

## Supporting information

### **ULTRASONIC, SPECTROPHOTOMETRIC AND DFT INVESTIGATION ON HALOGEN BONDED AND I<sub>2</sub>···π INTERACTION OF PHENOL···I<sub>2</sub>, ANISOLE···I<sub>2</sub> AND CHLOROBENZENE···I<sub>2</sub>**

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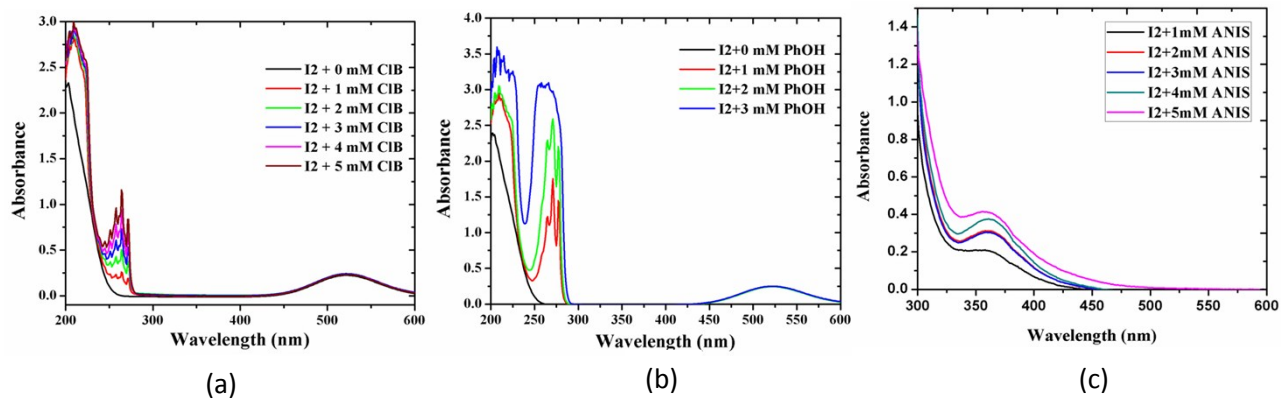
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**Figure S1.** Recorded UV - visible spectra for chlorobenzene, phenol and anisole with iodine in n-hexane medium at 303K. The concentration of acceptor iodine was kept constant at  $2 \times 10^{-5}$  M and the concentration of donor varied in excess.

Table S2. Calculated Cartesian coordinates of all the compounds in the present study.

Iodine				Chlorobenzene			
53	0.541132000	0.246914000	0.000000000	6	1.573788000	1.208351000	0.000000000
53	-2.151749000	0.246914000	0.000000000	6	0.177161000	1.217007000	0.000000000
				6	-0.507029000	0.000000000	0.000000000
				6	0.177161000	-1.217008000	0.000000000
				6	1.573788000	-1.208350000	0.000000000
				6	2.275084000	0.000000000	0.000000000
				1	2.113838000	2.156206000	0.000000000
				1	-0.379729000	2.153312000	0.000000000
				1	-0.379729000	-2.153313000	0.000000000
				1	2.113838000	-2.156205000	0.000000000
				1	3.365805000	-0.000001000	0.000000000
				17	-2.254472000	0.000000000	0.000000000
Phenol				Anisole			
6	-1.202834000	-1.168360000	0.000000000	6	0.004001000	0.000811000	-0.017929000
6	0.189875000	-1.232142000	0.000000000	6	1.402146000	0.004522000	-0.084347000
6	0.935363000	-0.046930000	0.000000000	6	2.088212000	1.226804000	-0.085483000
6	0.283384000	1.192457000	0.000000000	6	1.370380000	2.431836000	-0.020388000
6	-1.112124000	1.242146000	0.000000000	6	-0.018907000	2.410114000	0.045371000
6	-1.863051000	0.064800000	0.000000000	6	-0.713688000	1.193913000	0.047629000
1	-1.778595000	-2.095072000	0.000000000	1	-0.523298000	-0.954660000	-0.017282000
1	0.715330000	-2.187322000	0.000000000	1	1.941224000	-0.940354000	-0.134277000
1	0.868143000	2.116432000	0.000001000	1	1.925822000	3.370219000	-0.022135000
1	-1.612654000	2.211598000	0.000000000	1	-0.566460000	3.352564000	0.097010000
1	-2.952565000	0.107107000	-0.000001000	1	-1.802803000	1.180613000	0.100523000
8	2.303993000	-0.159730000	0.000001000	8	3.450955000	1.349496000	-0.146598000
1	2.687433000	0.735144000	-0.000002000	6	4.216025000	0.148375000	-0.204174000
				1	4.050740000	-0.477623000	0.688833000
				1	3.979391000	-0.438801000	-1.107612000
				1	5.264812000	0.463479000	-0.239904000
1a				1b			
6	3.221005000	-0.152944000	-1.217950000	6	4.182683000	1.332249000	-1.184470000
6	2.500081000	-1.345613000	-1.210336000	6	3.611370000	0.058289000	-1.140867000
6	2.124464000	-1.943617000	0.004020000	6	3.053714000	-0.380551000	0.058040000
6	2.481256000	-1.330373000	1.216552000	6	3.044686000	0.411445000	1.204853000
6	3.202331000	-0.137536000	1.220658000	6	3.619181000	1.682282000	1.142131000
6	3.564309000	0.440186000	0.000487000	6	4.187211000	2.144457000	-0.047883000
1	3.512658000	0.321425000	-2.153951000	1	4.621440000	1.688810000	-2.116761000
1	2.227931000	-1.815430000	-2.155781000	1	3.593167000	-0.583387000	-2.020604000
1	1.616489000	-2.908116000	0.006045000	1	2.588947000	0.041810000	2.122026000
1	2.194113000	-1.788668000	2.163388000	1	3.616009000	2.313742000	2.031127000
1	3.478858000	0.348305000	2.155149000	1	4.629000000	3.140135000	-0.090587000
53	-0.525766000	-0.559403000	0.001635000	53	-0.555110000	-0.699083000	0.010144000
53	-3.085202000	0.555532000	-0.002600000	53	-3.002265000	0.612599000	-0.050444000
17	4.458269000	1.933352000	-0.002606000	17	2.311720000	-1.970968000	0.118817000

