Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Photoswitchable Nonlinear Optical Properties of Azobenzene-Based Supramolecular Complexes: Insights From Density Functional Theory

Aqsa Nisar[1], Sobia Tabassum[2], Khurshid Ayub[3] , Tariq Mahmood[3, 4], Hamad AlMohamadi[5], Asim Laeeq Khan[6], Muhammad Yasin[6], R. Nawaz[7], Mazhar Amjad Gilani[1]*

[1]Department of Chemistry, COMSATS University Islamabad, Lahore Campus, Lahore-54600, Pakistan

[2]Interdisciplinary Research Centre in Biomedical Materials (IRCBM), COMSATS University Islamabad, Lahore Campus, Lahore-54600, Pakistan

[3]Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad-22060, Pakistan

[4]Department of Chemistry, College of Science, University of Bahrain, Bahrain

[5]Department of Chemical Engineering, Faculty of Engineering, Islamic University of Madinah, Madinah, Saudi Arabia

[6]Department of Chemical Engineering, COMSATS University Islamabad, Lahore Campus, Lahore-54600, Pakistan

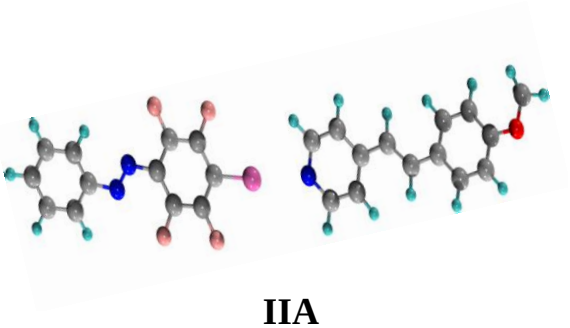
[7]Center for Applied Mathematics and Bioinformatics (CAMB), Gulf University for Science and Technology, 32093 Hawally, Kuwait

*Corresponding Author

Mazhar Amjad Gilani

Email: mazhargilani@cuilahore.edu.pk

Figures



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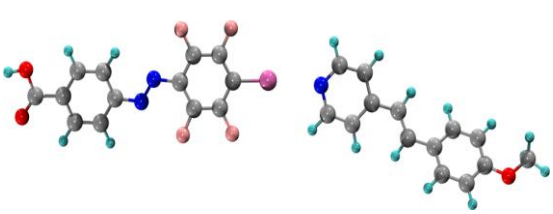

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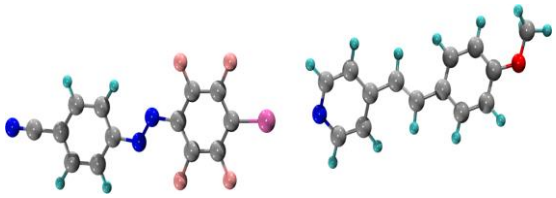

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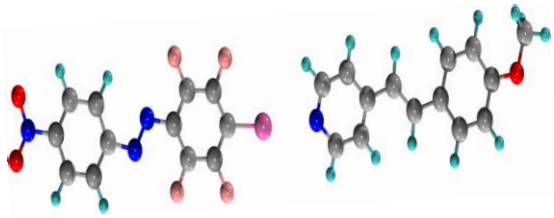

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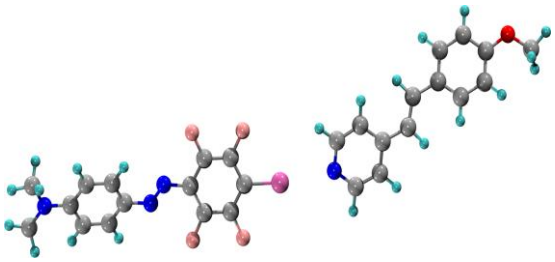

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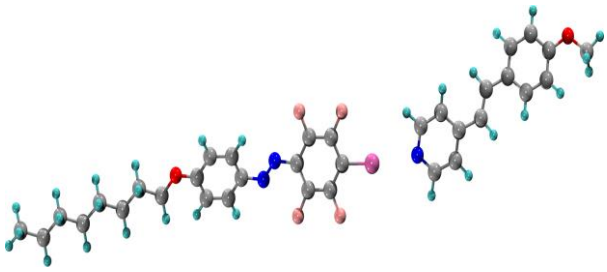

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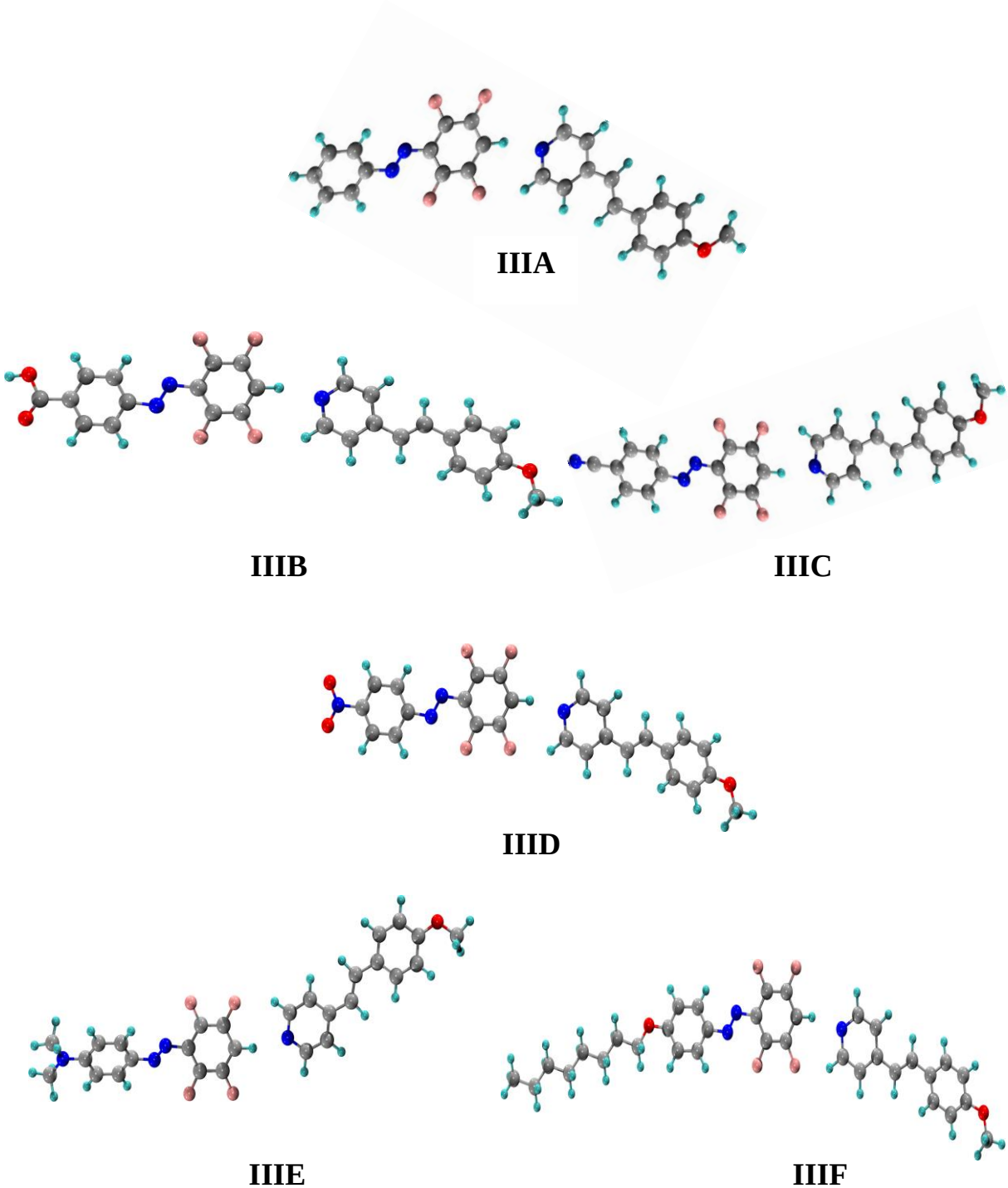
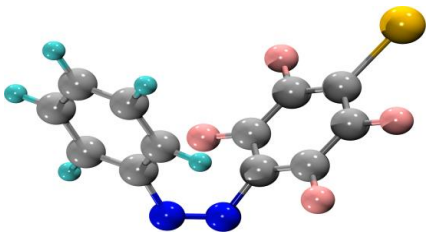
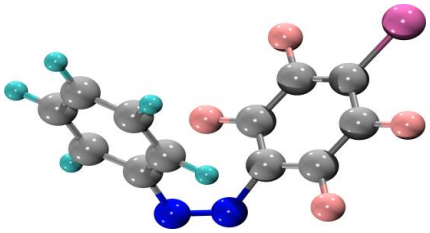


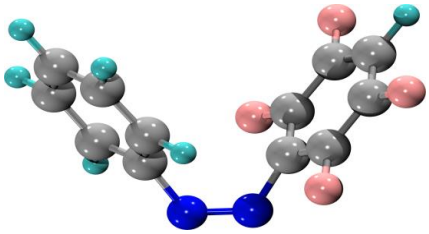
Fig. S1: Optimized geometries of **IIA-IIF** and **IIIA-IIIF** complexes



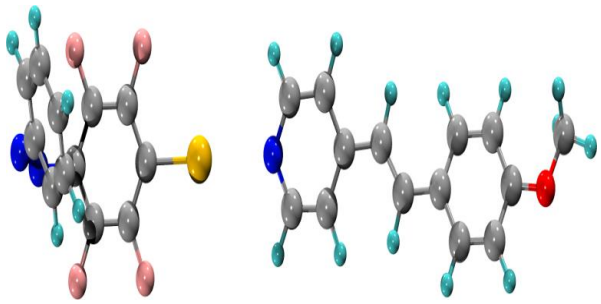
Cis Azo-I (i)



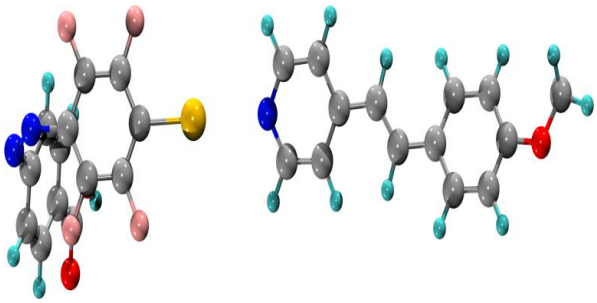
Cis Azo-Br (ii)



Cis Azo-H (iii)



iA



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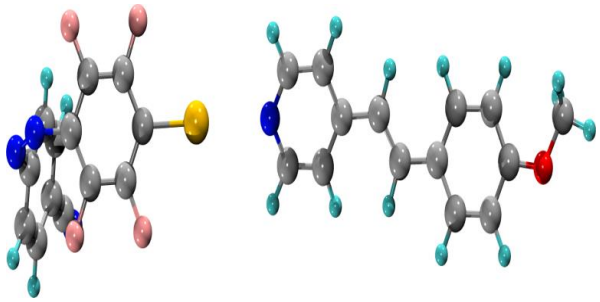

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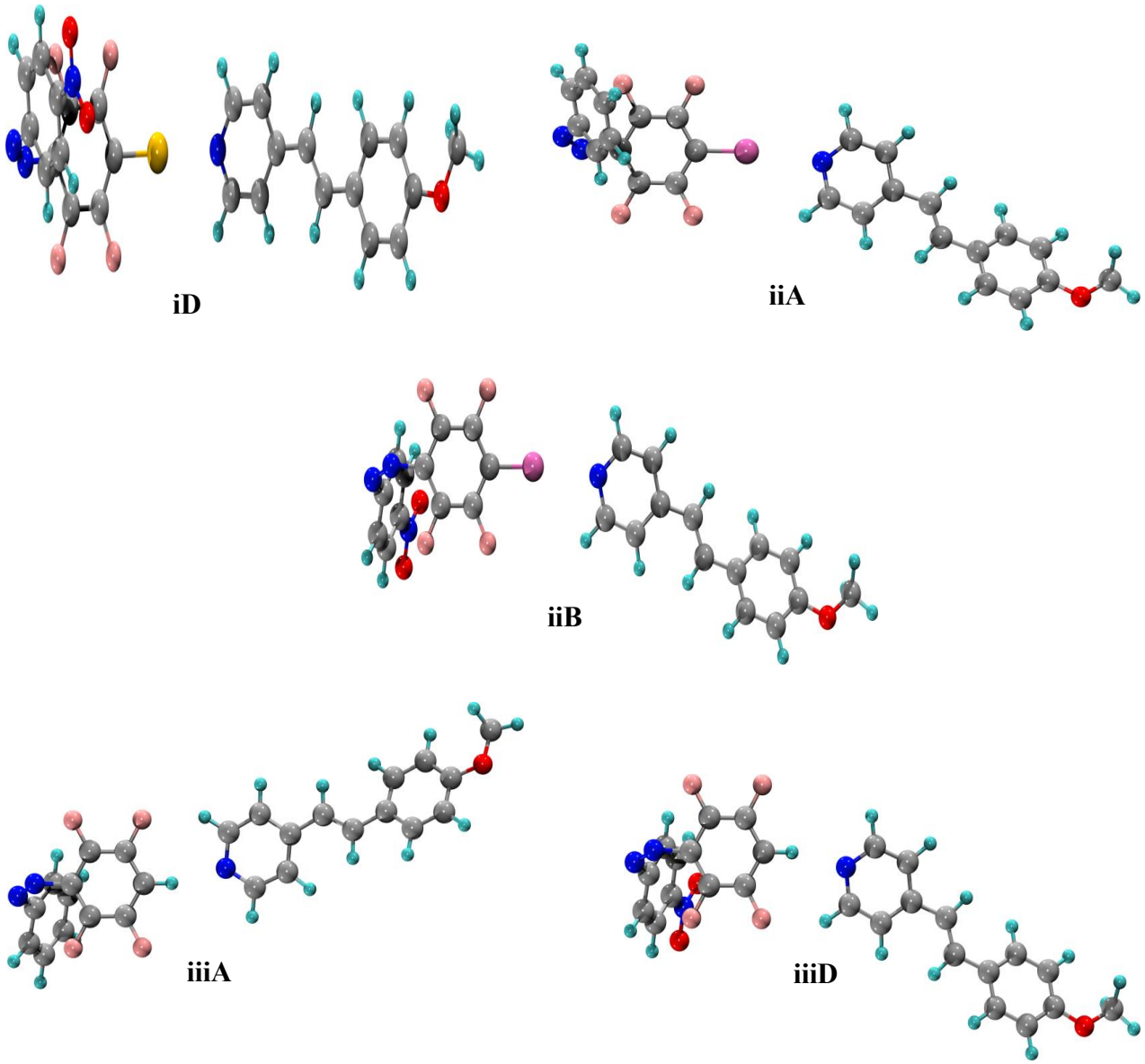
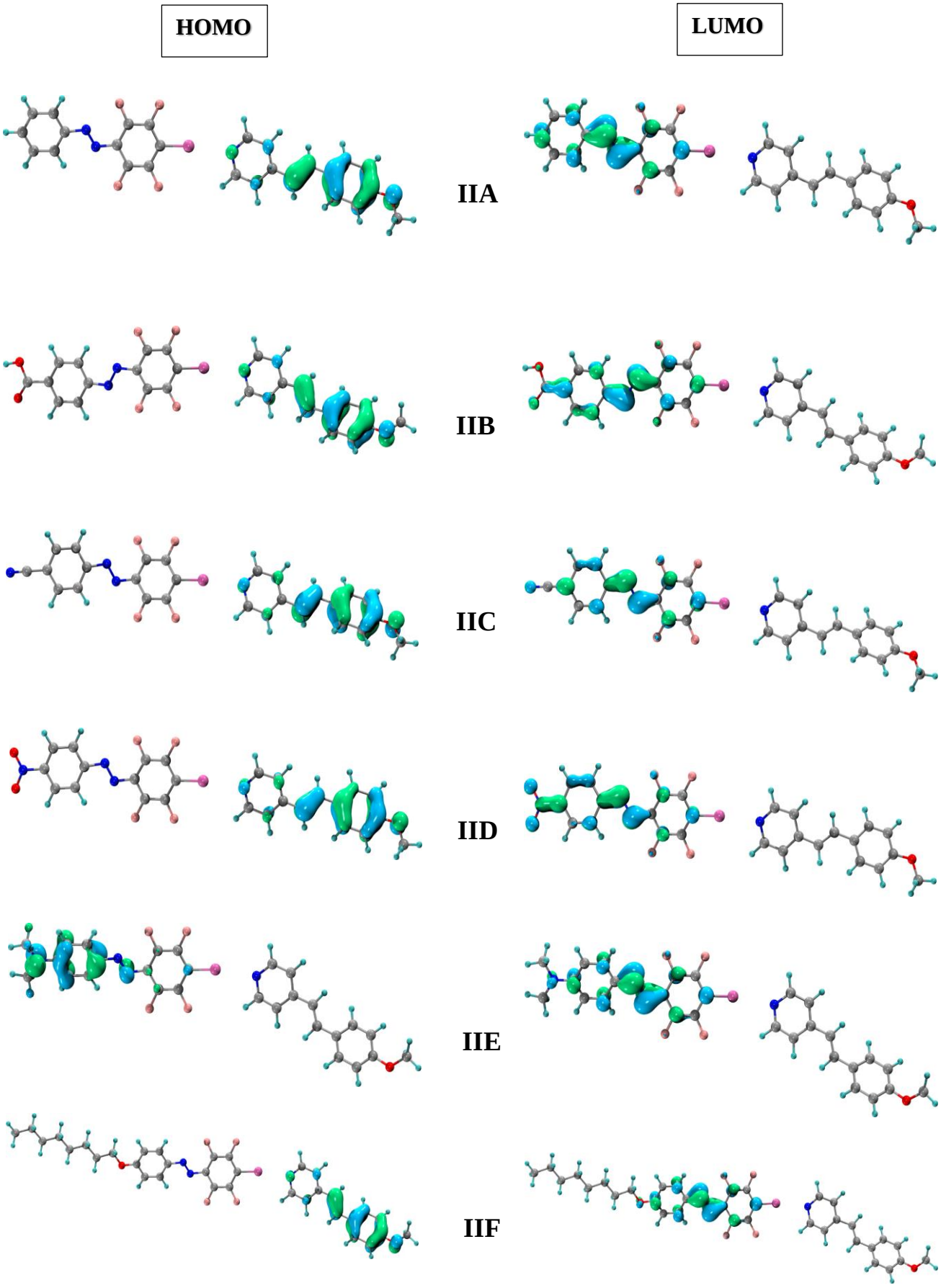


