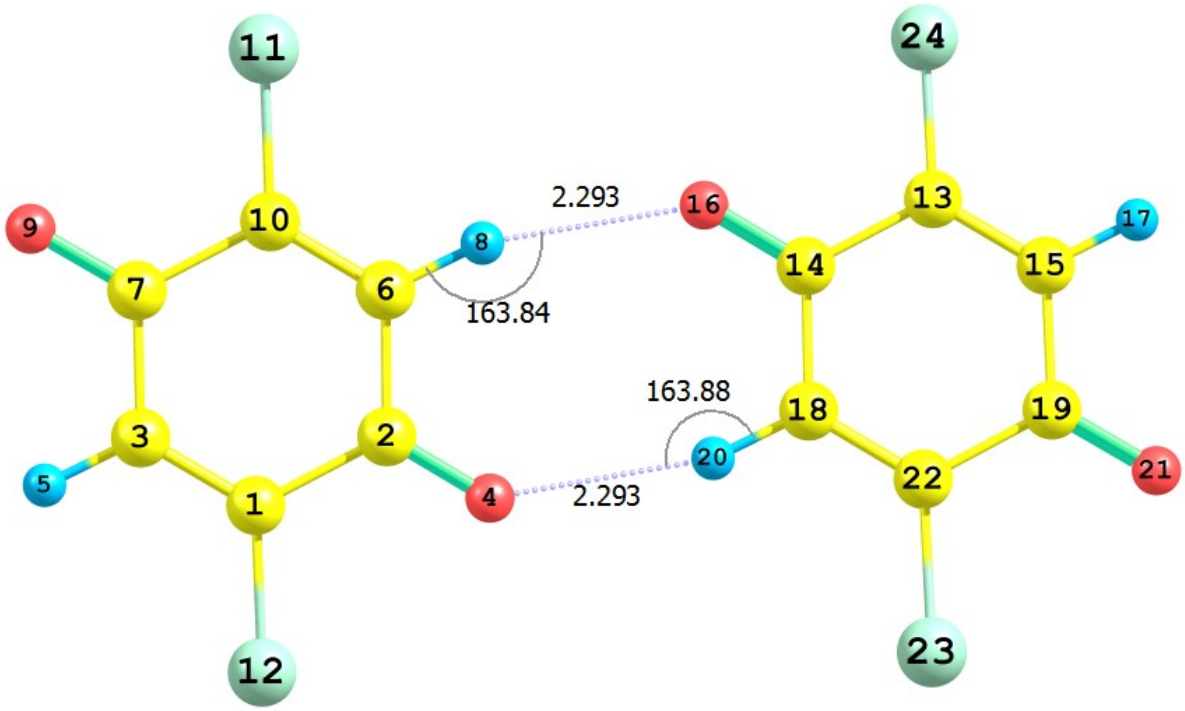

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