2a

6	3.717904000	-0.956013000	1.274942000
6	3.507439000	0.419327000	1.230193000
6	3.013076000	1.005607000	0.057761000
6	2.724308000	0.199758000	-1.062596000
6	2.946644000	-1.187645000	-0.997459000
6	3.438448000	-1.768537000	0.167605000
1	4.100421000	-1.404277000	2.192723000
1	3.714957000	1.055682000	2.089980000
1	2.404875000	0.662439000	-1.999375000
1	2.723003000	-1.801206000	-1.870595000
1	3.601613000	-2.844580000	0.218574000
8	2.837868000	2.357111000	0.052038000
1	2.403478000	2.619847000	-0.779686000
53	-0.140699000	-0.039025000	-0.300662000
53	-2.835494000	-0.025499000	0.219707000

2b

6	4.109353000	1.778110000	0.000001000
6	3.016941000	0.911351000	0.000001000
6	3.240191000	-0.467821000	0.000000000
6	4.540541000	-0.980391000	0.000000000
6	5.624835000	-0.100016000	0.000000000
6	5.416037000	1.280582000	0.000000000
1	3.933545000	2.854467000	0.000001000
1	1.993375000	1.287304000	0.000001000
1	4.705710000	-2.060891000	0.000000000
1	6.638924000	-0.501717000	0.000000000
1	6.265284000	1.964310000	0.000000000
8	2.133915000	-1.295781000	0.000000000
1	2.416874000	-2.226976000	0.000000000
53	-0.588411000	-0.481642000	0.000000000
53	-3.160879000	0.378224000	0.000000000

3a

6	-3.286948000	-0.412527000	1.366443000
6	-3.338635000	-1.767393000	1.070327000
6	-3.056517000	-2.237077000	-0.223172000
6	-2.714002000	-1.329383000	-1.214782000
6	-2.643349000	0.051847000	-0.938551000
6	-2.949264000	0.512229000	0.362299000
1	-3.504635000	-0.037203000	2.366388000
1	-3.601634000	-2.474113000	1.858467000
1	-3.099941000	-3.303328000	-0.442704000
1	-2.486691000	-1.674546000	-2.224119000
1	-2.458823000	0.753790000	-1.749538000
53	0.218141000	0.008566000	-0.308014000
53	2.980773000	-0.057716000	0.208751000
8	-2.952452000	1.817836000	0.730597000
6	-2.569395000	2.790111000	-0.248061000
1	-1.545462000	2.599457000	-0.606474000
1	-2.606903000	3.756075000	0.265315000
1	-3.270106000	2.795281000	-1.098238000

3b

6	4.622533000	-0.692969000	1.184355000
6	3.768597000	0.384867000	0.921076000
6	2.933035000	0.329622000	-0.197230000
6	2.943843000	-0.785297000	-1.043673000
6	3.797194000	-1.848858000	-0.766390000
6	4.641344000	-1.809491000	0.350082000
1	5.273381000	-0.652361000	2.058887000
1	3.763058000	1.244004000	1.588586000
1	2.276897000	-0.799450000	-1.905795000
1	3.801996000	-2.716262000	-1.427491000
1	5.306655000	-2.645961000	0.565115000
8	2.046863000	1.335047000	-0.548065000
53	-0.510691000	0.410835000	-0.257174000
53	-3.109020000	-0.457402000	0.226086000
6	2.090896000	2.550622000	0.214906000
1	1.359329000	3.217449000	-0.252307000
1	3.095672000	2.995507000	0.162712000
1	1.808142000	2.373755000	1.263768000