0469	0.0033	0.0013	-0.0021
3-H	0.0103	-0.0065	0.0019	-0.0037	0.0005	-0.0003	-0.0007
4-N	0.0353	0.1212	0.0782	0.0859	0.0016	0.0053	0.0038
5-C	0.0624	0.0137	0.0381	-0.0487	0.0027	0.0006	-0.0021
6-C	0.0373	0.1249	0.0811	0.0876	0.0016	0.0055	0.0039
7- H	0.0094	0.0160	0.0127	0.0066	0.0004	0.0007	0.0003
8-C	0.0216	-0.0257	0.0021	0.0041	0.0010	-0.0011	-0.0021
9-H	0.0207	0.0246	0.0227	0.0039	0.0009	0.0011	0.0002
10-C	0.0729	0.1272	0.1001	0.0543	0.0032	0.0056	0.0024
11-C	0.0264	0.0508	0.0386	0.0245	0.0012	0.0022	0.0011
12-H	0.0132	0.0165	0.0149	0.0033	0.0006	0.0007	0.0001
13-C	0.0337	0.0294	0.0316	-0.0043	0.0015	0.0013	-0.0002
14-H	0.0190	0.0224	0.0207	0.0034	0.0008	0.0010	0.0002
15-C	0.0299	0.0484	0.0392	0.0185	0.0013	0.0021	0.0008
16-H	0.0171	0.0208	0.0189	0.0037	0.0008	0.0009	0.0002
17-C	0.0268	0.0095	0.0182	-0.0173	0.0012	0.0004	-0.0008
18-H	0.0037	0.0064	0.0050	0.0027	0.0002	0.0003	0.0001
19-C	-0.0273	0.0151	0.0061	-0.0122	-0.0012	0.0007	0.0019

20-C	0.0094	-0.0308	0.0107	0.0214	0.0004	-0.0014	-0.0018
21-C	-0.0106	-0.0079	0.0092	-0.0027	-0.0005	-0.0003	0.0001
22-H	0.0191	0.0205	0.0198	0.0013	0.0008	0.0009	0.0001
23-H	0.0117	0.0118	0.0118	0.0001	0.0005	0.0005	0.0000
24-H	0.0110	0.0113	0.0111	0.0003	0.0005	0.0005	0.0000
25-C	0.0116	0.1094	0.0605	0.0977	0.0005	0.0048	0.0043
26-H	0.0203	0.0229	0.0216	0.0026	0.0009	0.0010	0.0001
27-C	0.0613	-0.0371	0.0121	-0.0242	0.0027	-0.0016	-0.0043
28-C	-0.0136	0.0474	0.0169	0.0338	-0.0006	0.0021	0.0027
29-H	0.0184	0.0042	0.0113	-0.0142	0.0008	0.0002	-0.0006
30-C	0.0817	0.0075	0.0446	-0.0743	0.0036	0.0003	-0.0033
31-C	0.0726	0.0651	0.0688	-0.0075	0.0032	0.0029	-0.0003
32-H	0.0247	0.0195	0.0221	-0.0052	0.0011	0.0009	-0.0002
33-C	0.0029	0.0206	0.0118	0.0177	0.0001	0.0009	0.0008
34-H	0.0270	0.0197	0.0233	-0.0073	0.0012	0.0009	-0.0003
35-C	0.0744	0.0208	0.0476	-0.0535	0.0033	0.0009	-0.0024
36-C	-0.0177	-0.0055	0.0116	-0.0122	-0.0008	-0.0002	0.0005
37-H	0.0270	0.0140	0.0205	-0.0130	0.0012	0.0006	-0.0006
38-H	0.0163	0.0060	0.0111	-0.0103	0.0007	0.0003	-0.0005
39-H	0.0203	0.0136	0.0169	-0.0067	0.0009	0.0006	-0.0003

Computational details (DFT and TD-DFT calculations)

$\mu=1/2(\varepsilon_H+\varepsilon_L)$ (1)

χ is the electronegativity

$\varepsilon_L-\varepsilon_H$ (2)

$\omega=\mu^2/2$ (3)

$\Delta N=\mu_{Nu}-\mu_E/2(\eta_{Nu}+\eta_E)$ (4)

$f^-_k=\rho_N(r)-\rho_{N-1}(r)\rightarrow$for electrophilic attack (5)

$f^+_k=\rho_{N+1}(r)-\rho_N(r)\rightarrow$for nucleophilic attack (6)

$f^0_k=1/2\rho_{N+1}(r)-\rho_{N-1}(r)\rightarrow$for radical attack (7)

Where, $\rho_N(r)$, $\rho_{N-1}(r)$ and $\rho_{N+1}(r)$ represent the electron density of a system at the N electron (neutral), N–1electron (cationic) and N+1electron (anionic) (N+1), respectively. It is argued that the reactive site ought to possess a higher value of FF in comparison to other sites.

$\omega^\alpha_k=\omega f^\alpha_k$ (8)

$\Delta f(r)=\rho_{N+1}(r)+\rho_{N-1}(r)-2\rho_N(r)$ (9)

The sign of dual descriptor $\Delta f(r)$ s an important criterion of reactivity site within a molecule: if $\Delta f(r)>0$ then the site is favourable for an nucleophilic attack, while if $\Delta f(r)<0$ then the site is favourable for an electrophilic attack.

The absorption spectra of the studied compounds was calculated with the TD–DFT methods in gas and solvent phases (namely n-hexane, dichloromethane, chloroform methanol, acetone and water), in order to predict the effect of solvent on linear optical properties (we used M06–2X/6–311+G(d) and IEFPCM).