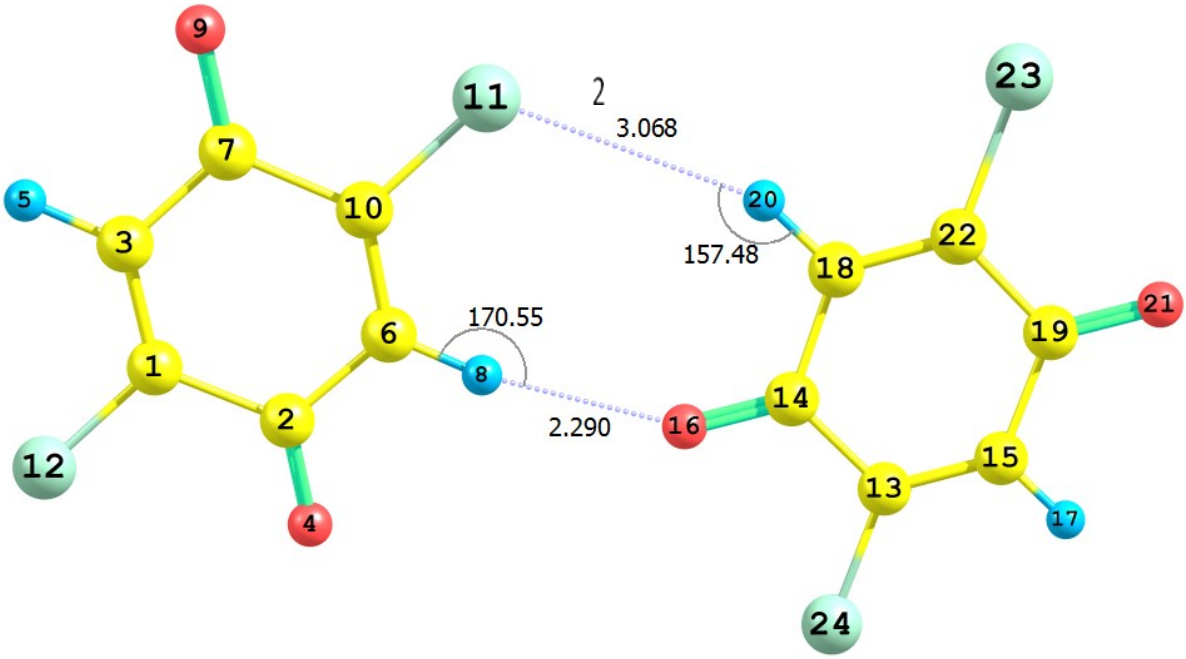

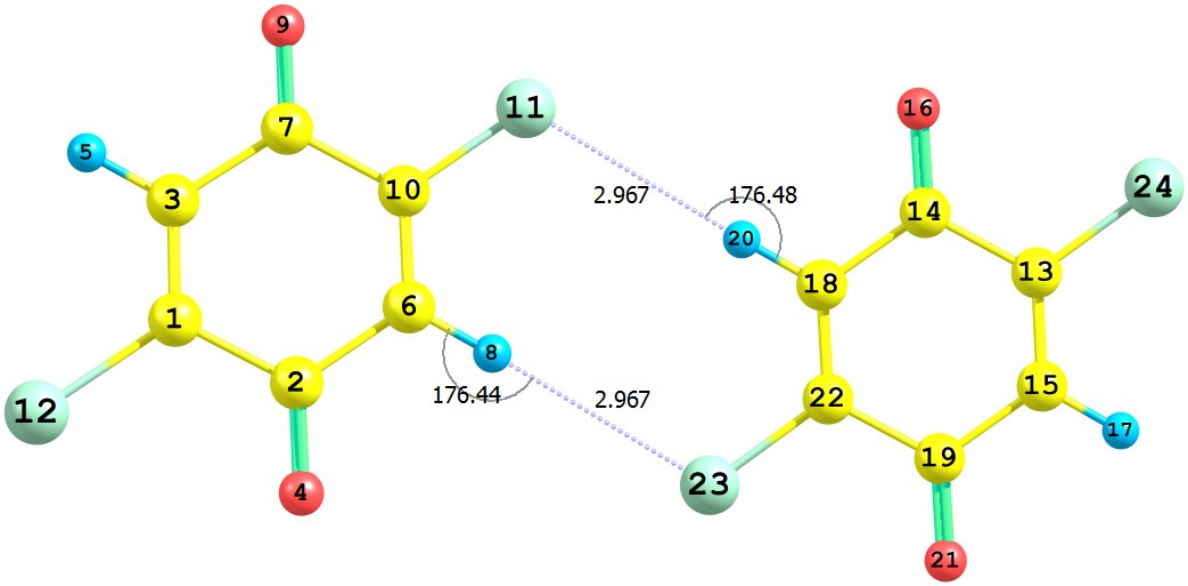