Fig. S2: Optimized geometries of *cis* Azo-X (where X=I, Br or H) and their supramolecular complexes


HOMO
LUMO
IIA
IIB
IIC
IID
IIE
IIF

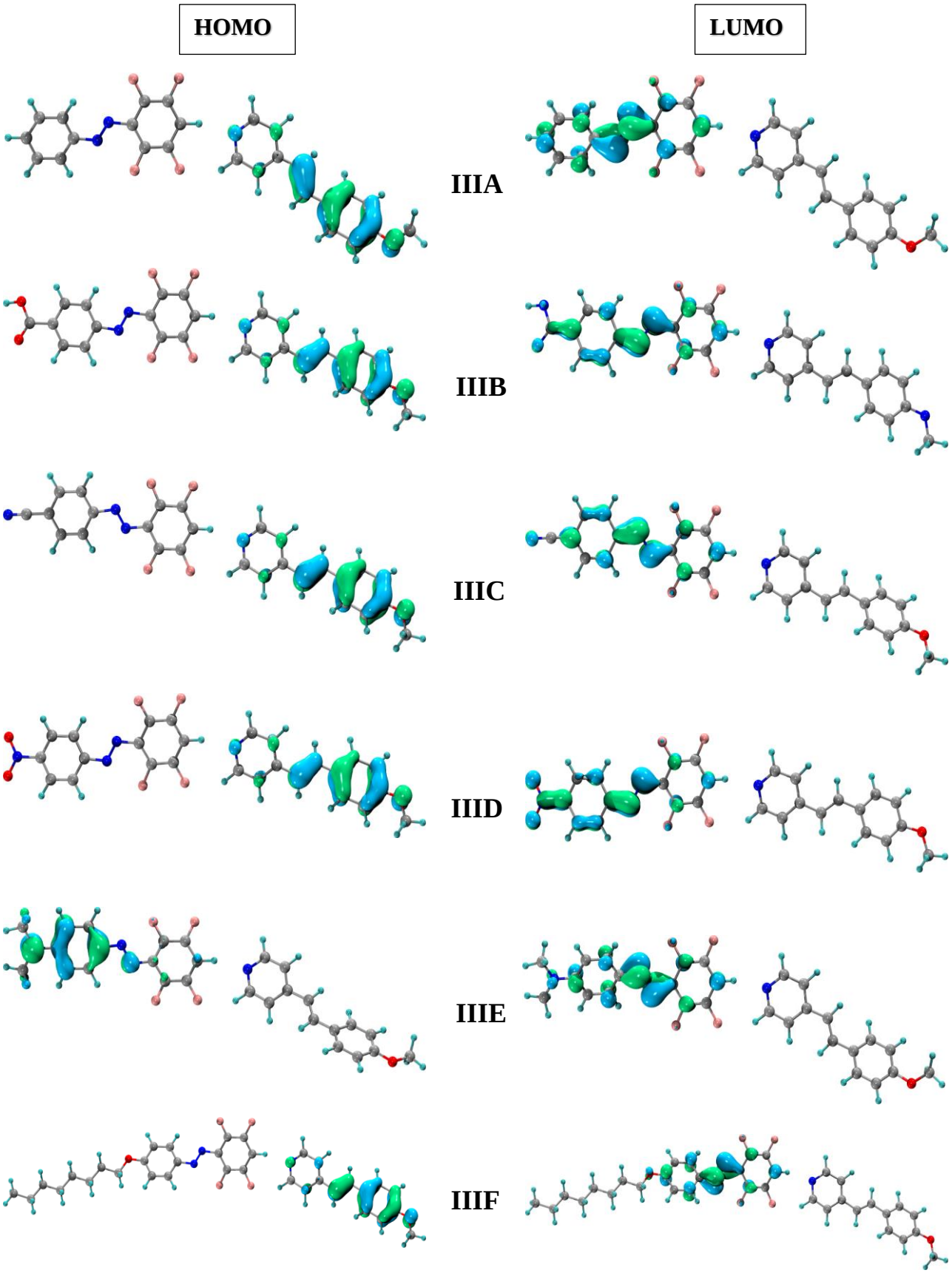
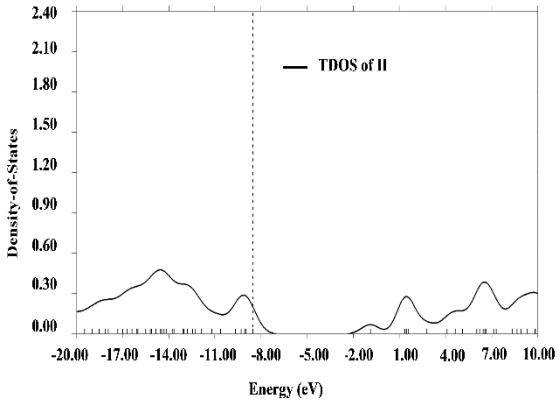
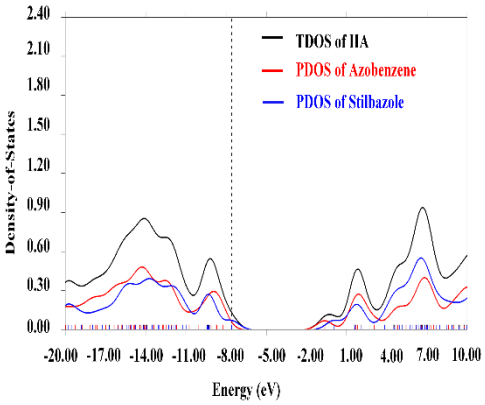
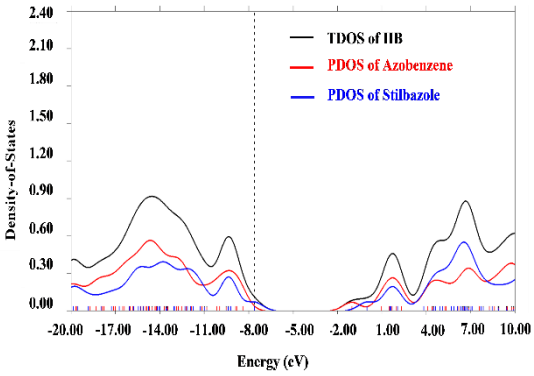
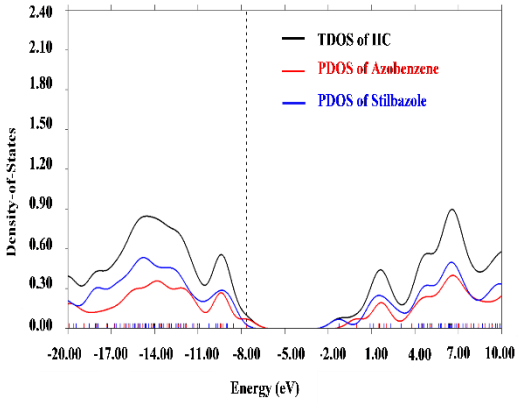


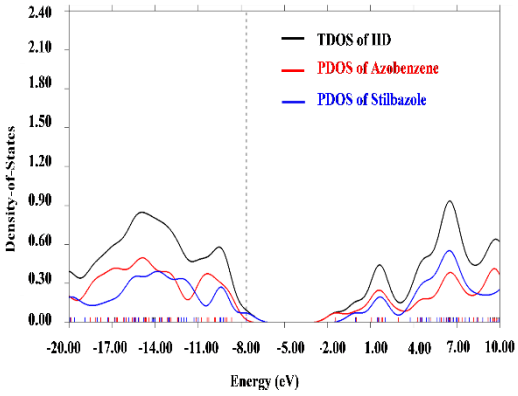
Fig. S3: HOMOs and LUMOs of **IIA-IIF** and **IIIA-IIIF** complexes

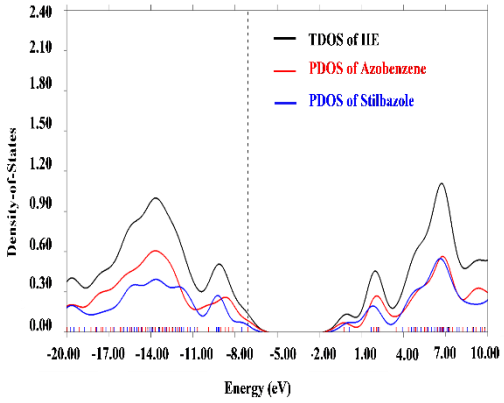

TDOS of II
Density-of-States
Energy (eV)

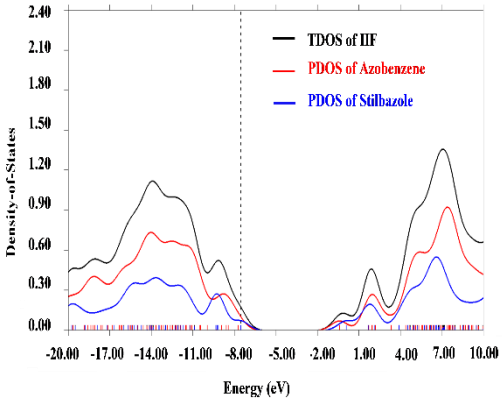

TDOS of IIA
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)


TDOS of IIB
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)


TDOS of IIC
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)


TDOS of IID
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)


TDOS of IIE
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)


TDOS of IIF
PDOS of Azobenzene
PDOS of Stilbazole
Density-of-States
Energy (eV)

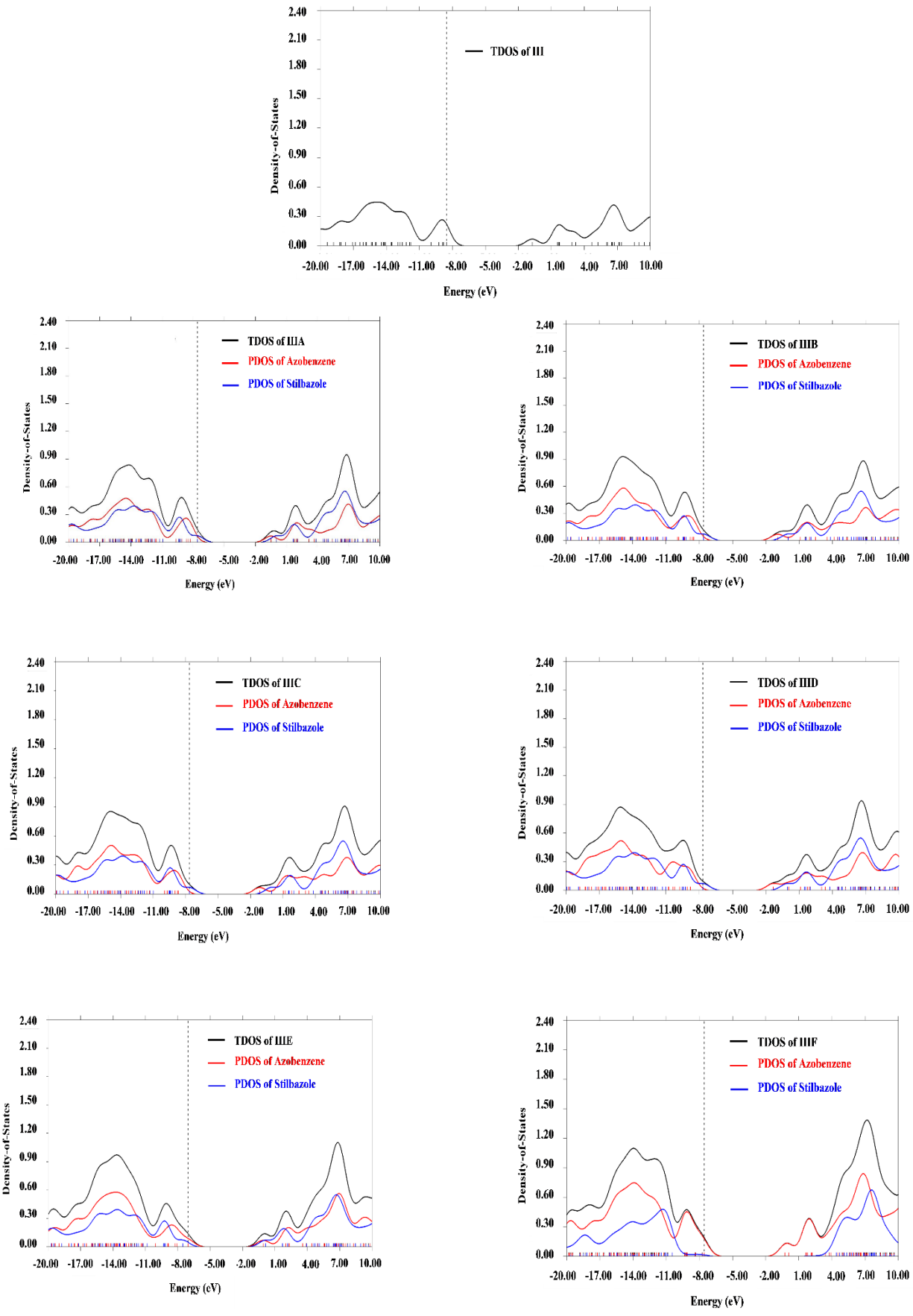
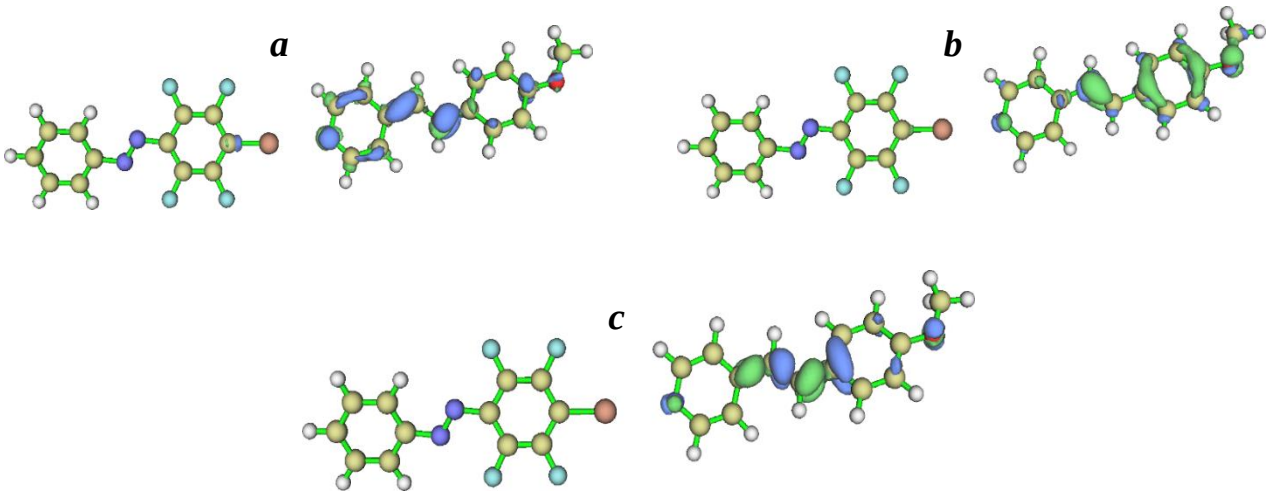


