Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Structural, Electronic and optical properties of 2, 5-dichloro-*p*-xylene: Experimental and theoretical calculations using DFT method

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Table S1: Total energies of DCPX, calculated by DFT B3LYP/6-31G*, B3LYP/6-311+G** methods in gaseous phase and B3LYP/6-311+G** methods in aqueous phase using DFT calculations

Method	Energies (Hartrees) Gases Phase	Energies (Hartrees) aqueous phase
6-31G*	-1229.95	-1229.54
6-311+G**	-1230.07	-1230.09

Table S2: Definition of internal coordinates of DCPX

No(i)	Symbol	Type	Definition
Stretching 1-6	r_i	C-C	C1-C2, C2-C3, C3-C4, C4-C5, C5-C6, C6-C1
7-8	S_i	C-H	C1-H7, C4-H10
9-10	p_i	C-Cl	C2-Cl8, C5-Cl11
11-12	P_i	C-C(m)	C3-C9, C6-C12
13-15	n_i	C-H(m)	C9-H13, C9-H14, C9-H15
16-18	N_i	C-H(m)	C12-H16, C12-H17, C12-H18
Bending 19-24	α_i	C-C-C	C1-C2-C3, C2-C3-C4, C3-C4-C5, C4-C5-C6, C5-C6-C1,C6-C1-C2
25-28	θ_i	C-C-H	C6-C1-H7, C2-C1-H7, C3-C4-H10, C5-C4-H10
29-32	β_i	C-C-Cl	C1-C2-Cl8, C3-C2-Cl8, C6-C5-Cl11, C4-C5-Cl11
33-36	Φ_i	C-C-C	C2-C3-C9, C4-C3-C9, C1-C6-C12, C5-C6-C12
37-39	μ_i	H-C-H	H13-C9-H14, H14-C9-H15, H15-C9-H13
40-42	ν_i	C-C-H	C3-C9-H13, C3-C9-H14, C3-C9-H15
43-45	ε_i	H-C-H	H16-C12-H17, H17-C12-H18, H18-C12-H16
46-48	ι_i	C-C-H	C6-C12-H16, C6-C12-H17, C6-C12-H18
Out-of-plane 49-51	ω_i	C-H	H7-C1-C6-C2, H10-C4-C5-C3
52	ξ_i	C-Cl	Cl8-C2-C3-C1, Cl11-C5-C6-C4
53-54	Ω_i	C-C	C9-C3-C2-C4, C12-C6-C5-C1
Torsion 55-60	τ_i	C-C	C1-C2-C3-C4, C2-C3-C4-C5, C3-C4-C5-C6,C4-C5-C6-C1, C5-C6-C1-C2, C6-C1-C2,C3
61	τ_i	C-H	C2-C3-C9-(H13,H14,H15)
62	τ_i	C-H	C1-C6-C12-(H16,H17,H18)

*for numbering of atom refer Fig.1

Table S3: Definition of local symmetry coordinates and the values corresponding to scale factors used to correct the force fields for DCPX