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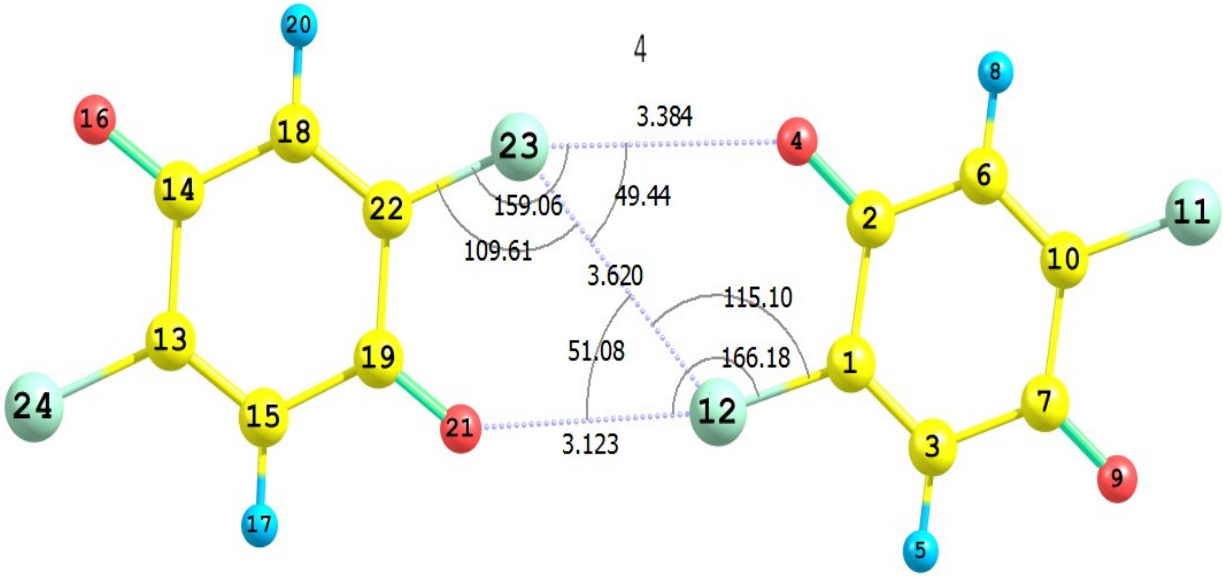
21