Fig. S4: TDOS and PDOS of Azo-Br, Azo-H, **IIA-IIF** and **IIIA-IIIF** complexes



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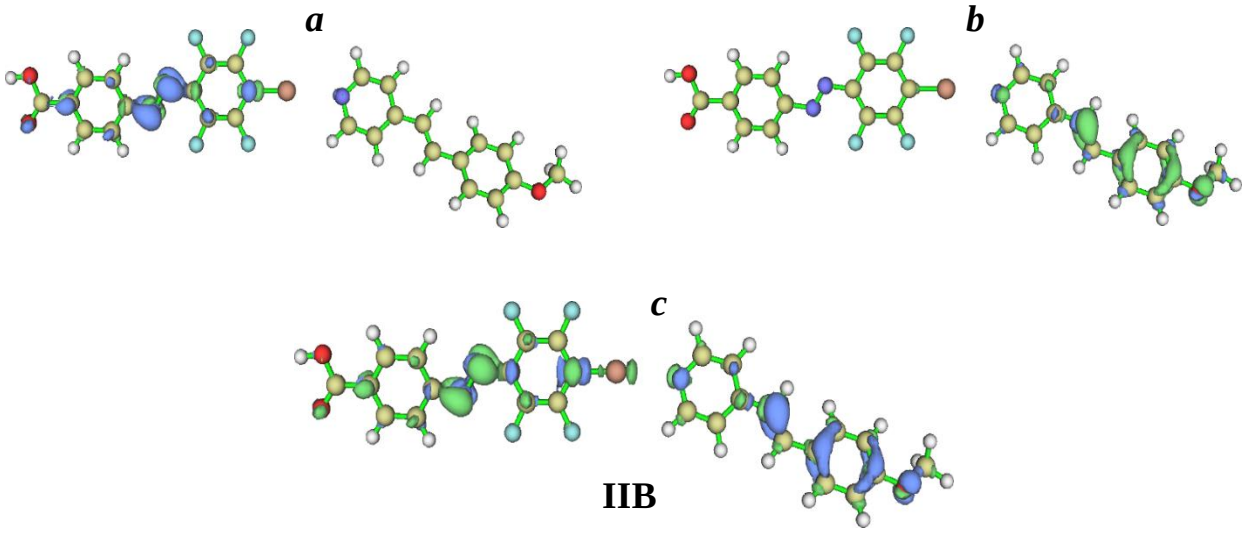

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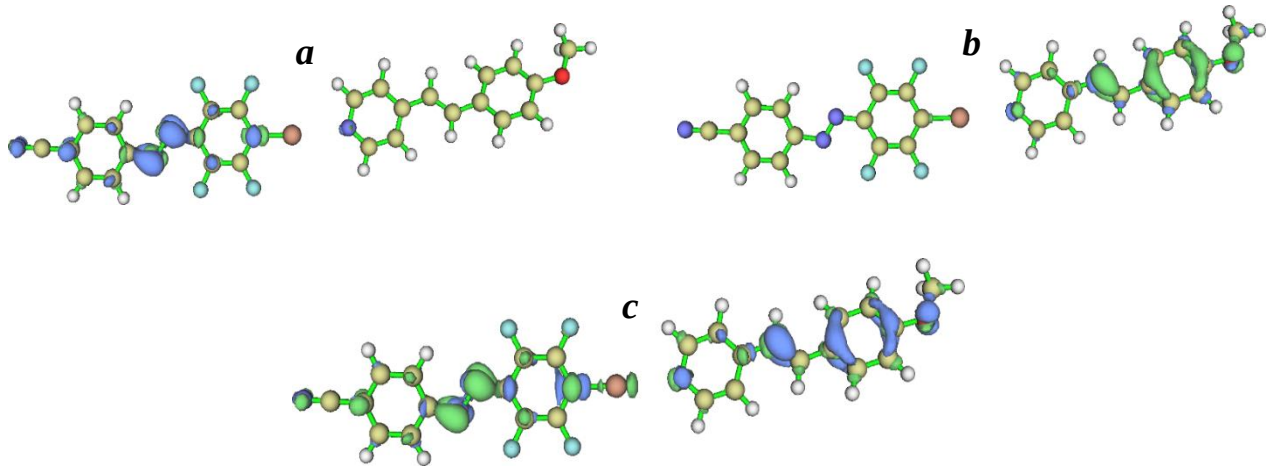

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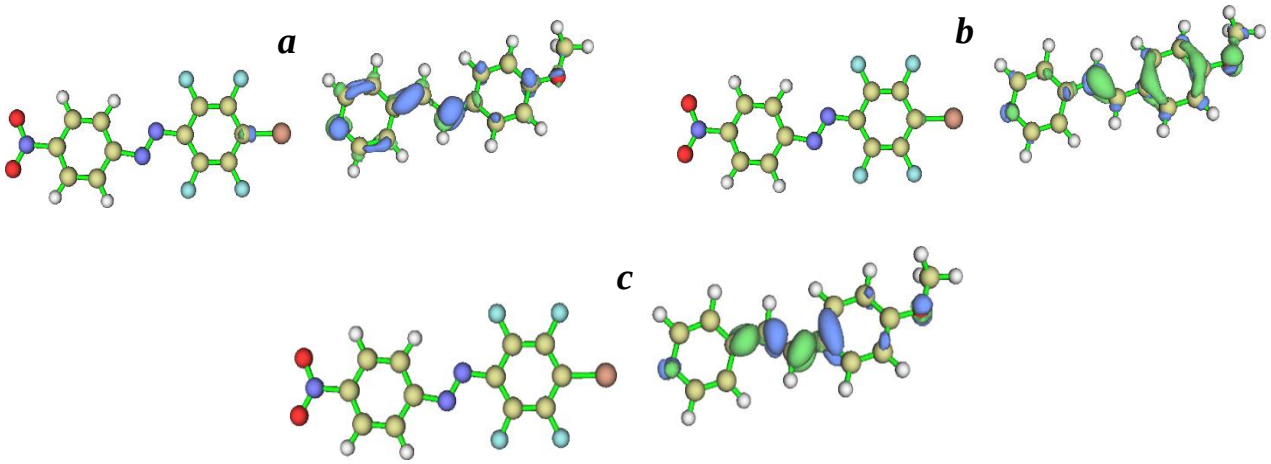

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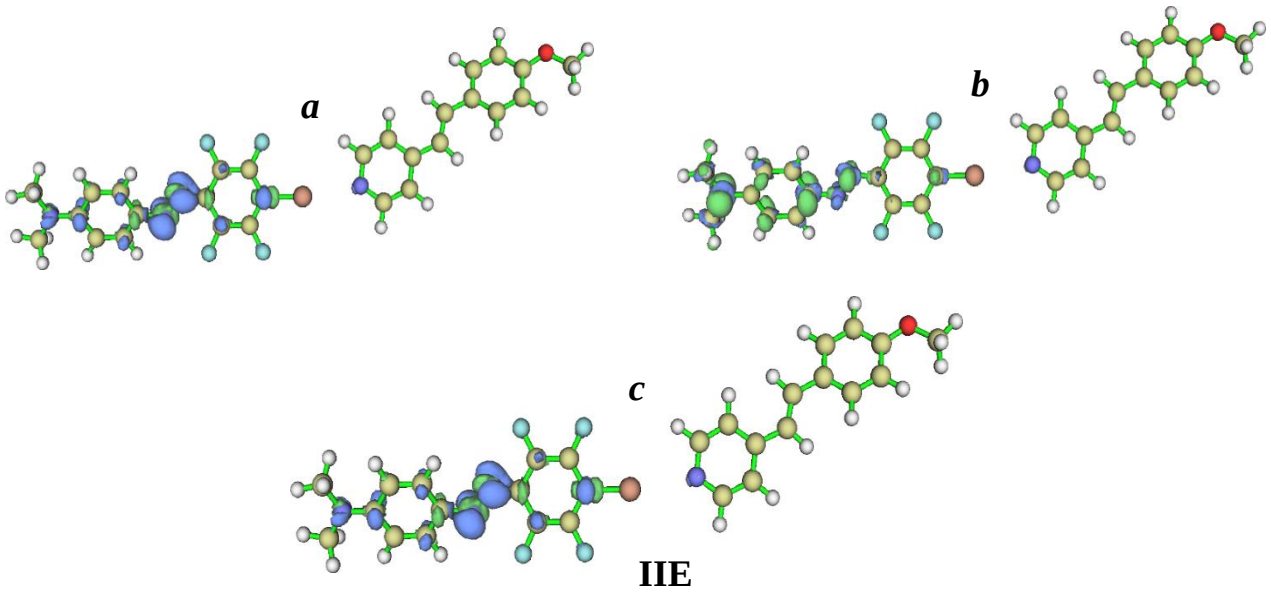
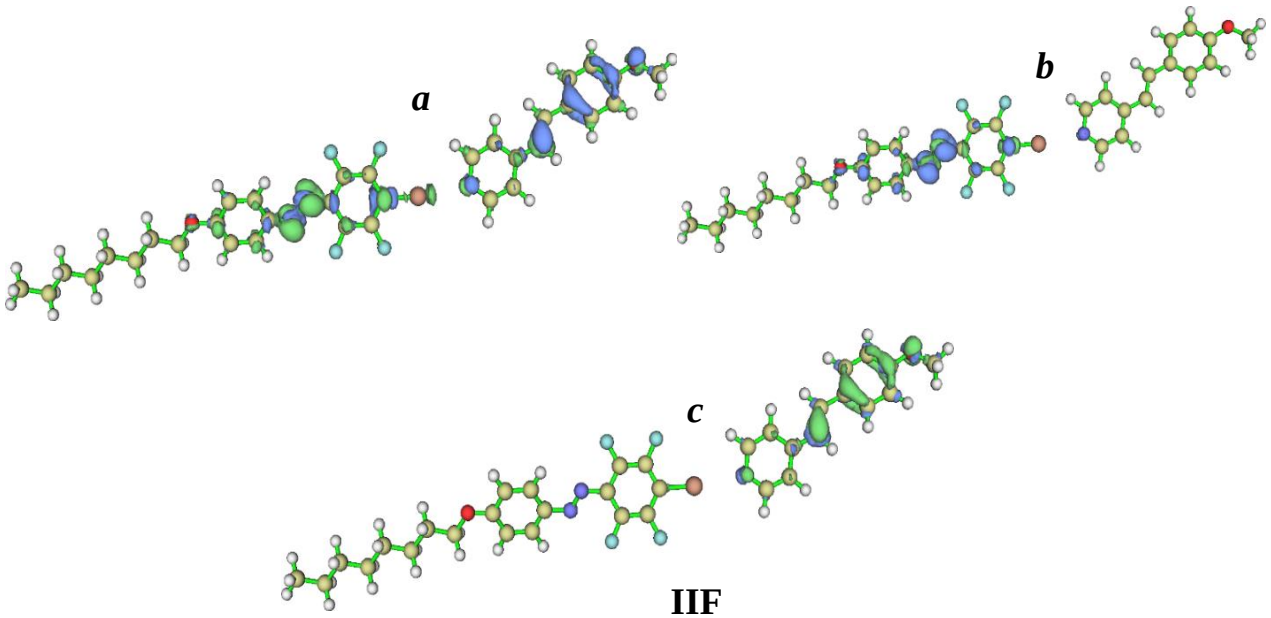


IIE



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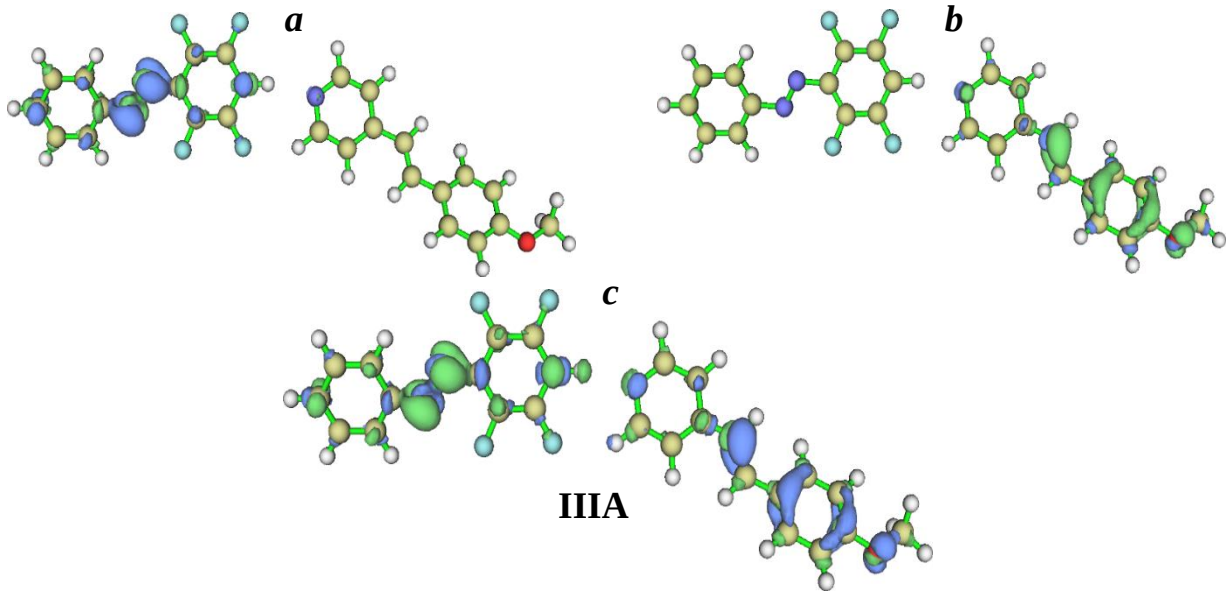
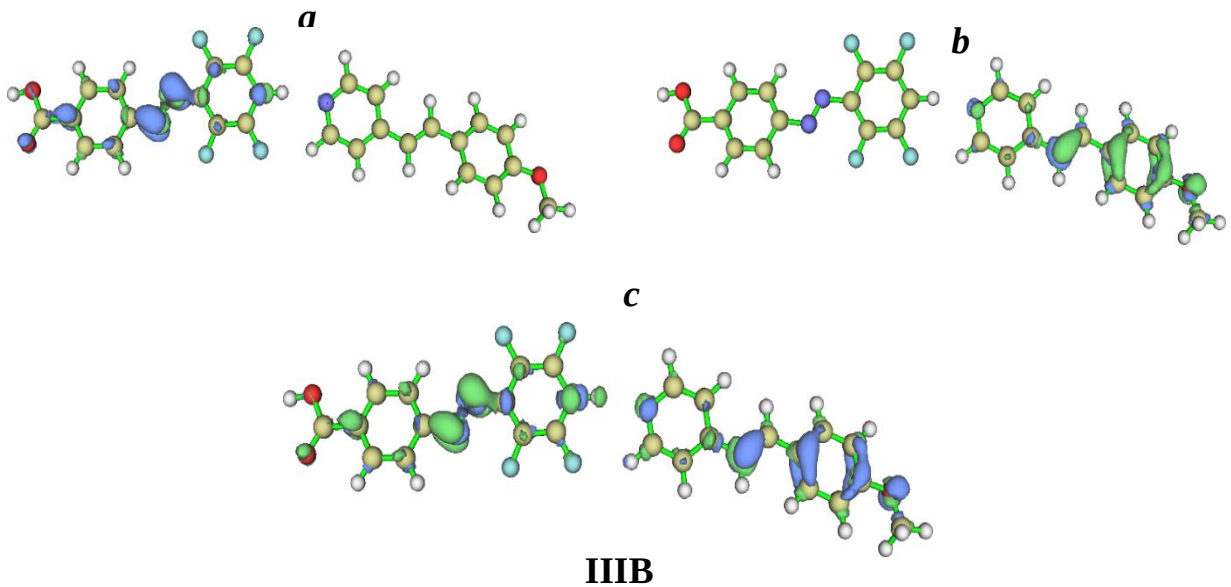