No.(i)	Symbol[a]	Definition[b]	Scale factors used in calculation
1-6	C-C	r1,r2,r3,r4,r5,r6	0.914
7-8	C-H	S7,S8	0.914
9-10	C-Cl	p9,p10	0.992
11-12	C-Cm	P11,P12	0.992
13	mss1	(n13+n14+n15)/ √3	0.995
14	mips1	(2n14-n13-n15)/ √6	0.992
15	mops1	(n14-n15)/ √2	0.919
16	mss2	(N16+N17+N18)/ √3	0.919
17	mips2	(2N17-N16-N18)/ √6	0.919
18	mops2	(N17-N18)/ √2	0.919
19	C-C-C	(α19-α20+α21-α22+α23-α24)/ √6	0.992
20	C-C-C	(2α19-α20-α21+2α22-α23-α24)/ √12	0.992
21	C-C-C	(α20-α21+α23-α24)/2	0.992
22-23	C-C-H	(θ25-θ26)/√2,(θ27-θ28)/√2	0.916
24-25	C-C-Cl	(β31-β32)/√2, (β33-β34)/√2	0.923
26-27	C-C-C	(Φ33- Φ34)/√2, (Φ35- Φ36)/√2	0.923
28	msb1	(μ37+μ38+μ39-ν40-ν41-ν42)/ √6	0.990
29	mipb1	(2μ39-μ37-μ38)/ √6	0.990
30	mopb1	(μ37-μ39)/ √2	0.990
31	mipr1	(2ν41-ν40-ν42)/ √6	0.990
32	mopr1	(ν40-ν42)/ √2	0.990
33	msb2	(ε43+ε44+ε45-ι46-ι47-ι48)/ √6	0.990
34	mipb2	(2ε45-ε43-ε44)/ √6	0.990
35	mopb2	(ε43-ε45)/ √2	0.990
36	mipr2	(2ι47-ι46-ι48)/ √6	0.990
37	mopr2	(ι46-ι48)/ √2	0.990
38-39	C-H	ω49, ω50	0.994
40-41	C-Cl	ξ51, ξ52	0.962
42-43	C-C	Ω53, Ω54	0.962
44	Tring	(τ55-τ56+τ57-τ58+τ59-τ60)/√6	0.994
45	Tring	(τ55-τ57+τ58-τ60)/2	0.994
46	Tring	(-τ55+2τ56-τ57-τ58+2τ59-τ60)/√12	0.994

47	C-H	τ61/3	0.979
48	C-H	τ62/3	0.979

[a] These symbols are used for description of the normal modes by PED in Table 2.

[b] The internal coordinates used here are defined in Table S2

Table S4: Calculated Mulliken atomic charges of DCPX using B3LYP/6-311G**

Atoms	Mullikens Charges
C1	0.13787
C2	-0.3028
C3	-0.0477
C4	0.13787
C5	-0.3028
C6	-0.0477
C11	-0.0386
C12	-0.0386
H8	0.20899
H9	0.20899
H13	0.22045
H14	0.22044
H15	0.20531
H16	0.22044
H17	0.20531
H18	0.22045
Cl9	-0.0386
Cl10	-0.0386

Table S5: The dipole moment (μ) and first-order hyperpolarizibility (β) of DCPX calculated using DFT calculations

β_{xxx}	-20.447
β_{xxy}	-2282.2
β_{xyy}	29.076
β_{yyy}	-3212.9
β_{zxx}	-282.3
β_{xyz}	7449.2
β_{zyy}	195.31
β_{xzz}	8228.1
β_{yzz}	-1623.2
β_{zzz}	752.83
β_{total}	11.583
μ_x	0.00023171
μ_y	1.0851E-06
μ_z	8.0457E-06
μ	0.01551893

Dipole moment (μ) in Debye, hyperpolarizibility $\beta(-2\omega;\omega,\omega)$ 10^{-30}esu.

Table S6: Calculated absorption wavelength (λ_{ng}), energy (E_{ng}), oscillator strength (f_n) and its major contribution

N	λ_{ng}	E_{ng}	f_n	Major contribution
1	202.5	6.12	0.0294	H-0->L+0(+53%), H-1->L+1(+26%)
2	196.7	6.30	0.0239	H-0->L+1(+41%), H-1->L+0(37%)
3	168.4	7.36	0.0002	H-0->L+2(+71%)

(Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)