3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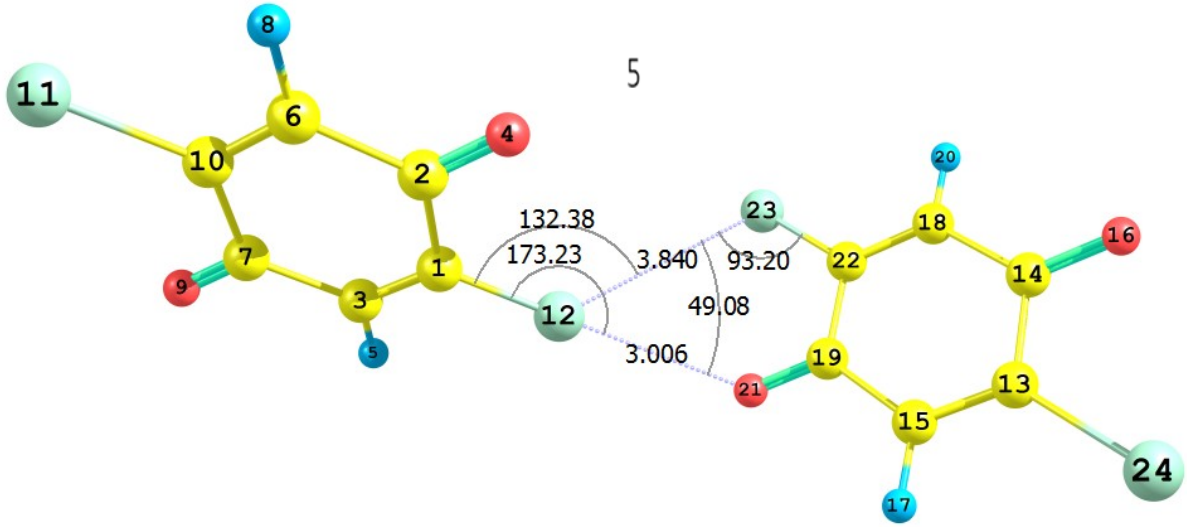
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