IIIA



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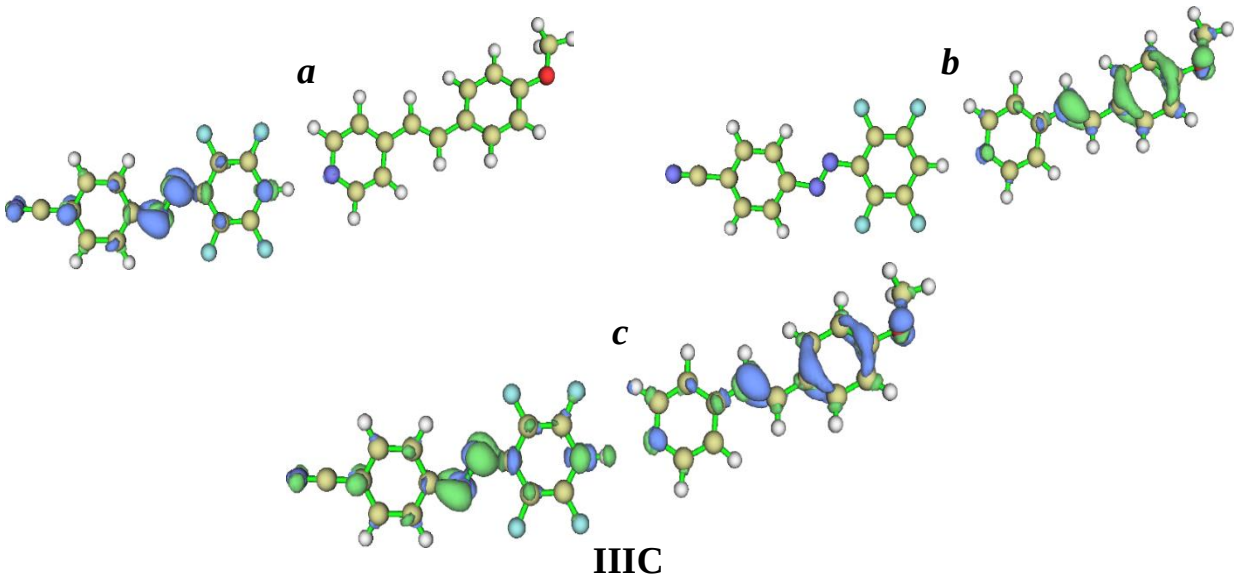

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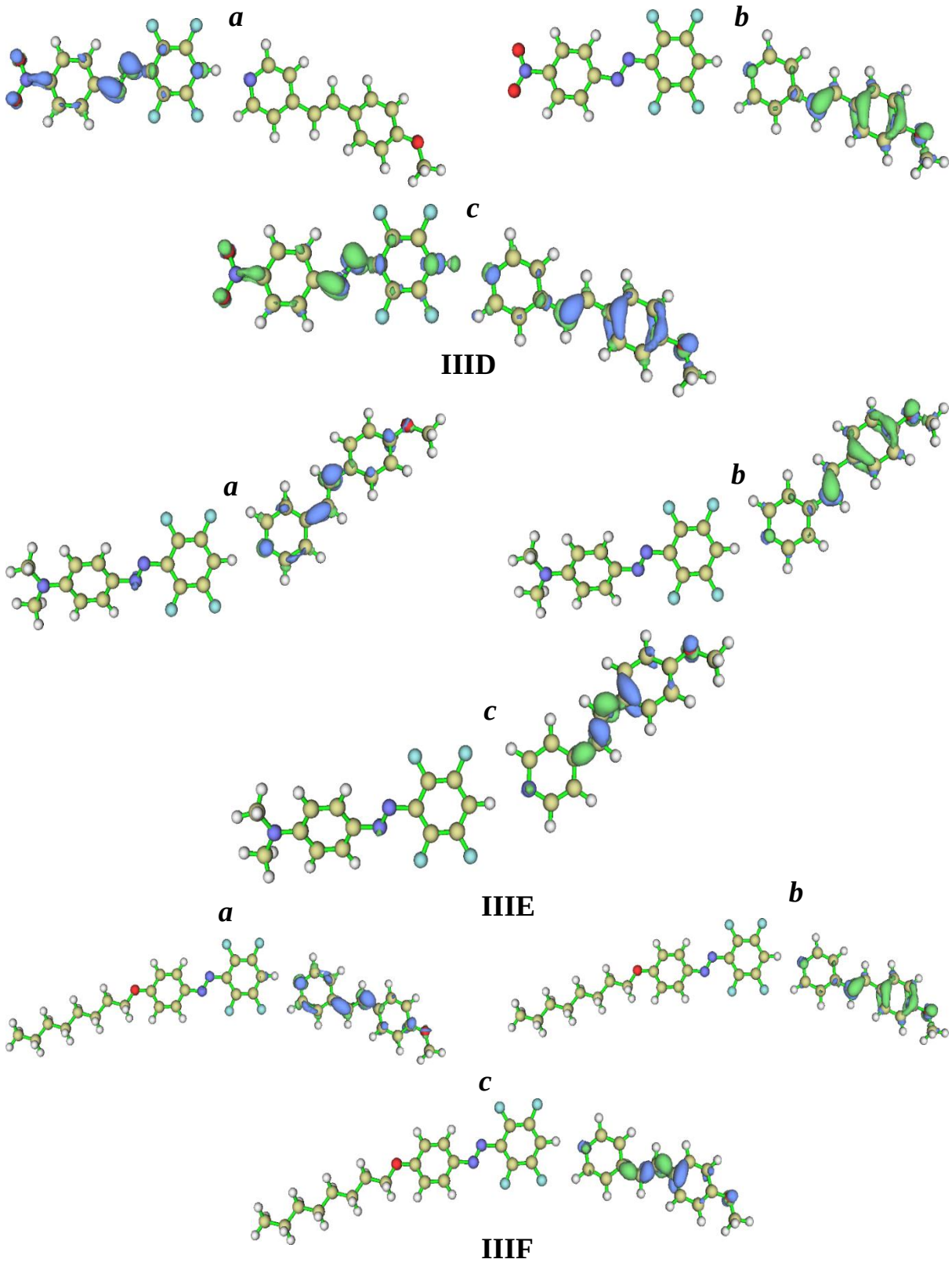
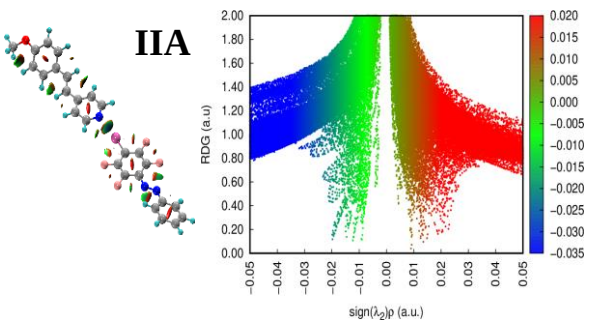
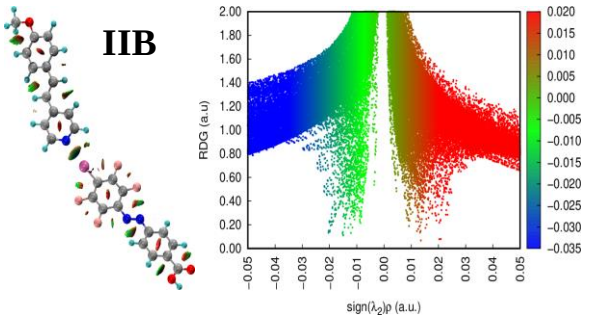
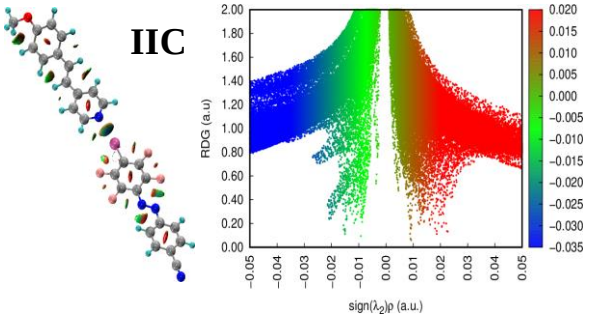
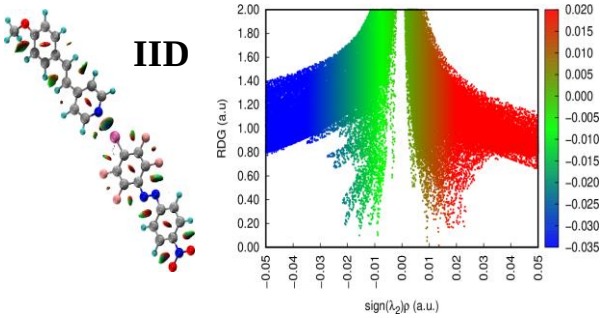


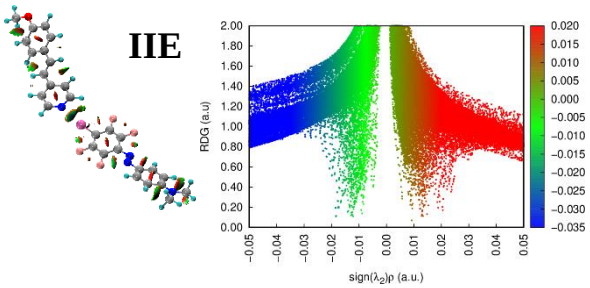
Fig. S5: a) & **b)** f^+ & f^- Fukui functions of **IIA-IIF** and **IIIA-IIIF** complexes, respectively
c) Dual descriptor (Δf) of **IIA-IIF** and **IIIA-IIIF** complexes

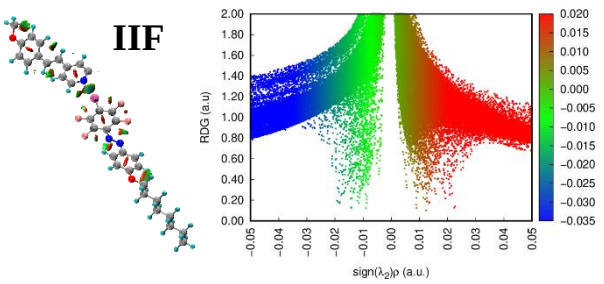

IIA
RDG (a.u)
sign(λ2)ρ (a.u.)


IIB
RDG (a.u)
sign(λ2)ρ (a.u.)


IIC
RDG (a.u)
sign(λ2)ρ (a.u.)


IID
RDG (a.u)
sign(λ2)ρ (a.u.)


IIE
RDG (a.u)
sign(λ2)ρ (a.u.)


IIF
RDG (a.u)
sign(λ2)ρ (a.u.)

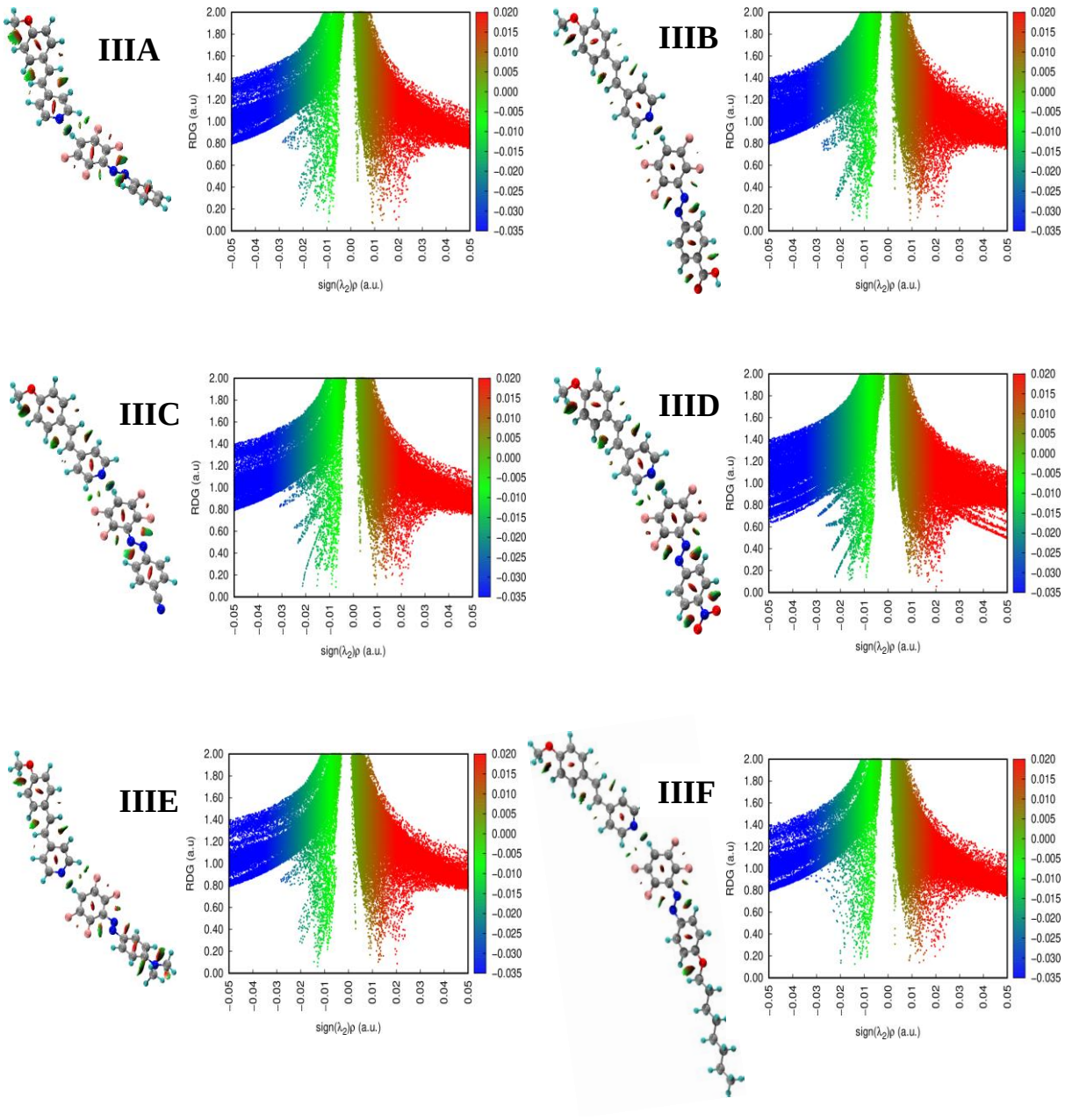


Fig. S6: 3D isosurfaces and 2D-RDG graphs of **IIA-IIF** and **IIIA-IIIF** complexes

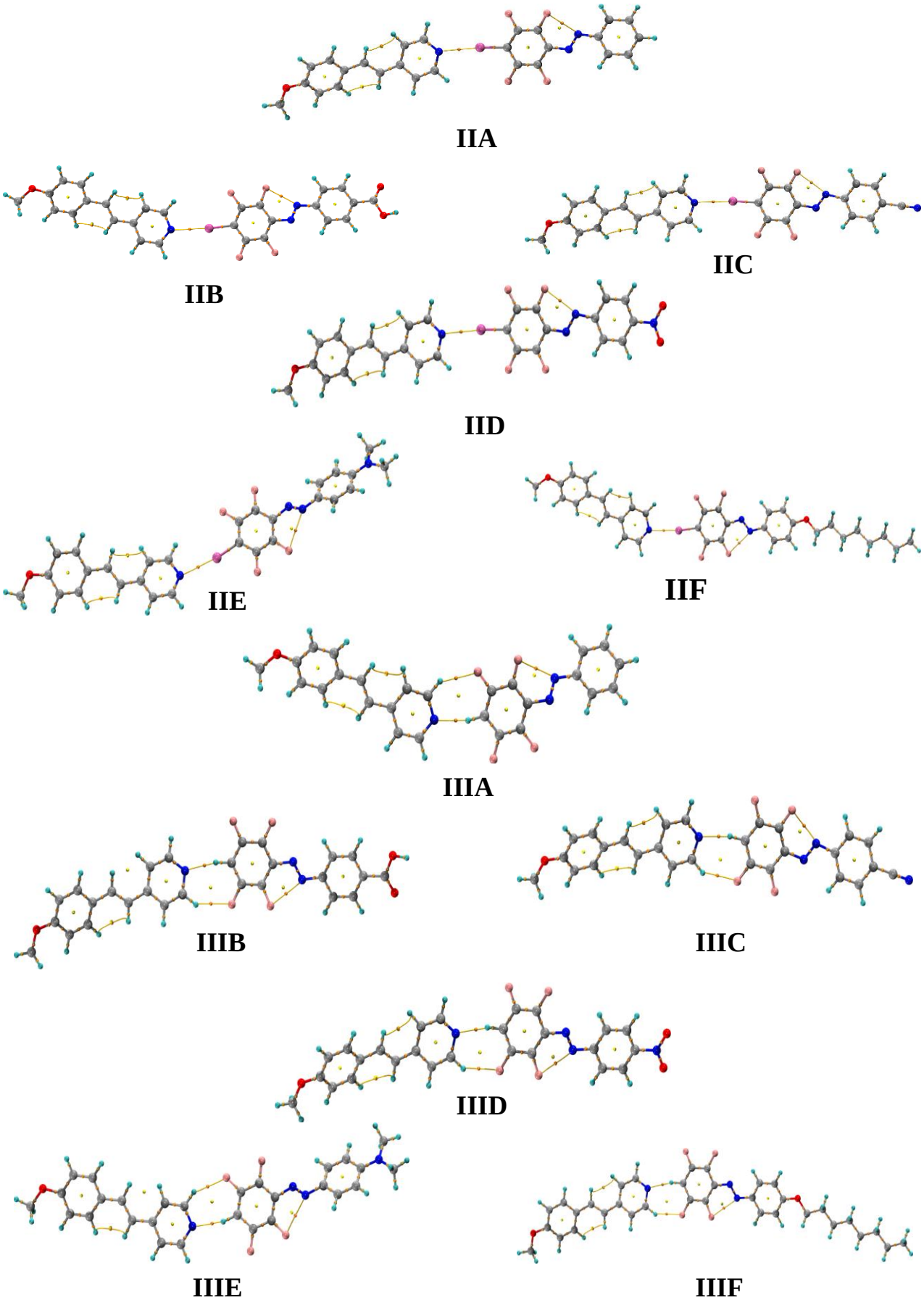


Fig. S7: Topological figures of **IIA-IIF** and **IIIA-IIIF** complexes (orange dots represent BCPs)