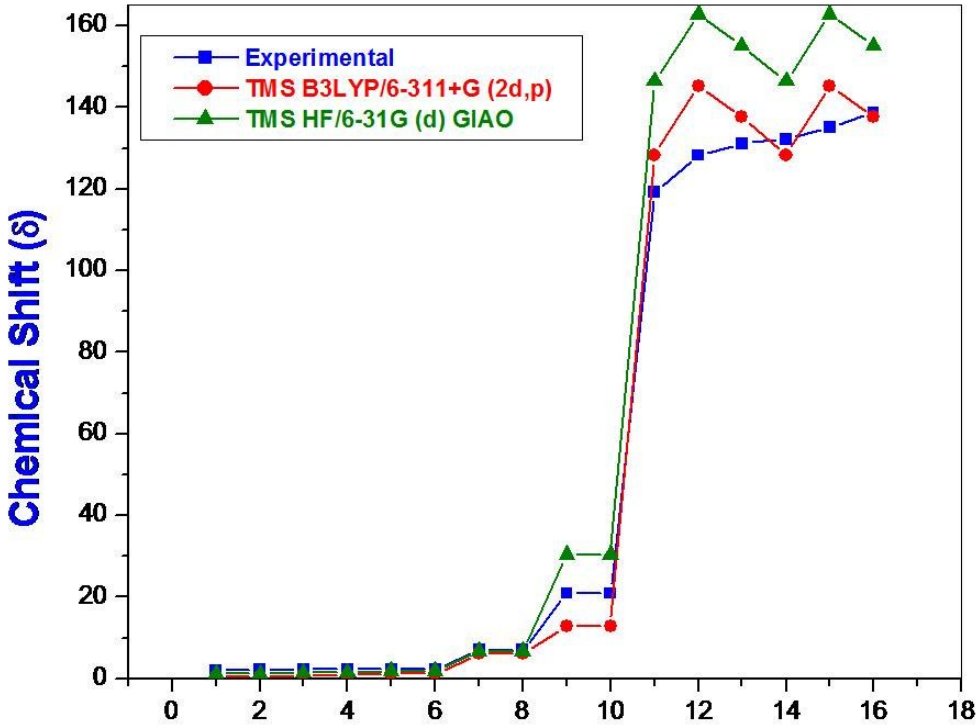

Fig. S1: ^{13}C and ^{1}H NMR of 2, 5 Dichloro P-xylene

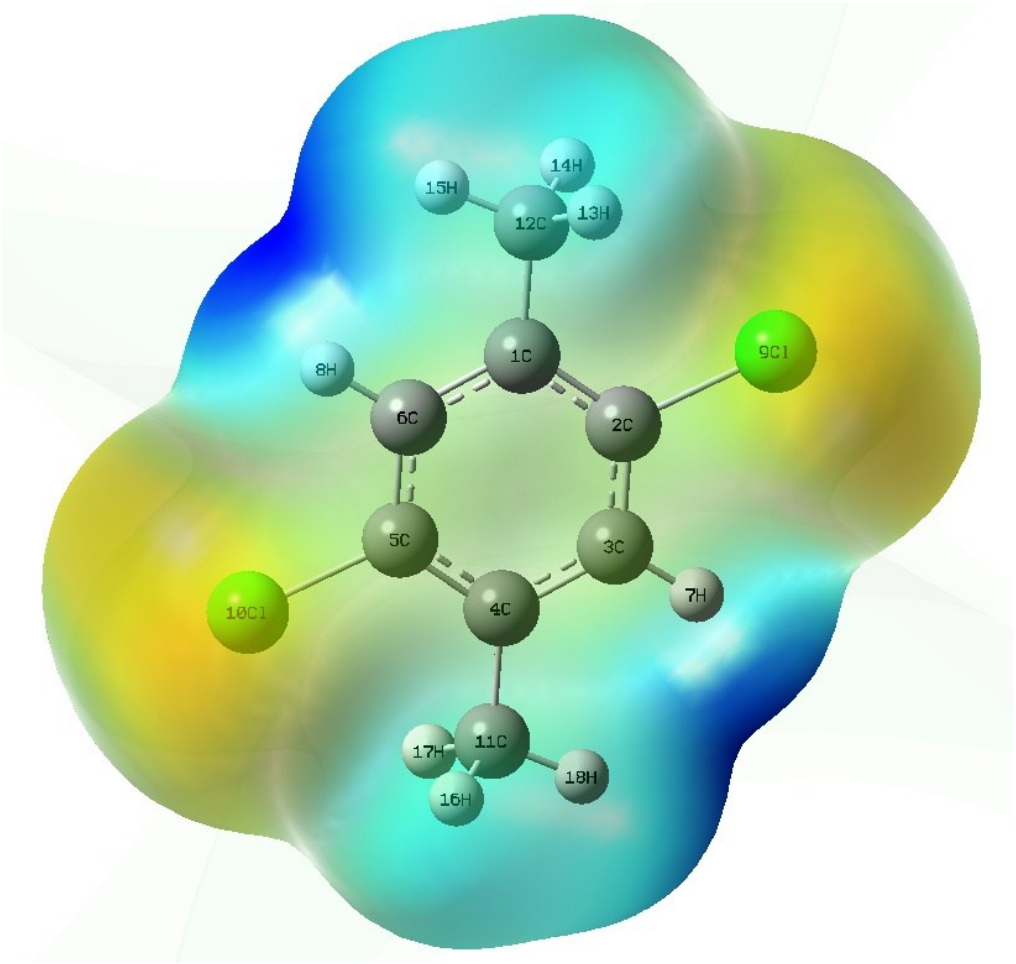

Fig. S2: MEP Diagram of 2, 5 Dichloro P-xylene