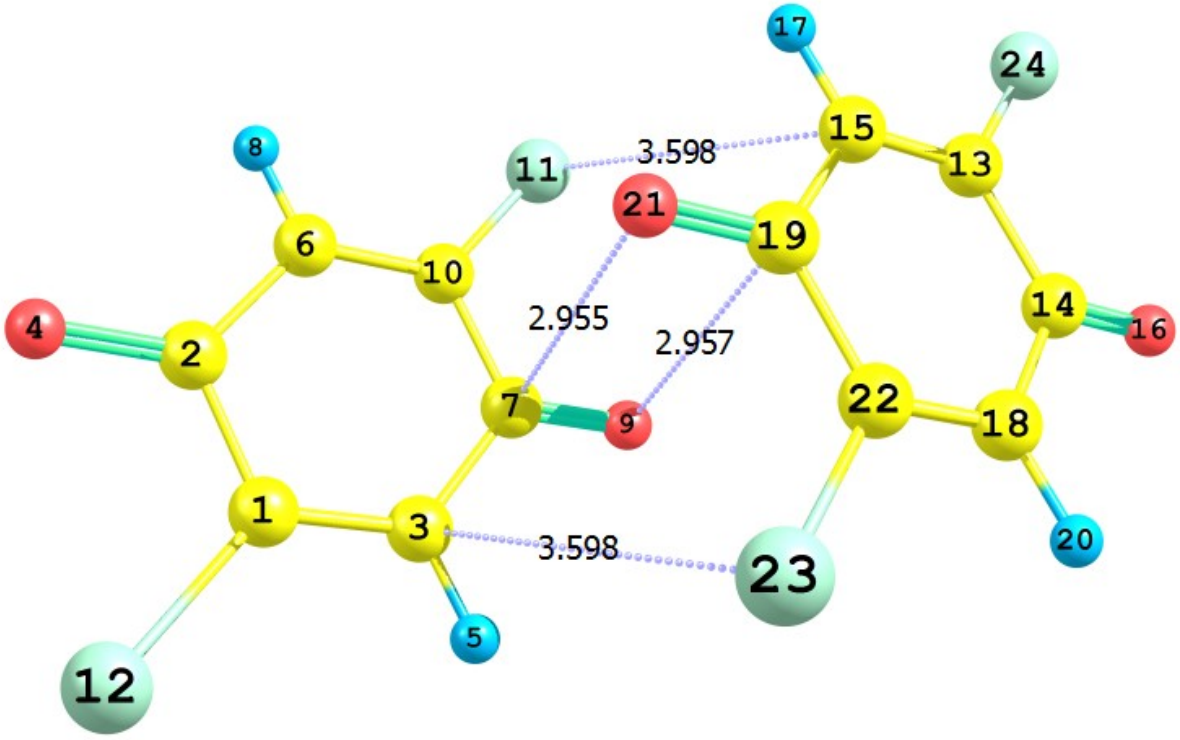
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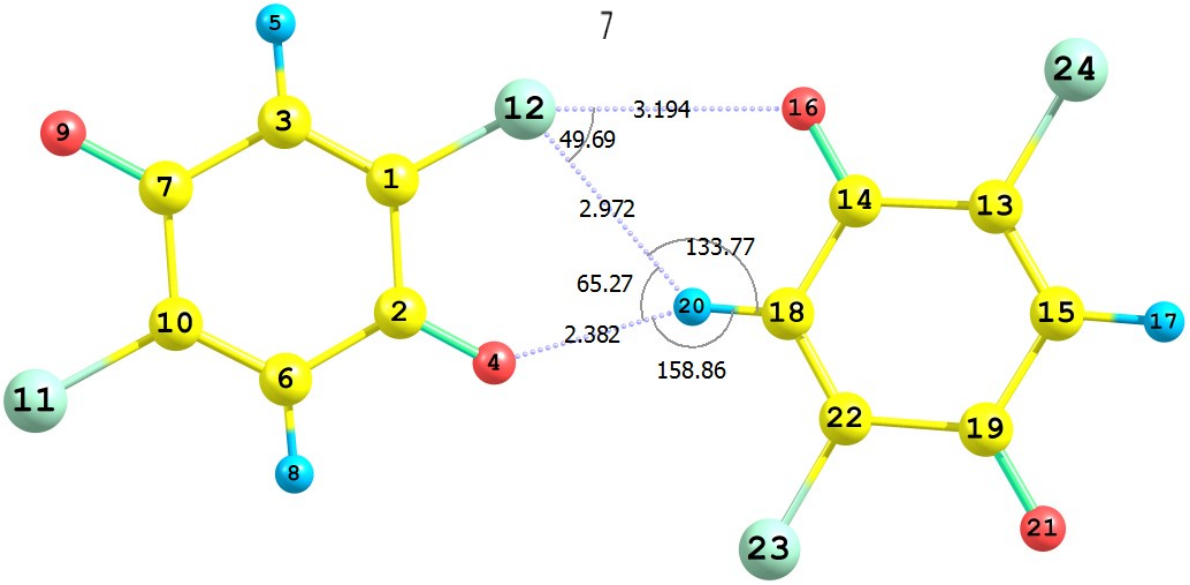
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