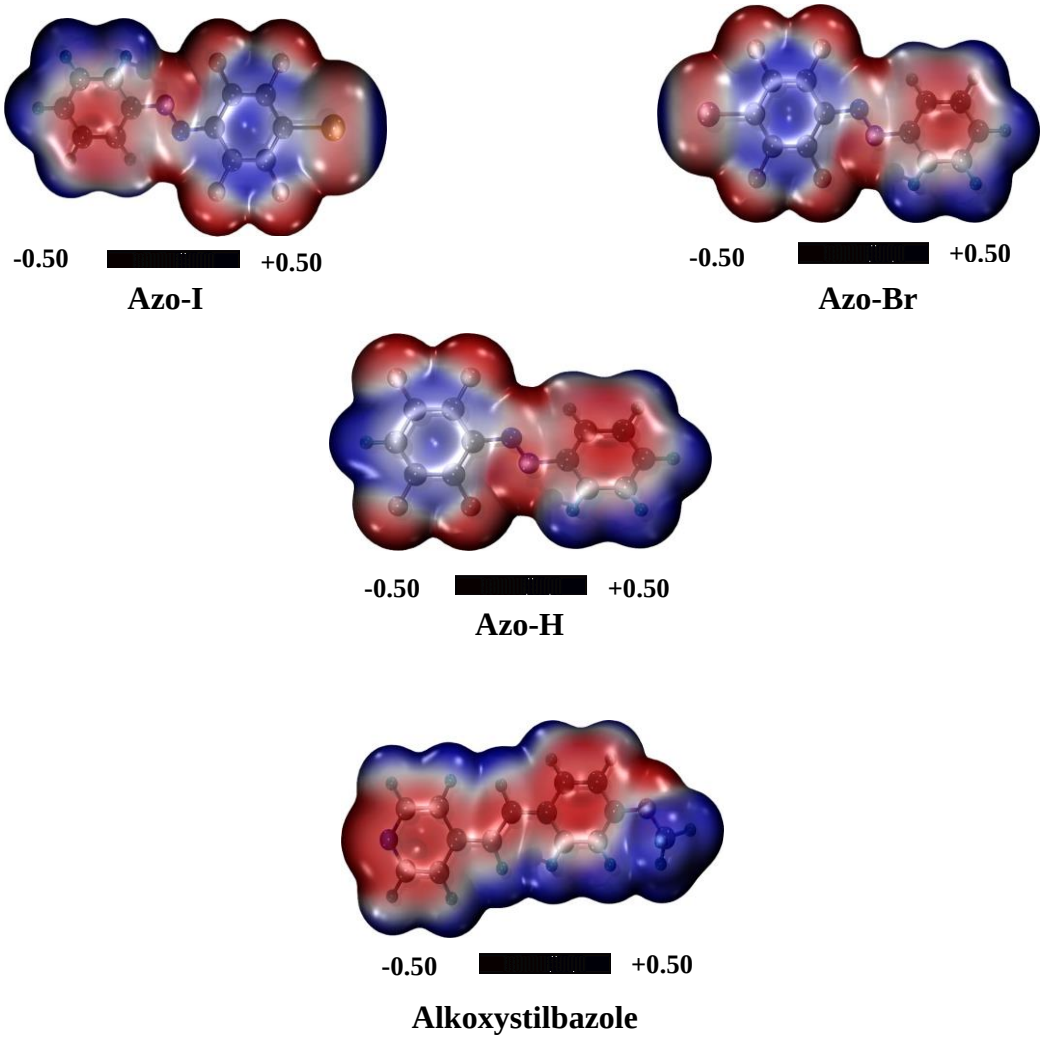
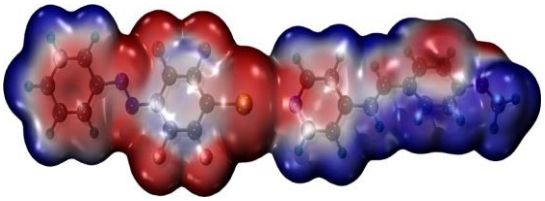
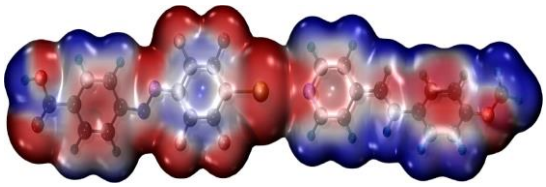


Fig. S8 (a): Molecular electrostatic potential plots for Azo-X (where X=I, Br and H) and alkoxystilbazole molecule



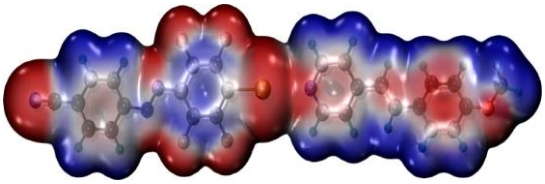
-0.50 +0.50

IA



-0.50 +0.50

IB



-0.50 +0.50

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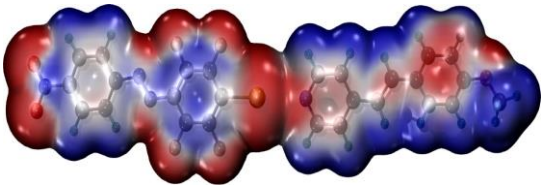

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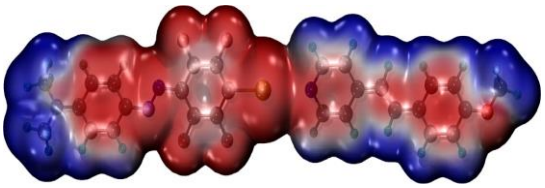
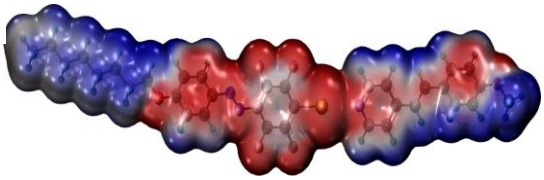
ID



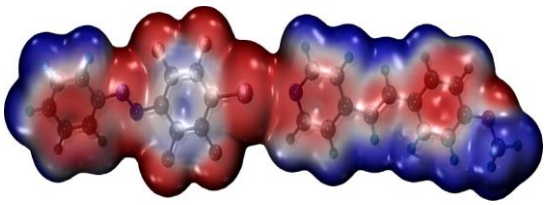
-0.50 +0.50

IE



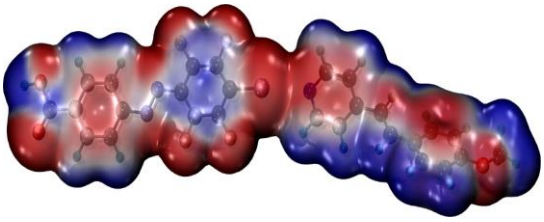
-0.50 +0.50

IF



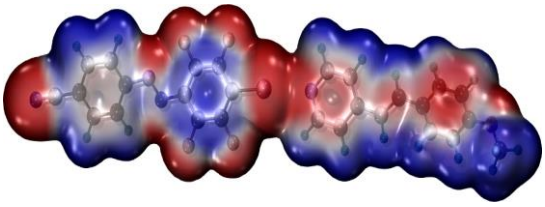
-0.50 +0.50

IIA



-0.50 +0.50

IIB



-0.50 +0.50

IIC

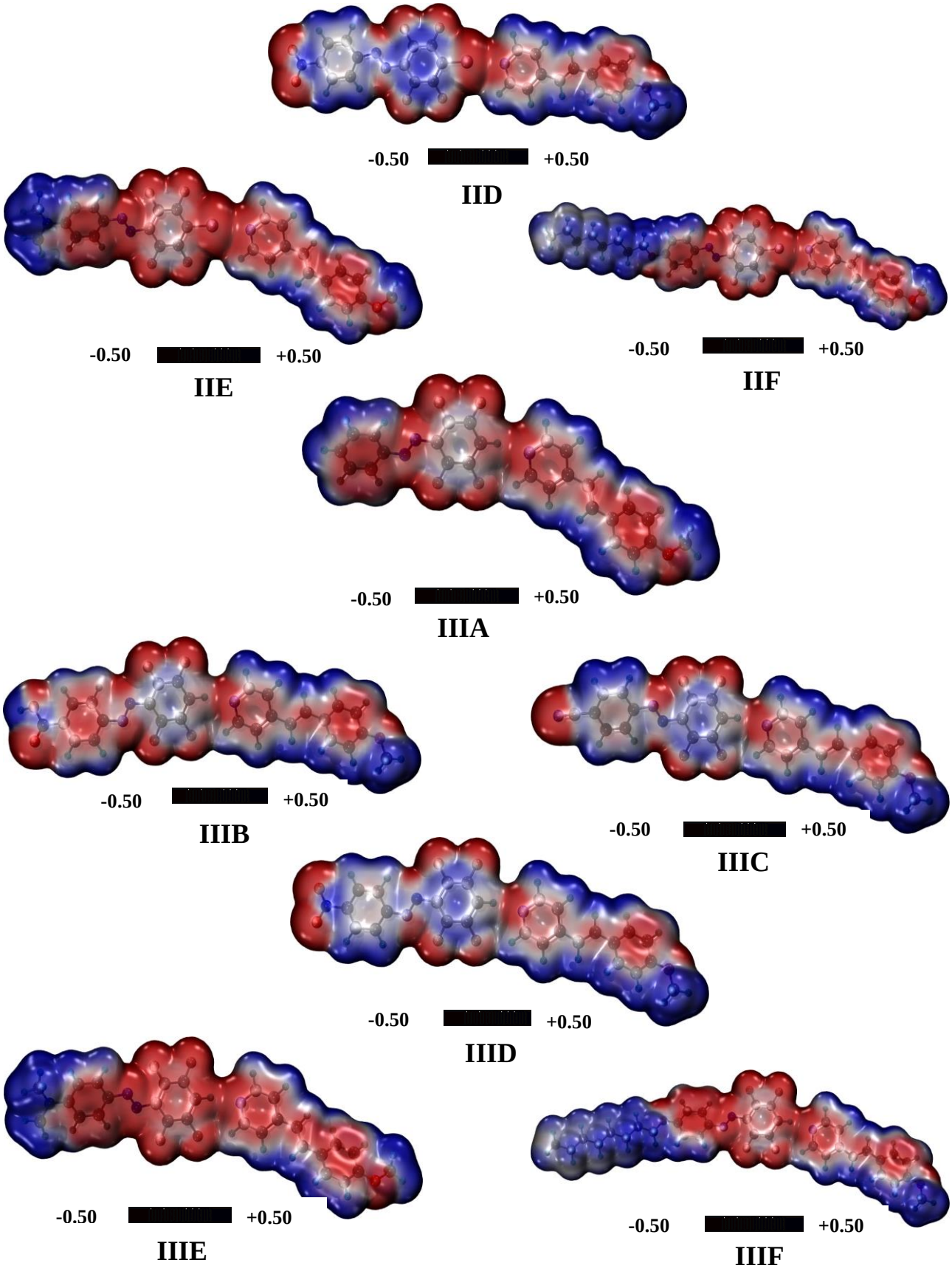


Fig. S8 (b): Molecular electrostatic potential plots for **IA-IF**, **IIA-IIF** and **IIIA-IIIF** complexes

Tables

Table S1: First frequencies v_1 (cm^{-1}), Halogen/Hydrogen bond lengths (Å) and interaction energies (*kcal/mol*) of *cis* Azo-X complexes

Complexes	**v_1**	**X_{I-N}**	**E_{int}**
iA	4.76	2.92	-1.7
iB	3.45	2.91	-1.9
iC	1.86	2.90	-2.3
iD	3.61	2.90	-2.3
iiA	3.51	2.85	-7.1
iiD	3.13	2.83	-7.7
iiiA	4.27	2.17	-7.1
iiiD	2.48	2.15	-7.6

Table S2: Energy decomposition analysis of IB, IC, ID and IID complexes (units of all are in *kcal/mol*)

	IB	**IC**	**ID**	**IID**
Pauli Repulsion	13.41	13.77	13.91	10.86
Steric Interaction	-0.86	-1.07	-1.00	-0.39
Orbital Interactions	-6.71	-6.94	-7.02	-5.36
Bonding Energy	-7.57	-8.01	-8.02	-5.74

Table S3: Energies of frontier molecular orbitals E_{HOMO} (*eV*), E_{LUMO} (*eV*), HOMO-LUMO energy gaps G_{H-L} (*eV*), % G_{HL} and Fermi level E_{FL} (*eV*) of all the complexes

Complex	**E_{HOMO}**	**E_{LUMO}**	**G_{H-L}**	**% G_{HL}**	**E_{FL}**
Azobenzene	-8.54	-0.74	7.80		
IA	-7.89	-0.96	6.93	9.90	-4.43
IB	-7.68	-0.99	6.69	17.75	-4.34
IC	-7.71	-1.21	6.51	15.43	-4.46
ID	-7.72	-1.39	6.33	13.02	-4.56

IE	-7.06	-0.18	6.88	10.61	-3.62
IF	-7.62	-0.36	7.26	5.62	-3.99
IIA	-7.59	-0.64	6.95	9.73	-4.12
IIB	-7.62	-1.04	6.57	19.22	-4.33
IIC	-7.66	-1.27	6.39	17.00	-4.46
IID	-7.66	-1.45	6.22	14.56	-4.56
IIE	-7.10	-0.24	6.86	10.91	-3.67
IIF	-7.56	-0.42	7.14	7.25	-3.99
IIIA	-7.59	-0.51	7.09	7.92	-4.05
IIIB	-7.63	-0.93	6.70	17.86	-4.28
IIIC	-7.66	-1.15	6.51	15.40	-4.41
IIID	-7.67	-1.35	6.32	12.96	-4.51
IIIE	-7.05	-0.09	6.96	9.55	-3.57
IIIF	-7.57	-0.28	7.29	5.28	-3.92

Table S4: Ionization potential I (eV), electron affinity A (eV), hardness μ (eV), chemical potential μ (eV), softness S (eV^{-1}), and electrophilicity ω (eV) of all the complexes

Complex	**I**	**A**	**ŋ**	**μ**	**S**	**ω**
Azobenzene	8.54	0.74	3.9	-4.64	0.13	2.76
IA	7.89	0.96	3.46	-4.43	0.15	2.83
IB	7.68	0.99	3.34	-4.34	0.15	2.82
IC	7.71	1.21	3.25	-4.46	0.15	3.06
ID	7.72	1.39	3.16	-4.56	0.16	3.29
IE	7.06	0.18	3.44	-3.62	0.14	1.90
IF	7.62	0.36	3.63	-3.99	0.14	2.19
IIA	7.59	0.64	3.48	-4.12	0.14	2.44
IIB	7.62	1.04	3.29	-4.33	0.15	2.85
IIC	7.66	1.27	3.20	-4.46	0.15	3.11
IID	7.66	1.45	3.11	-4.56	0.16	3.34
IIE	7.10	0.24	3.43	-3.67	0.15	1.96
IIF	7.56	0.42	3.57	-3.99	0.14	2.23

IIIA	7.59	0.51	3.54	-4.05	0.14	2.31
IIIB	7.63	0.93	3.35	-4.28	0.15	2.73
IIIC	7.66	1.15	3.26	-4.41	0.15	2.99
IIID	7.67	1.35	3.16	-4.51	0.16	3.22
IIIE	7.05	0.09	3.48	-3.57	0.14	1.83
IIIF	7.57	0.28	3.65	-3.92	0.14	2.11