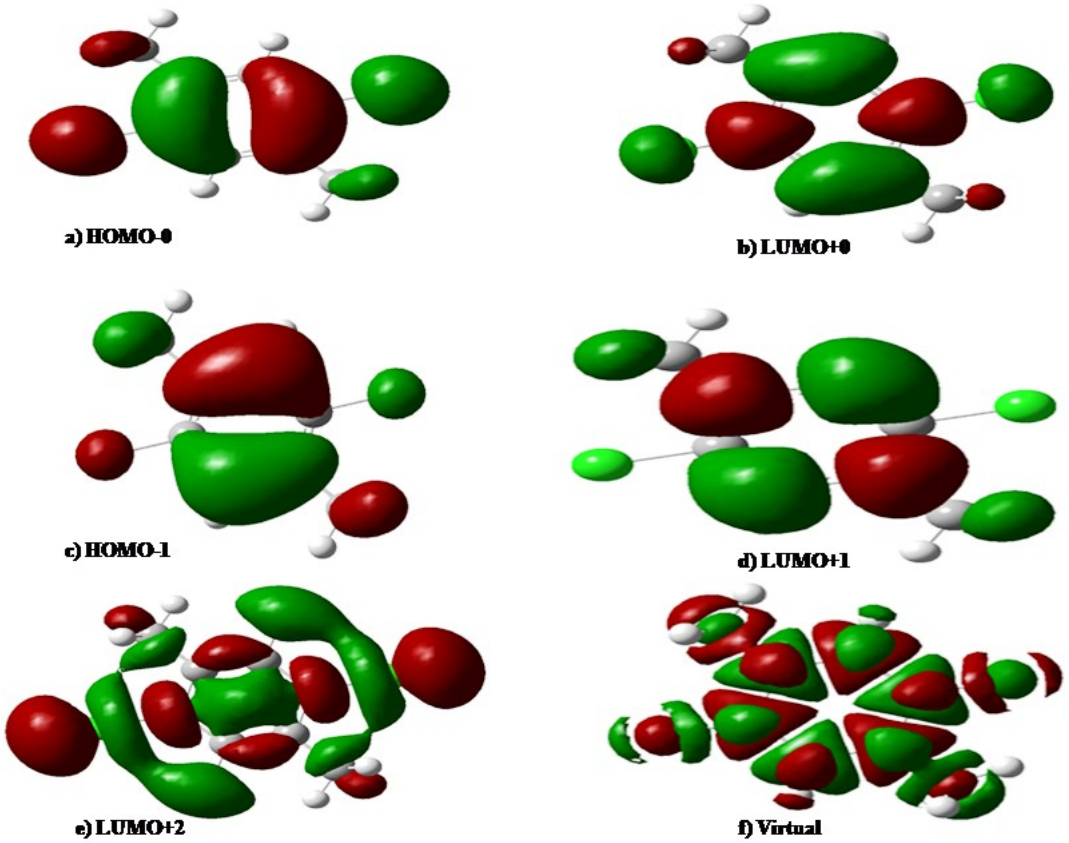

Fig. S3: Representation of the orbitals involved in the electronic transition for (a) HOMO−0 (b) LUMO+0 (c) HOMO-1 (d) LUMO+1 (e) LUMO+2 f) virtual