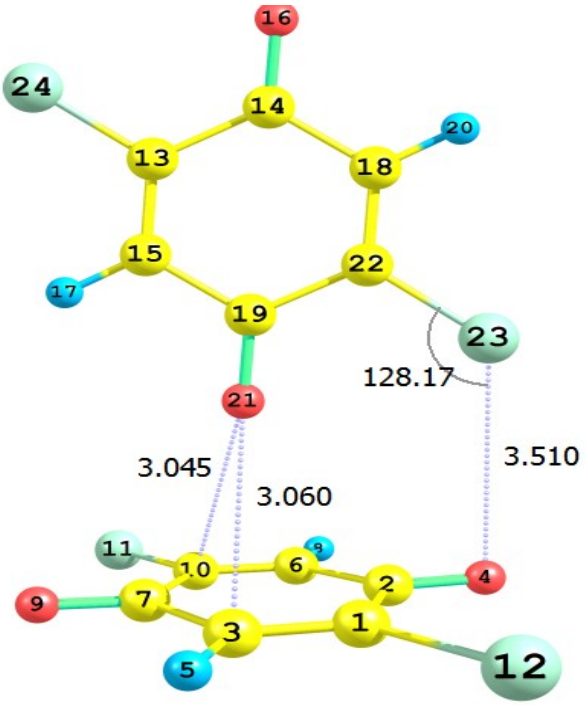
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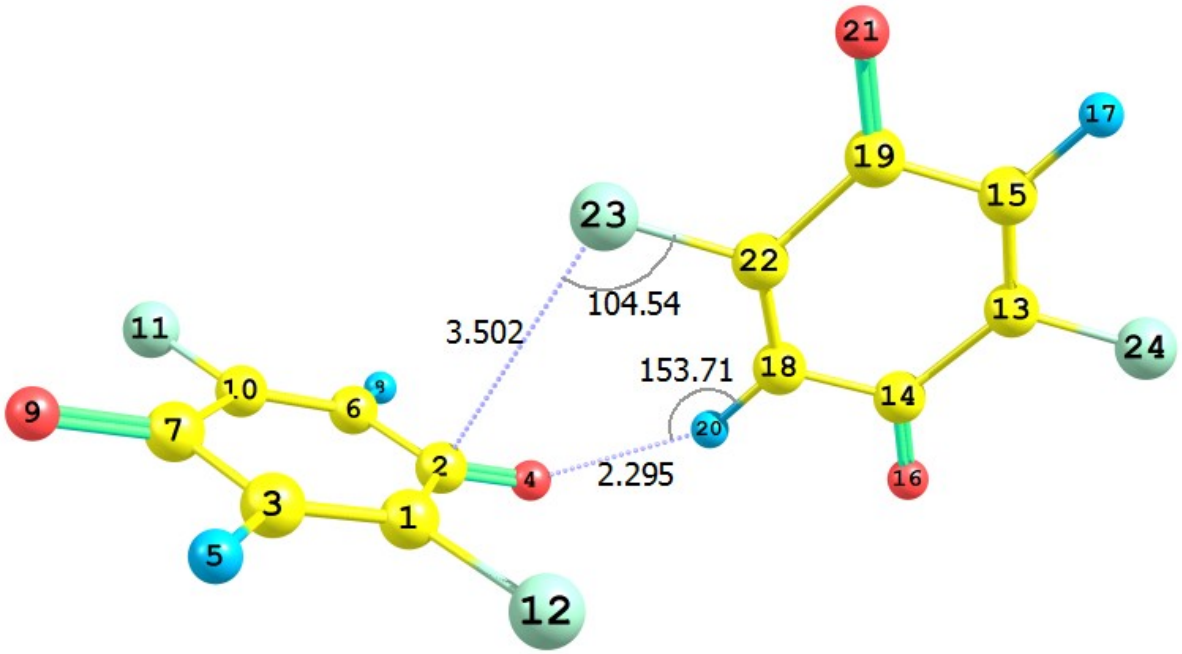