Table S5: Condensed atomic charges($\boldsymbol{q}$), Fukui functions ($\boldsymbol{f^-}$) and dual descriptors ($\Delta\boldsymbol{f}$) of **IA-IF**, **IIA-IIF** and **IIIA-IIIF** complexes

Atoms	**IA**			**IIA**			**IIIA**		
	$\boldsymbol{q}$	$\boldsymbol{f^-}$	$\Delta\boldsymbol{f}$	$\boldsymbol{q}$	$\boldsymbol{f^-}$	$\Delta\boldsymbol{f}$	$\boldsymbol{q}$	$\boldsymbol{f^-}$	$\Delta\boldsymbol{f}$
1 N	-0.058	-0.002	0.003	-0.058	-0.002	0.002	-0.057	-0.002	0.130
2 N	-0.050	0.005	0.007	-0.050	0.005	0.004	-0.050	0.004	0.133
3 C	0.001	0.006	0.004	0.000	0.006	0.002	0.000	0.006	0.007
4 C	0.020	-0.001	0.001	0.019	-0.001	0.000	0.019	-0.002	0.012
5 C	-0.034	0.002	0.001	-0.034	0.002	0.001	-0.035	0.002	0.040
6 C	0.086	0.003	0.002	0.087	0.002	0.002	0.084	0.004	0.032
7 C	0.087	0.002	0.002	0.089	0.003	0.002	0.085	0.001	0.034
8 C	-0.037	0.001	0.001	-0.037	0.001	0.001	-0.038	0.002	0.041
9 C	-0.039	0.003	0.001	-0.039	0.003	0.001	-0.040	0.003	0.029
10 C	0.074	0.001	0.002	0.077	0.000	0.001	0.086	0.000	0.031
11 C	0.074	0.001	0.002	0.078	0.001	0.001	0.084	-0.005	0.033
12 C	-0.042	0.003	0.001	-0.041	0.003	0.001	-0.042	0.003	0.033
13 C	-0.033	0.006	0.002	-0.033	0.006	0.002	-0.034	0.006	0.062
14 C	-0.078	0.003	0.005	-0.034	-0.001	0.002	-0.062	-0.010	0.078
15 H	0.053	0.001	0.000	0.054	0.001	0.001	0.053	0.000	0.024
16 H	0.048	0.000	0.000	0.048	0.000	0.000	0.048	0.001	0.021
17 H	0.050	0.002	0.000	0.050	0.002	0.001	0.050	0.003	0.024
18 H	0.050	0.002	0.000	0.050	0.003	0.001	0.050	0.003	0.025
19 H	0.050	0.003	0.000	0.050	0.003	0.001	0.050	0.004	0.031
20 F	-0.092	0.000	0.001	-0.087	0.001	0.001	-0.092	-0.006	0.035

21	**F**	-0.084	0.004	0.002	-0.083	0.004	0.002	-0.088	0.003	0.024
22	**F**	-0.092	0.000	0.001	-0.088	-0.002	0.001	-0.097	0.000	0.031
23	**F**	-0.085	0.004	0.002	-0.084	0.004	0.002	-0.088	0.005	0.022
24	**I/Br/H**	0.038	-0.018	-0.002	0.001	-0.019	-0.001	0.046	-0.006	0.032
25	**C**	-0.019	0.064	-0.058	-0.019	0.063	-0.054	-0.019	0.064	-0.066
26	**C**	-0.027	0.036	0.055	-0.028	0.038	0.055	-0.028	0.038	-0.030
27	**C**	0.018	-0.002	0.052	0.016	-0.001	0.050	0.016	-0.001	0.008
28	**C**	-0.051	0.095	-0.038	-0.050	0.095	-0.032	-0.051	0.096	-0.100
29	**C**	-0.035	0.047	-0.011	-0.036	0.047	-0.010	-0.036	0.047	-0.045
30	**C**	-0.036	0.041	-0.013	-0.037	0.042	-0.012	-0.037	0.042	-0.040
31	**C**	-0.070	0.045	-0.023	-0.070	0.044	-0.022	-0.071	0.044	-0.041
32	**C**	-0.059	0.051	-0.025	-0.060	0.051	-0.024	-0.060	0.051	-0.048
33	**C**	-0.049	0.031	0.010	-0.051	0.032	0.010	-0.052	0.032	-0.026
34	**C**	0.082	0.066	-0.019	0.081	0.066	-0.018	0.081	0.067	-0.061
35	**C**	0.025	0.024	0.028	0.022	0.025	0.025	0.023	0.026	-0.027
36	**C**	0.025	0.023	0.020	0.023	0.024	0.018	0.022	0.025	-0.034
37	**H**	0.044	0.023	0.009	0.044	0.023	0.009	0.044	0.023	-0.023
38	**H**	0.042	0.027	0.002	0.042	0.027	0.002	0.042	0.027	-0.025
39	**H**	0.046	0.025	-0.009	0.046	0.025	-0.008	0.046	0.025	-0.024
40	**H**	0.048	0.028	-0.011	0.047	0.028	-0.011	0.048	0.028	-0.028
41	**H**	0.043	0.027	-0.009	0.043	0.027	-0.009	0.043	0.027	-0.025
42	**H**	0.052	0.031	-0.010	0.052	0.031	-0.010	0.052	0.031	-0.029
43	**H**	0.051	0.014	0.011	0.050	0.015	0.010	0.049	0.015	-0.009
44	**H**	0.050	0.019	0.013	0.046	0.019	0.011	0.050	0.020	-0.020
45	**H**	0.050	0.018	0.011	0.051	0.019	0.010	0.043	0.018	-0.026
46	**N**	-0.138	0.046	0.025	-0.145	0.050	0.026	-0.140	0.051	-0.070
47	**C**	-0.047	0.026	0.018	-0.049	0.026	0.018	-0.049	0.027	-0.025
48	**O**	-0.136	0.070	-0.044	-0.137	0.069	-0.043	-0.137	0.069	-0.066
49	**H**	0.050	0.011	0.012	0.049	0.011	0.011	0.049	0.012	-0.009
50	**C**	0.006	0.018	-0.008	0.005	0.018	-0.008	0.005	0.018	-0.016
51	**H**	0.040	0.019	-0.009	0.040	0.019	-0.009	0.040	0.019	-0.018
52	**H**	0.052	0.023	-0.007	0.052	0.023	-0.008	0.052	0.023	-0.020

53	**H**	0.040	0.019	-0.009	0.040	0.019	-0.009	0.040	0.019	-0.018

Atoms		**IB**			**IIB**			**IIIB**		
		q	f^-	Δf	q	f^-	Δf	q	f^-	Δf
1	**C**	-0.019	0.065	-0.067	-0.052	-0.002	0.120	-0.051	-0.002	0.123
2	**C**	-0.026	0.036	-0.028	-0.051	0.005	0.113	-0.051	0.005	0.114
3	**C**	0.019	-0.002	0.009	-0.001	0.006	0.003	-0.001	0.005	0.003
4	**C**	-0.051	0.096	-0.100	0.030	-0.002	0.015	0.030	-0.002	0.019
5	**C**	-0.035	0.047	-0.045	-0.032	0.002	0.037	-0.033	0.002	0.038
6	**C**	-0.036	0.041	-0.040	0.090	0.003	0.030	0.087	0.003	0.030
7	**C**	-0.070	0.045	-0.042	0.091	0.002	0.031	0.087	0.001	0.031
8	**C**	-0.059	0.051	-0.049	-0.037	0.001	0.037	-0.037	0.002	0.039
9	**C**	-0.049	0.031	-0.028	-0.029	0.002	0.025	-0.029	0.002	0.026
10	**C**	0.082	0.066	-0.062	0.078	0.001	0.022	0.087	-0.001	0.028
11	**C**	0.025	0.024	-0.027	0.077	0.000	0.021	0.085	-0.004	0.030
12	**C**	0.025	0.023	-0.026	-0.024	0.002	0.031	-0.024	0.002	0.033
13	**H**	0.044	0.023	-0.022	-0.013	0.005	0.049	-0.014	0.005	0.051
14	**H**	0.042	0.027	-0.025	-0.032	-0.001	0.046	-0.059	-0.011	0.073
15	**H**	0.046	0.025	-0.025	0.057	0.000	0.022	0.056	0.000	0.023
16	**H**	0.048	0.028	-0.028	0.050	0.000	0.019	0.050	0.000	0.020
17	**H**	0.043	0.027	-0.025	0.052	0.002	0.019	0.052	0.002	0.020
18	**H**	0.052	0.031	-0.029	0.057	0.002	0.021	0.056	0.002	0.022
19	**H**	0.051	0.014	-0.010	-0.087	-0.002	0.026	-0.091	-0.006	0.032
20	**H**	0.050	0.019	-0.020	-0.081	0.003	0.021	-0.085	0.003	0.021
21	**H**	0.050	0.018	-0.020	-0.086	0.001	0.025	-0.095	0.000	0.029
22	**N**	-0.138	0.046	-0.058	-0.082	0.005	0.020	-0.086	0.005	0.020
23	**C**	-0.047	0.026	-0.022	0.215	0.001	0.025	0.047	-0.006	0.029
24	**O**	-0.136	0.070	-0.067	-0.283	0.004	0.044	0.215	0.001	0.027
25	**H**	0.050	0.011	-0.007	-0.174	0.002	0.019	-0.284	0.005	0.046
26	**C**	0.006	0.018	-0.016	0.192	0.002	0.017	-0.175	0.002	0.020
27	**H**	0.040	0.019	-0.018	0.005	-0.020	0.096	0.192	0.002	0.018
28	**H**	0.053	0.023	-0.021	-0.019	0.064	-0.066	-0.019	0.064	-0.067

29	**H**	0.040	0.019	-0.018	-0.028	0.038	-0.031	-0.028	0.037	-0.029
30	**N**	-0.052	-0.002	0.120	0.017	-0.001	0.008	0.017	-0.001	0.008
31	**N**	-0.051	0.006	0.113	-0.051	0.095	-0.100	-0.050	0.096	-0.101
32	**C**	0.000	0.006	0.002	-0.036	0.047	-0.045	-0.036	0.047	-0.046
33	**C**	0.031	-0.002	0.016	-0.037	0.041	-0.040	-0.037	0.042	-0.040
34	**C**	-0.032	0.002	0.036	-0.070	0.044	-0.042	-0.070	0.045	-0.042
35	**C**	0.088	0.003	0.029	-0.060	0.051	-0.048	-0.060	0.051	-0.048
36	**C**	0.090	0.002	0.030	-0.051	0.032	-0.028	-0.050	0.032	-0.030
37	**C**	-0.037	0.001	0.037	0.082	0.066	-0.062	0.082	0.067	-0.062
38	**C**	-0.029	0.002	0.025	0.024	0.025	-0.026	0.022	0.026	-0.034
39	**C**	0.074	0.001	0.021	0.022	0.024	-0.030	0.022	0.024	-0.026
40	**C**	0.075	0.001	0.019	0.044	0.023	-0.022	0.044	0.023	-0.021
41	**C**	-0.024	0.002	0.031	0.042	0.027	-0.025	0.042	0.027	-0.026
42	**C**	-0.013	0.004	0.049	0.046	0.025	-0.024	0.046	0.025	-0.025
43	**C**	-0.076	0.003	0.037	0.048	0.028	-0.028	0.047	0.028	-0.027
44	**H**	0.057	0.000	0.022	0.043	0.027	-0.025	0.043	0.028	-0.026
45	**H**	0.050	0.000	0.020	0.052	0.031	-0.029	0.052	0.031	-0.029
46	**H**	0.052	0.002	0.020	0.049	0.015	-0.010	0.050	0.015	-0.012
47	**H**	0.056	0.002	0.021	0.051	0.020	-0.020	0.044	0.019	-0.026
48	**F**	-0.091	0.000	0.023	0.046	0.019	-0.023	0.050	0.019	-0.020
49	**F**	-0.082	0.004	0.019	-0.144	0.049	-0.064	-0.140	0.050	-0.069
50	**F**	-0.091	0.000	0.024	-0.048	0.026	-0.024	-0.050	0.026	-0.021
51	**F**	-0.083	0.004	0.019	-0.136	0.069	-0.066	-0.136	0.070	-0.066
52	**C**	0.216	0.001	0.025	0.049	0.011	-0.009	0.049	0.011	-0.007
53	**O**	-0.284	0.004	0.044	0.005	0.018	-0.016	0.005	0.018	-0.016
54	**O**	-0.175	0.001	0.019	0.040	0.019	-0.018	0.040	0.019	-0.018
55	**H**	0.192	0.002	0.017	0.052	0.023	-0.021	0.052	0.023	-0.021
56	**I/Br/H**	0.042	-0.019	0.100	0.040	0.019	-0.018	0.040	0.019	-0.018

Atoms		**IC**			**IIC**			**IIIC**		
		q	f^-	Δf	q	f^-	Δf	q	f^-	Δf
1	**C**	-0.019	0.065	-0.068	-0.019	0.064	-0.066	-0.049	-0.003	0.124

2	**C**	-0.026	0.035	-0.028	-0.028	0.037	-0.029	-0.052	0.006	0.111
3	**C**	0.019	-0.002	0.009	0.017	-0.001	0.008	-0.001	0.005	0.003
4	**C**	-0.051	0.096	-0.100	-0.051	0.096	-0.100	0.033	-0.002	0.020
5	**C**	-0.035	0.047	-0.045	-0.036	0.047	-0.045	-0.028	0.002	0.037
6	**C**	-0.036	0.041	-0.040	-0.037	0.041	-0.040	0.088	0.001	0.033
7	**C**	-0.070	0.045	-0.043	-0.070	0.045	-0.042	0.090	0.003	0.031
8	**C**	-0.059	0.051	-0.049	-0.060	0.051	-0.048	-0.032	0.001	0.040
9	**C**	-0.049	0.031	-0.027	-0.050	0.032	-0.029	-0.020	0.002	0.027
10	**C**	0.083	0.066	-0.062	0.082	0.066	-0.062	0.086	-0.004	0.032
11	**C**	0.025	0.024	-0.027	0.022	0.025	-0.030	0.087	-0.001	0.026
12	**C**	0.025	0.023	-0.026	0.023	0.024	-0.026	-0.021	0.003	0.033
13	**H**	0.044	0.023	-0.022	0.044	0.023	-0.022	0.017	0.005	0.053
14	**H**	0.042	0.027	-0.025	0.042	0.027	-0.026	-0.056	-0.011	0.074
15	**H**	0.046	0.025	-0.025	0.046	0.025	-0.025	0.060	0.001	0.022
16	**H**	0.048	0.028	-0.028	0.047	0.028	-0.027	0.053	0.000	0.021
17	**H**	0.043	0.028	-0.026	0.043	0.027	-0.026	0.062	0.002	0.022
18	**H**	0.052	0.031	-0.029	0.052	0.031	-0.029	0.062	0.003	0.023
19	**H**	0.051	0.014	-0.010	0.050	0.015	-0.011	-0.094	-0.001	0.028
20	**H**	0.050	0.019	-0.020	0.046	0.019	-0.023	-0.083	0.005	0.021
21	**H**	0.050	0.018	-0.020	0.051	0.019	-0.020	-0.090	-0.005	0.033
22	**N**	-0.138	0.046	-0.058	-0.145	0.049	-0.064	-0.085	0.003	0.022
23	**C**	-0.047	0.025	-0.022	-0.049	0.026	-0.022	0.067	0.001	0.023
24	**O**	-0.136	0.070	-0.067	-0.136	0.069	-0.066	-0.211	0.009	0.076
25	**H**	0.050	0.011	-0.007	0.049	0.011	-0.007	0.048	-0.006	0.030
26	**C**	0.006	0.018	-0.017	0.006	0.018	-0.016	-0.019	0.065	-0.067
27	**H**	0.040	0.019	-0.018	0.040	0.019	-0.018	-0.028	0.037	-0.028
28	**H**	0.053	0.023	-0.021	0.052	0.023	-0.021	0.017	-0.001	0.008
29	**H**	0.040	0.019	-0.018	0.040	0.019	-0.018	-0.051	0.096	-0.101
30	**N**	-0.050	-0.002	0.121	-0.050	-0.002	0.120	-0.036	0.047	-0.046
31	**N**	-0.053	0.006	0.111	-0.052	0.006	0.111	-0.037	0.042	-0.040
32	**C**	0.000	0.006	0.001	-0.002	0.006	0.002	-0.070	0.045	-0.042
33	**C**	0.033	-0.002	0.017	0.032	-0.002	0.016	-0.059	0.051	-0.048
34	**C**	-0.028	0.002	0.036	-0.028	0.002	0.036	-0.050	0.032	-0.030