9

Fig. S1 Geometrical figures of nine isomers with noncovalent parameter computed at the M05-2X/6-31++G (d,p) level of theory.

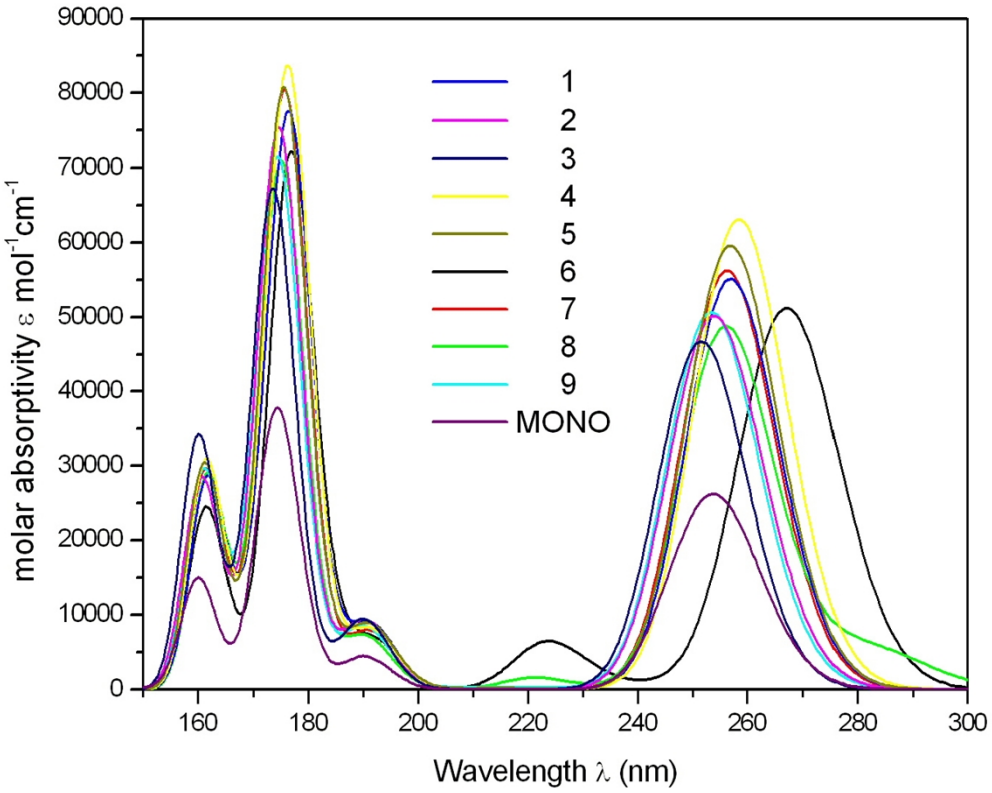

Fig. S2 Absorption spectrum for 9 isomers calculated at TD- M05-2X/6-31++G (d, p) level of theory.

Table S1: Comparison of geometrical parameters at ground and excited states. Lengths in Å

State	1			2		
	Covalent length	Non covalent length	Bond angle	Covalent length	Non covalent length	Bond angle
S_0	C6-H8 1.0839 C18-H20 1.0839	H8---O16 2.292 H20---O4 2.293	C6-H8---O16 163.840 C18-H20---O4 163.882	C18-H20 1.0822 C6-H8 1.0835	H20---Cl11 3.025 H8---O16 2.290	C18-H20---Cl11 157.483 C6-H8---O16 170.554
S_1	C6-H8 1.0854 C18-H20 1.0843	H8---O16 2.196 H20---O4 2.293	C6-H8---O16 167.590 C18-H20---O4 163.345	C18-H20 1.0825 C6-H8 1.0817	H20---Cl11 3.068 H8---O16 2.241	C18-H20---Cl11 163.182 C6-H8---O16 179.613
State	3			4		
	Covalent length	Non covalent length	Bond angle	Covalent length	Non covalent length	Bond angle
S_0	C6-H8 1.0823 C18-H20 1.0823	H8---Cl23 2.967 H20---Cl11 2.967	C6-H8---Cl23 176.439 C18-H20---Cl11 176.479	C22-Cl23 1.7109 C1-Cl12 1.7107	Cl23---O4 3.384 Cl12---O21 3.123 Cl12---Cl23 3.619	C22-Cl23---O4 159.058 C22-Cl23---C12 109.613 C1-Cl12---O21 166.177 C1-Cl12---Cl23 115.102
S_1	C6-H8 1.0805 C18-H20 1.0825	H8---Cl23 2.987 H20---Cl11 2.971	C6-H8---Cl23 172.784 C18-H20---Cl11 174.929	C22-Cl23 1.7090 C1-Cl12 1.7137	Cl23---O4 3.009 Cl12---O21 3.419 Cl12---Cl23 3.559	C22-Cl23---O4 169.451 C22-Cl23---C12 116.677 C1-Cl12---O21 157.133 C1-Cl12---Cl23 107.392
State	5			6		
	Covalent length	Non covalent length	Bond angle	Covalent length	Non covalent length	Bond angle
S_0	C1-Cl12 1.7121 C22-Cl23 1.7137	Cl12---O21 3.006 Cl12---Cl23 3.840	C1-Cl12---O21 173.225 C1-Cl12---Cl23 132.379 C22-Cl23---C12 93.199	C7-O9 1.2137 C19-O21 1.2137 C22-Cl23 1.7164 C10-Cl11 1.7164	O9---C19 2.956 O21---C7 2.955 Cl11---C15 3.598 Cl23---C3 3.598	C7-O9---C19 93.306 C19-O21---C7 93.441 C22-Cl23-C3 96.488 C10-Cl11---C15 96.478
S_1	C1-Cl12 1.7149	Cl12---O21 3.498	C1-Cl12---O21 125.619	C7-O9 1.2138 C19-O21 1.2286 C22-Cl23	O9---C19 3.023 O21---C7 2.857 Cl11---C15	C7-O9---C19 87.312 C19-O21---C7 94.887 C22-Cl23-C15