35	**C**	0.090	0.002	0.030	0.091	0.002	0.032	0.082	0.067	-0.062
36	**C**	0.091	0.002	0.031	0.093	0.002	0.032	0.022	0.026	-0.034
37	**C**	-0.031	0.001	0.038	-0.031	0.001	0.038	0.022	0.024	-0.026
38	**C**	-0.020	0.002	0.025	-0.020	0.002	0.025	0.044	0.023	-0.021
39	**C**	0.075	0.001	0.021	0.078	0.000	0.023	0.042	0.027	-0.026
40	**C**	0.075	0.001	0.019	0.079	0.001	0.020	0.046	0.025	-0.025
41	**C**	-0.021	0.002	0.032	-0.021	0.002	0.031	0.047	0.028	-0.027
42	**C**	0.017	0.005	0.051	0.017	0.005	0.051	0.043	0.028	-0.026
43	**C**	-0.075	0.003	0.038	-0.030	-0.001	0.047	0.052	0.032	-0.029
44	**H**	0.060	0.001	0.022	0.060	0.001	0.021	0.050	0.015	-0.012
45	**H**	0.054	0.000	0.020	0.053	0.000	0.020	0.043	0.019	-0.026
46	**H**	0.062	0.002	0.021	0.062	0.002	0.021	0.050	0.019	-0.020
47	**H**	0.063	0.002	0.022	0.063	0.002	0.022	-0.140	0.050	-0.069
48	**F**	-0.090	0.000	0.023	-0.085	0.000	0.024	-0.049	0.026	-0.021
49	**F**	-0.081	0.004	0.020	-0.079	0.004	0.021	-0.136	0.070	-0.066
50	**F**	-0.089	0.000	0.024	-0.086	-0.002	0.027	0.049	0.011	-0.007
51	**F**	-0.082	0.004	0.019	-0.081	0.004	0.021	0.006	0.018	-0.016
52	**C**	0.067	0.001	0.021	0.067	0.001	0.021	0.040	0.019	-0.018
53	**N**	-0.211	0.008	0.073	0.008	-0.020	0.097	0.052	0.023	-0.021
54	**I/Br/H**	0.045	-0.019	0.101	-0.210	0.008	0.073	0.040	0.019	-0.018

Atoms		**ID**			**IID**			**IIID**		
		q	f^-	Δf	q	f^-	Δf	q	f^-	Δf
1	**C**	-0.019	0.065	-0.068	-0.048	-0.002	0.000	-0.047	-0.002	0.116
2	**C**	-0.026	0.035	-0.028	-0.052	0.006	0.003	-0.052	0.006	0.095
3	**C**	0.019	-0.002	0.009	-0.002	0.006	0.002	-0.001	0.005	0.000
4	**C**	-0.051	0.096	-0.100	0.035	-0.002	0.000	0.035	-0.002	0.026
5	**C**	-0.035	0.047	-0.045	-0.027	0.002	0.001	-0.028	0.002	0.036
6	**C**	-0.036	0.041	-0.040	0.092	0.002	0.001	0.089	0.003	0.028
7	**C**	-0.070	0.045	-0.043	0.093	0.002	0.001	0.089	0.001	0.029
8	**C**	-0.059	0.052	-0.049	-0.031	0.001	0.001	-0.031	0.001	0.038
9	**C**	-0.049	0.031	-0.028	-0.027	0.002	0.001	-0.028	0.002	0.027

10	**C**	0.083	0.066	-0.062	0.078	0.000	0.001	0.088	-0.001	0.026
11	**C**	0.025	0.024	-0.027	0.079	0.001	0.001	0.086	-0.004	0.028
12	**C**	0.025	0.023	-0.026	-0.028	0.002	0.001	-0.028	0.002	0.036
13	**H**	0.044	0.023	-0.022	0.028	0.004	0.001	0.028	0.005	0.044
14	**H**	0.042	0.027	-0.025	-0.030	-0.001	0.002	-0.056	-0.011	0.069
15	**H**	0.046	0.025	-0.025	0.061	0.001	0.000	0.061	0.000	0.023
16	**H**	0.048	0.028	-0.028	0.054	0.000	0.000	0.054	0.000	0.021
17	**H**	0.043	0.028	-0.026	0.060	0.002	0.001	0.060	0.002	0.020
18	**H**	0.052	0.031	-0.029	0.061	0.002	0.001	0.060	0.002	0.022
19	**H**	0.051	0.014	-0.010	-0.085	0.000	0.001	-0.090	-0.006	0.030
20	**H**	0.050	0.019	-0.020	-0.079	0.004	0.002	-0.084	0.003	0.020
21	**H**	0.050	0.018	-0.020	-0.086	-0.002	0.001	-0.093	0.000	0.027
22	**N**	-0.138	0.046	-0.057	-0.080	0.004	0.002	-0.084	0.005	0.018
23	**C**	-0.047	0.025	-0.022	0.009	-0.020	-0.002	0.048	-0.006	0.028
24	**O**	-0.136	0.070	-0.067	0.257	0.001	0.001	0.257	0.001	0.029
25	**H**	0.050	0.011	-0.007	-0.204	0.005	0.002	-0.203	0.005	0.064
26	**C**	0.006	0.018	-0.017	-0.203	0.004	0.002	-0.204	0.005	0.064
27	**H**	0.040	0.019	-0.018	-0.019	0.064	-0.056	-0.019	0.065	-0.067
28	**H**	0.053	0.023	-0.021	-0.028	0.037	0.058	-0.027	0.036	-0.028
29	**H**	0.040	0.019	-0.018	0.017	-0.001	0.053	0.017	-0.001	0.008
30	**N**	-0.048	-0.002	0.114	-0.051	0.095	-0.034	-0.051	0.096	-0.101
31	**N**	-0.053	0.006	0.097	-0.036	0.047	-0.010	-0.035	0.047	-0.046
32	**C**	-0.001	0.006	-0.001	-0.037	0.041	-0.013	-0.037	0.042	-0.040
33	**C**	0.036	-0.002	0.022	-0.070	0.045	-0.023	-0.070	0.045	-0.043
34	**C**	-0.027	0.002	0.035	-0.059	0.051	-0.025	-0.059	0.052	-0.048
35	**C**	0.091	0.002	0.028	-0.050	0.032	0.011	-0.050	0.032	-0.030
36	**C**	0.092	0.002	0.029	0.082	0.066	-0.019	0.082	0.067	-0.062
37	**C**	-0.031	0.001	0.036	0.022	0.025	0.027	0.022	0.026	-0.033
38	**C**	-0.028	0.002	0.026	0.023	0.024	0.020	0.022	0.024	-0.026
39	**C**	0.075	0.001	0.020	0.044	0.023	0.009	0.044	0.023	-0.021
40	**C**	0.075	0.001	0.018	0.042	0.027	0.002	0.042	0.027	-0.026
41	**C**	-0.028	0.002	0.034	0.046	0.025	-0.009	0.046	0.025	-0.025
42	**C**	0.028	0.004	0.043	0.047	0.028	-0.011	0.047	0.028	-0.027

43	**C**	-0.074	0.003	0.035	0.043	0.027	-0.010	0.043	0.028	-0.026
44	**H**	0.061	0.001	0.022	0.052	0.031	-0.010	0.052	0.032	-0.029
45	**H**	0.054	0.000	0.020	0.050	0.015	0.011	0.050	0.015	-0.012
46	**H**	0.060	0.002	0.019	0.046	0.019	0.012	0.044	0.019	-0.025
47	**H**	0.060	0.002	0.021	0.051	0.019	0.011	0.050	0.019	-0.020
48	**F**	-0.089	0.000	0.022	-0.145	0.049	0.028	-0.140	0.050	-0.067
49	**F**	-0.080	0.004	0.019	-0.049	0.026	0.019	-0.049	0.026	-0.021
50	**F**	-0.089	0.000	0.022	-0.136	0.070	-0.044	-0.136	0.070	-0.067
51	**F**	-0.081	0.004	0.018	0.049	0.011	0.012	0.049	0.011	-0.007
52	**I/Br/H**	0.047	-0.019	0.097	0.006	0.018	-0.008	0.006	0.018	-0.016
53	**N**	0.257	0.001	0.026	0.040	0.019	-0.010	0.040	0.019	-0.018
54	**O**	-0.203	0.004	0.059	0.052	0.023	-0.008	0.052	0.023	-0.021
55	**O**	-0.204	0.004	0.059	0.040	0.019	-0.010	0.040	0.019	-0.018

Atoms		**IE**			**IIE**			**IIIE**		
		q	f^-	Δf	q	f^-	Δf	q	f^-	Δf
1	**N**	-0.077	0.056	-0.031	-0.054	0.001	0.132	-0.054	0.004	0.017
2	**N**	-0.055	0.001	0.037	-0.077	0.056	0.055	-0.076	-0.005	0.012
3	**C**	0.002	0.003	0.008	-0.003	0.083	-0.083	-0.003	-0.001	0.000
4	**C**	-0.002	0.082	-0.083	0.001	0.003	0.012	0.001	0.006	0.004
5	**C**	-0.033	0.031	-0.019	-0.035	0.028	0.012	-0.035	0.001	0.005
6	**C**	0.082	0.018	-0.007	0.085	0.016	0.017	0.082	0.003	0.005
7	**C**	0.083	0.015	-0.005	-0.032	0.031	0.008	-0.033	0.002	0.005
8	**C**	-0.035	0.029	-0.017	0.083	0.018	0.015	0.080	0.001	0.005
9	**C**	-0.070	0.054	-0.046	-0.070	0.055	-0.031	-0.070	0.002	0.003
10	**C**	0.072	0.012	-0.003	0.076	0.012	0.011	0.084	-0.001	0.004
11	**C**	0.073	0.011	-0.004	-0.076	0.061	-0.039	-0.076	0.002	0.003
12	**C**	-0.076	0.061	-0.053	0.075	0.012	0.013	0.082	-0.005	0.004
13	**C**	0.057	0.029	-0.013	0.057	0.029	0.019	0.056	0.004	0.006
14	**C**	-0.082	0.023	-0.008	-0.038	0.026	0.021	-0.068	-0.011	0.006
15	**H**	0.053	0.026	-0.020	0.048	0.023	-0.003	0.048	0.000	0.002
16	**H**	0.048	0.023	-0.017	0.053	0.026	-0.005	0.053	0.001	0.003

17	**H**	0.039	0.026	-0.020	0.040	0.026	-0.007	0.039	0.002	0.002
18	**H**	0.039	0.028	-0.021	0.039	0.028	-0.009	0.039	0.002	0.002
19	**F**	-0.094	0.015	-0.008	-0.087	0.012	0.012	-0.091	0.005	0.004
20	**F**	-0.088	0.011	-0.002	-0.089	0.015	0.010	-0.100	0.000	0.004
21	**F**	-0.094	0.015	-0.008	-0.088	0.014	0.012	-0.092	0.003	0.004
22	**F**	-0.089	0.013	-0.003	-0.091	0.016	0.011	-0.095	-0.006	0.003
23	**I/Br/H**	0.031	0.062	-0.059	-0.002	0.056	0.022	-0.054	0.004	0.003
24	**N**	-0.053	0.110	-0.101	-0.053	0.112	-0.087	-0.031	0.001	0.001
25	**C**	-0.031	0.023	-0.020	-0.031	0.024	-0.014	0.037	0.001	0.002
26	**H**	0.037	0.031	-0.027	0.038	0.032	-0.019	0.045	0.002	0.002
27	**H**	0.045	0.025	-0.019	0.045	0.025	-0.009	0.037	0.001	0.002
28	**H**	0.037	0.032	-0.027	0.037	0.032	-0.020	-0.031	0.001	0.001
29	**C**	-0.031	0.023	-0.020	-0.031	0.023	-0.013	0.037	0.002	0.002
30	**H**	0.037	0.032	-0.027	0.037	0.032	-0.019	0.045	0.002	0.002
31	**H**	0.045	0.025	-0.019	0.045	0.025	-0.010	0.037	0.001	0.002
32	**H**	0.037	0.031	-0.027	0.037	0.032	-0.019	0.045	-0.007	0.004
33	**C**	-0.019	-0.002	0.007	-0.019	-0.002	-0.001	-0.019	0.063	-0.054
34	**C**	-0.027	0.005	0.067	-0.029	0.005	0.002	-0.029	0.039	0.046
35	**C**	0.018	0.005	0.036	0.016	0.005	0.002	0.016	0.000	0.045
36	**C**	-0.050	-0.003	0.047	-0.050	-0.003	-0.001	-0.050	0.095	-0.039
37	**C**	-0.035	0.001	0.027	-0.036	0.001	0.000	-0.036	0.047	-0.013
38	**C**	-0.037	0.001	0.021	-0.037	0.001	0.000	-0.037	0.042	-0.015
39	**C**	-0.070	0.002	0.015	-0.071	0.002	0.001	-0.071	0.044	-0.024
40	**C**	-0.060	0.002	0.018	-0.060	0.002	0.001	-0.060	0.050	-0.026
41	**C**	-0.050	0.003	0.030	-0.052	0.003	0.001	-0.052	0.032	0.005
42	**C**	0.082	0.004	0.033	0.081	0.004	0.001	0.081	0.066	-0.022
43	**C**	0.025	-0.002	0.041	0.023	-0.001	0.000	0.022	0.026	0.020
44	**C**	0.025	-0.002	0.034	0.021	-0.005	-0.002	0.023	0.025	0.013
45	**H**	0.044	0.001	0.023	0.044	0.000	0.000	0.044	0.023	0.005
46	**H**	0.042	0.001	0.021	0.041	0.001	0.000	0.041	0.027	-0.001
47	**H**	0.046	0.000	0.012	0.046	0.000	0.000	0.046	0.025	-0.010
48	**H**	0.048	0.000	0.013	0.047	0.000	0.000	0.048	0.028	-0.012
49	**H**	0.043	0.002	0.012	0.042	0.002	0.000	0.042	0.027	-0.011

50	**H**	0.052	0.002	0.015	0.052	0.002	0.001	0.052	0.031	-0.011
51	**H**	0.050	0.003	0.017	0.049	0.004	0.001	0.049	0.015	0.008
52	**H**	0.050	-0.001	0.024	0.051	0.000	0.000	0.050	0.020	0.009
53	**H**	0.050	-0.001	0.023	0.044	-0.004	-0.001	0.043	0.018	0.006
54	**N**	-0.138	-0.008	0.062	-0.146	-0.010	-0.005	-0.140	0.052	0.018
55	**C**	-0.048	0.002	0.032	-0.049	0.001	0.001	-0.049	0.027	0.013
56	**O**	-0.136	0.003	0.017	-0.137	0.003	0.001	-0.137	0.068	-0.045
57	**H**	0.050	0.003	0.015	0.049	0.002	0.001	0.049	0.012	0.009
58	**C**	0.006	0.001	0.007	0.005	0.001	0.000	0.005	0.018	-0.008
59	**H**	0.040	0.001	0.006	0.040	0.001	0.000	0.040	0.019	-0.010
60	**H**	0.052	0.002	0.010	0.052	0.002	0.001	0.052	0.023	-0.009
61	**H**	0.040	0.001	0.007	0.040	0.001	0.000	0.040	0.019	-0.010

Atoms		**IF**			**IIF**			**IIIF**		
		q	f^-	Δf	q	f^-	Δf	q	f^-	Δf
1	**N**	-0.068	-0.003	0.014	-0.068	-0.003	0.121	-0.019	0.063	-0.055
2	**N**	-0.052	0.004	0.018	-0.052	0.004	0.131	-0.029	0.039	0.053
3	**C**	0.001	0.006	0.003	0.000	0.006	0.008	0.016	0.000	0.046
4	**C**	0.005	-0.001	0.000	0.005	-0.001	0.005	-0.050	0.095	-0.034
5	**C**	-0.030	0.002	0.006	-0.030	0.002	0.040	-0.036	0.047	-0.009
6	**C**	0.084	0.003	0.005	0.085	0.002	0.032	-0.037	0.042	-0.012
7	**C**	0.085	0.002	0.005	0.086	0.003	0.031	-0.071	0.044	-0.021
8	**C**	-0.033	0.001	0.005	-0.033	0.001	0.036	-0.060	0.051	-0.023
9	**C**	-0.056	0.003	0.004	-0.056	0.002	0.025	-0.051	0.033	0.009
10	**C**	0.073	0.001	0.004	0.076	0.000	0.026	0.081	0.066	-0.017
11	**C**	0.073	0.001	0.004	0.077	0.001	0.022	0.023	0.026	0.027
12	**C**	-0.072	0.002	0.003	-0.072	0.002	0.023	0.022	0.025	0.019
13	**C**	0.089	0.004	0.007	0.089	0.004	0.049	0.043	0.023	0.010
14	**C**	-0.080	0.003	0.008	-0.036	-0.001	0.049	0.042	0.027	0.004
15	**H**	0.054	0.001	0.003	0.055	0.001	0.021	0.046	0.025	-0.007
16	**H**	0.050	0.000	0.002	0.050	0.000	0.019	0.047	0.028	-0.009
17	**H**	0.052	0.002	0.003	0.053	0.002	0.021	0.043	0.027	-0.008