				1.7174 C10-Cl11 1.7172	3.599 Cl23---C3 3.571	94.928 C10-Cl11---C3 93.004
State	7			8		
	Covalent length	Non covalent length	Bond angle	Covalent length	Non covalent length	Bond angle
S_0	C1-Cl12 1.7119 C18-H20 1.0841	Cl12---O16 3.194 H20---Cl12 2.972 H20---O4 2.382	C1-Cl12---O16 151.041 C18-H20---Cl12 133.768 C18-H20---O4 158.861	C19-O21 1.2137 C22-Cl23 1.7129	O21---C10 3.045 O21---C3 3.060 Cl23---O4 3.510	C19-O21---C10 158.547 C19-O21---C3 151.530 C22-Cl23---O4 128.171
S_1	C1-Cl12 1.7104 C18-H20 1.0842	Cl12---O16 3.023 H20---Cl12 2.874 H20---O4 2.415	C1-Cl12---O16 156.067 C18-H20---Cl12 130.110 C18-H20---O4 162.156	C19-O21 1.2278 C22-Cl23 1.7149	O21---C10 3.020 O21---C3 3.051 Cl23---O4 3.510	C19-O21---C10 157.973 C19-O21---C3 151.827 C22-Cl23---O4 125.720
	9					
State	Covalent length	Non covalent length	Bond angle	------ ------	------ ------	------ ------
S_0	C18-H20 1.0834 C22-Cl23 1.7207	H20---O4 2.295 Cl23---C2 3.502	C18-H20---O4 153.711 C22-Cl23---C2 104.542	------ ------	------ ------	------ ------
S_1	C18-H20 1.0821 C22-Cl23 1.7223	H20---O4 2.254 Cl23---C1 3.467	C18-H20---O4 158.392 C22-Cl23---C1 110.114	------ ------	------ ------	------ ------

S_0 – ground state S_1- low lying first excited state

Table S2: Monomer geometrical parameters. Lengths in Å

State	monomer
	Covalent length
S_0	C1-Cl12 1.7138 C10-Cl11 1.7137 C2-O4 1.2104 C7-O9 1.2105 C3-H5 1.0822 C6-H8 1.0822
S_1	C1-Cl12 1.7209 C10-Cl11 1.7210 C2-O4 1.2465 C7-O9 1.2468 C3-H5 1.0805 C6-H8 1.0805

S_0 – ground state S_1- low lying first excited state

Table S3: Comparison of length shift and frequency shift.

$\Delta R_{x\text{-}h}$ – donor covalent bond length shift (in angstroms). Δ^{w_e} - Frequency shift (in cm^{-1}).

Isomer	Bond	**interactions**	$\Delta \mathbf{R_{x\text{-}h}}$ **(**Å)	Δ^{w_e} (cm^{-1})
1	C6-H8	H-bond	0.00172	-31.33
	C18-H20	H-bond	0.00173	-31.33
2	C18-H20	H-bond	0.00002	-18.89
	C6-H8	H-bond	0.00135	-27.62
3	C6-H8	H-bond	-0.0017	17.58
	C18-H20	H-bond	-0.0003	17.58
4	C22-Cl23	X-bond	-0.00276	3.69
	C1-Cl12	X-bond	-0.00312	12.32
5	C1-Cl12	X-bond	-0.0017	6.31
	C22-Cl23	X-bond	0	2.95
6	C22-Cl23	C-bond	-0.00268	1.05
	C10-Cl11	C-bond	-0.00265	1.05
7	C1-Cl12	X-bond	-0.0019	4.47
	C18-H20	H-bond	0.0019	-16.54
	C18-H20	H-bond	0.0019	-16.54
8	C22-Cl23	X-bond	-0.00076	3.94
9	C18-H20	H-bond	0.00163	-20.72
	C22-Cl2	C-bond	0.00655	5.11