18	**H**	0.044	0.002	0.003	0.044	0.002	0.019	0.052	0.031	-0.008
19	**F**	-0.093	0.000	0.004	-0.088	0.001	0.025	0.050	0.015	0.012
20	**F**	-0.086	0.004	0.004	-0.085	0.004	0.020	0.044	0.019	0.013
21	**F**	-0.093	0.000	0.004	-0.090	-0.003	0.030	0.050	0.020	0.012
22	**F**	-0.087	0.004	0.004	-0.086	0.003	0.023	-0.140	0.051	0.030
23	**O**	-0.128	0.003	0.004	-0.128	0.003	0.024	-0.050	0.026	0.017
24	**C**	0.035	0.000	0.001	0.035	0.000	0.005	-0.137	0.069	-0.043
25	**H**	0.034	0.001	0.001	0.034	0.001	0.007	0.048	0.012	0.012
26	**H**	0.034	0.001	0.001	0.034	0.001	0.007	0.005	0.018	-0.007
27	**C**	-0.053	0.000	0.000	-0.053	0.000	0.002	0.040	0.019	-0.009
28	**H**	0.036	0.000	0.001	0.036	0.000	0.004	0.052	0.023	-0.007
29	**H**	0.036	0.001	0.001	0.036	0.000	0.004	0.040	0.019	-0.009
30	**C**	-0.050	0.000	0.000	-0.049	0.000	0.001	-0.067	-0.003	0.004
31	**H**	0.028	0.000	0.000	0.028	0.000	0.002	-0.053	0.004	0.007
32	**H**	0.028	0.000	0.000	0.028	0.000	0.002	0.000	0.006	0.004
33	**C**	-0.050	0.000	0.000	-0.050	0.000	0.001	0.005	-0.002	0.001
34	**H**	0.029	0.000	0.000	0.029	0.000	0.002	-0.031	0.002	0.001
35	**H**	0.029	0.000	0.000	0.029	0.000	0.002	0.082	0.003	0.002
36	**C**	-0.052	0.000	0.000	-0.052	0.000	0.001	0.083	0.001	0.002
37	**H**	0.027	0.000	0.000	0.027	0.000	0.001	-0.033	0.001	0.001
38	**H**	0.027	0.000	0.000	0.027	0.000	0.001	-0.057	0.003	0.000
39	**C**	-0.052	0.000	0.000	-0.052	0.000	0.001	0.085	-0.001	0.000
40	**H**	0.027	0.000	0.000	0.027	0.000	0.001	0.083	-0.004	-0.002
41	**H**	0.027	0.000	0.000	0.027	0.000	0.001	-0.073	0.002	0.000
42	**C**	-0.051	0.000	0.000	-0.051	0.000	0.001	0.088	0.005	0.001
43	**H**	0.027	0.000	0.000	0.027	0.000	0.001	-0.065	-0.011	-0.004
44	**H**	0.027	0.000	0.000	0.027	0.000	0.001	0.054	0.000	-0.001
45	**C**	-0.092	0.000	0.000	-0.092	0.000	0.001	0.050	0.000	-0.001
46	**H**	0.030	0.000	0.000	0.030	0.000	0.001	0.052	0.003	0.000
47	**H**	0.032	0.001	0.000	0.032	0.001	0.002	0.043	0.002	0.000
48	**H**	0.030	0.000	0.000	0.030	0.000	0.001	-0.094	-0.006	-0.003
49	**I/Br/H**	0.034	-0.018	0.009	0.000	-0.019	0.099	-0.090	0.003	0.001

50	**C**	-0.019	0.064	-0.057	-0.019	0.063	-0.065	-0.098	0.000	-0.001
51	**C**	-0.027	0.037	0.047	-0.029	0.039	-0.032	-0.090	0.005	0.001
52	**C**	0.018	-0.002	0.048	0.016	-0.001	0.007	0.046	-0.007	0.000
53	**C**	-0.051	0.095	-0.043	-0.050	0.095	-0.099	-0.128	0.003	0.000
54	**C**	-0.035	0.047	-0.014	-0.036	0.047	-0.045	0.035	0.000	0.000
55	**C**	-0.036	0.041	-0.016	-0.037	0.042	-0.040	0.034	0.001	0.000
56	**C**	-0.070	0.044	-0.025	-0.071	0.044	-0.041	0.034	0.001	0.000
57	**C**	-0.059	0.051	-0.028	-0.060	0.050	-0.048	-0.053	0.000	0.000
58	**C**	-0.050	0.031	0.006	-0.052	0.032	-0.027	0.036	0.001	0.000
59	**C**	0.082	0.066	-0.024	0.081	0.066	-0.061	0.036	0.001	0.000
60	**C**	0.025	0.024	0.021	0.023	0.025	-0.026	-0.049	0.000	0.000
61	**C**	0.025	0.023	0.015	0.021	0.024	-0.030	0.028	0.000	0.000
62	**H**	0.044	0.023	0.005	0.044	0.023	-0.023	0.028	0.000	0.000
63	**H**	0.042	0.027	-0.001	0.042	0.027	-0.025	-0.050	0.000	0.000
64	**H**	0.046	0.025	-0.011	0.046	0.025	-0.024	0.029	0.000	0.000
65	**H**	0.048	0.028	-0.013	0.048	0.028	-0.028	0.029	0.000	0.000
66	**H**	0.043	0.027	-0.012	0.042	0.027	-0.025	-0.052	0.000	0.000
67	**H**	0.052	0.031	-0.012	0.052	0.031	-0.029	0.027	0.000	0.000
68	**H**	0.050	0.015	0.008	0.049	0.015	-0.010	0.027	0.000	0.000
69	**H**	0.050	0.019	0.008	0.051	0.020	-0.020	-0.052	0.000	0.000
70	**H**	0.050	0.018	0.007	0.045	0.019	-0.024	0.027	0.000	0.000
71	**N**	-0.138	0.047	0.017	-0.146	0.050	-0.065	0.027	0.000	0.000
72	**C**	-0.048	0.026	0.014	-0.049	0.027	-0.024	-0.051	0.000	0.000
73	**O**	-0.136	0.069	-0.046	-0.137	0.068	-0.065	0.027	0.000	0.000
74	**H**	0.050	0.011	0.010	0.049	0.012	-0.009	0.027	0.000	0.000
75	**C**	0.006	0.018	-0.009	0.005	0.017	-0.016	-0.092	0.000	0.000
76	**H**	0.040	0.019	-0.011	0.040	0.019	-0.018	0.030	0.000	0.000
77	**H**	0.052	0.023	-0.009	0.052	0.023	-0.021	0.032	0.001	0.000
78	**H**	0.040	0.019	-0.011	0.040	0.019	-0.018	0.030	0.000	0.000

Table S6: NBO charges Q (|*e*|), Donor (i)-acceptor (j) NBO transitions, stabilization energies $E^{(2)}$, E(j)-E(i) energy differences and their Fock matrix element F (i,j)

Complex	Q	Donor NBO (i)	Acceptor NBO (j)	$E^{(2)}$ *kcal/mol*	E(j)-E(i) *(au)*	F (i,j) *(au)*
IA	0.043	CR (1) C_{50}	BD* (2)C_7-C_{11}	163.01	10.24	1.292
		BD* (2)C_7-C_{11}	RY* (6)H_{53}	138.47	0.06	0.181
IB	0.046	LP (1) N_{22}	BD* (1)C_{43}-I_{56}	12.05	0.58	0.076
		BD (1)C_{43}-I_{56}	RY* (1)N_{22}	0.29	1.69	0.020
IC	0.048	LP (1)N_{22}	BD*(1)C_{43}-I_{54}	12.41	0.58	0.077
		BD (1)C_{43}-I_{54}	RY*(1)N_{22}	0.29	1.69	0.020
ID	0.047	LP (1)N_{22}	BD*(1)C_{43}-I_{52}	12.54	0.58	0.077
		BD (1)C_{43}-I_{52}	RY*(1)N_{22}	0.29	1.69	0.020
IE	0.065	LP (1)N_{54}	BD*(1)C_{14}-I_{23}	10.95	0.59	0.072
		BD (1)C_{14}-I_{23}	RY*(1)N_{54}	0.29	1.68	0.020
IF	0.066	LP (1)N_{71}	BD*(1)C_{14}-I_{49}	11.28	0.59	0.073
		BD (1)C_{14}-I_{49}	RY*(1)N_{71}	0.29	1.68	0.020
IIA	0.028	LP (1) N_{46}	BD* (1)C_{14}-Br_{24}	7.12	0.61	0.060
		BD (1)C_{14}-Br_{24}	RY* (1) N_{46}	1.13	1.85	0.041
IIB	0.030	LP (1)N_{49}	BD*(1)C_{14}-Br_{27}	7.54	0.61	0.061
		BD (1)C_{14}-Br_{27}	RY*(1)N_{49}	1.17	1.86	0.042
IIC	0.033	LP (1)N_{22}	BD*(1)C_{43}-Br_{53}	7.72	0.61	0.062
		BD (1)C_{43}-Br_{53}	RY*(1)N_{22}	1.19	1.86	0.042
IID	0.033	LP (1)N_{48}	BD*(1)C_{14}-Br_{23}	7.81	0.61	0.062
		BD (1)C_{14}-Br_{23}	RY*(1)N_{48}	1.20	1.87	0.042
IIE	0.021	LP (1)N_{54}	BD*(1)C_{14}-Br_{23}	6.20	0.62	0.056
		BD (1)C_{14}-Br_{23}	RY*(1)N_{54}	1.03	1.84	0.039
IIF	0.025	LP (1)N_{71}	BD*(1)C_{14}-Br_{49}	6.56	0.62	0.057
		BD (1)C_{14}-Br_{49}	RY*(1)N_{71}	1.07	1.84	0.040
IIIA	0.017	LP (1) N_{46}	BD* (1)C_{14}-H_{24}	10.38	1.01	0.093
		LP (2) F_{20}	BD* (1)C_{36}-H_{45}	1.15	1.09	0.032
IIIB	0.018	LP (1)N_{49}	BD*(1)C_{14}-H_{23}	10.87	1.01	0.095
		LP (2)F_{19}	BD*(1)C_{38}-H_{47}	1.05	1.09	0.030
IIIC	0.021	LP (1)N_{47}	BD*(1)C_{14}-H_{25}	11.09	1.01	0.096
		LP (2)F_{21}	BD*(1)C_{36}-H_{45}	1.07	1.09	0.031

IIID	0.020	LP (1)N_{48}	BD*(1)C_{14}-H_{23}	11.33	1.01	0.097
		LP (2)F_{19}	BD*(1)C_{37}-H_{46}	0.99	1.09	0.029
IIIE	0.012	LP (1)N_{54}	BD*(1)C_{14}-H_{32}	9.69	1.02	0.090
		LP (2)F_{22}	BD*(1)C_{44}-H_{53}	1.26	1.09	0.033
IIIF	0.005	LP (1)N_{22}	BD*(1)C_{43}-H_{52}	10.03	1.02	0.091
		LP (2)F_{48}	BD*(1)C_{11}-H_{20}	1.22	1.09	0.033

BD for bonding orbitals, BD* label for anti-bonding orbitals, CR for core electrons, LP for valence lone pair orbitals and RY for Rydberg state

Table S7: Electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), Lagrangian kinetic energy *G(r)*, Potential energy density *V(r)*, electron energy density *H(r)* and the ratio of the kinetic to potential electron density *G(r)/V(r)* (all are in *au*)

Complexes	**Interaction**	***ρ***	***∇²ρ***	***G(r)***	***V(r)***	***H(r)***	***-G(r)/V(r)***
IA	I-N	0.210	0.652	0.144	-0.132	0.124	1.09
IB	I-N	0.217	0.669	0.153	-0.146	0.755	1.05
IC	I-N	0.220	0.679	0.156	-0.148	0.729	1.05
ID	I-N	0.222	0.682	0.157	-0.149	0.720	1.05
IE	I-N	0.206	0.638	0.146	-0.137	0.826	1.07
IF	I-N	0.209	0.647	0.148	-0.140	0.807	1.06
IIA	Br-N	0.198	0.627	0.140	-0.123	0.1657	1.14
IIB	Br-N	0.203	0.644	0.144	-0.127	0.166	1.13
IIC	Br-N	0.206	0.650	0.146	-0.129	0.165	1.13
IID	Br-N	0.207	0.653	0.146	-0.130	0.165	1.12
IIE	Br-N	0.185	0.591	0.131	-0.114	0.164	1.15
IIF	Br-N	0.190	0.606	0.135	-0.118	0.165	1.14
IIIA	H-N	0.205	0.498	0.129	-0.134	-0.467	0.96
	F-H	0.762	0.318	0.681	-0.565	0.116	1.21
IIIB	H-N	0.211	0.510	0.132	-0.137	-0.510	0.96
	F-H	0.727	0.308	0.652	-0.532	0.119	1.23
IIIC	H-N	0.213	0.514	0.134	-0.139	-0.529	0.96
	F-H	0.368	0.311	0.660	-0.541	0.118	1.22
IIID	H-N	0.216	0.520	0.135	-0.141	-0.548	0.96
	F-H	0.704	0.301	0.633	-0.512	0.121	1.24

IIIE	H-N	0.198	0.483	0.124	-0.128	-0.403	0.97
	F-H	0.796	0.328	0.708	-0.595	0.112	1.19
IIIF	H-N	0.201	0.490	0.127	-0.131	-0.438	0.97
	F-H	0.788	0.326	0.703	-0.589	0.113	1.19

Table S8: First hyperpolarizability β_o (*au*) values of Azo-X with different electron-withdrawing and electron-donating groups

Code(X)	**Substituent**	β_o
I	**A**	3.2×10^2
	B	1.0×10^3
	C	8.8×10^2
	D	2.3×10^3
	E	6.0×10^3
	F	3.5×10^4
II	**A**	2.2×10^2
	B	9.0×10^2
	C	6.4×10^2
	D	2.2×10^3
	E	6.6×10^3
	F	4.0×10^3
III	**A**	7.1×10^2
	B	4.1×10^1
	C	3.3×10^2
	D	6.1×10^3
	E	3.9×10^3
	F	2.8×10^3

Table S9: First hyperpolarizability β_o (*au*) values for urea, *p*-nitroaniline and various stilbenes calculated at different DFT functionals/**6-311++G(2d, 2p)** level of theory

Reference Molecules	*ω*B97XD	B3LYP	CAM-B3LYP	B3LYP-D3	LC-BLYP	BHandHLYP
Urea	$5.3x10^1$	$9.0x10^1$	$5.7\ x10^1$	$9.0\ x10^1$	$3.2\ x10^1$	$5.5\ x10^1$
***p*-Nitroaniline**	$1.2\ x10^3$	$1.6x10^3$	$1.3x10^3$	$1.6x10^3$	$1.1x10^3$	$1.2x10^3$
4-Nitrostilbene	$3.3x10^3$	$8.1x10^3$	$4.1x10^3$	$8.0x10^3$	$2.8x10^3$	$4.2x10^3$
4-(*N*,*N*-dimethylamino) stilbene	$4.8x10^3$	$5.0x10^3$	$5.0x10^3$	$5.0x10^3$	$4.3x10^3$	$4.6x10^3$
4-[*N*,*N*-dimethylamino]-4′-Nitro stilbene	$1.2x10^4$	$2.9\ x10^4$	$1.5x10^4$	$2.9x10^4$	$8.3x10^3$	$1.5x10^4$
4-Amine-4′-nitro stilbene	$8.5x10^3$	$2.0x10^4$	$1.1x10^4$	$2.0x10^4$	$6.1x10^3$	$1.1x10^4$
4-Bromo-4′ -nitro stilbene	$4.3x10^3$	$1.1x10^4$	$5.3x10^3$	$1.1x10^4$	$2.8x10^3$	$5.4x10^3$
4-Alkoxy-4′ -nitro stilbene	$6.7x10^3$	$1.6x10^4$	$8.2x10^3$	$1.6x10^4$	$4.6x10^3$	$8.1x10^3$

Table S10: First hyperpolarizability β_o (*au*) values for urea, *p*-nitroaniline and various stilbenes calculated at **CAM-B3LYP**/different basis sets level of theory

Reference Molecules	6-31+G(d, p)	6-311+G(d, p)	6-311++G(2d, 2p)	6-311++G(3d, 3p)
Urea	$2.9x10^1$	$4.2x10^1$	$5.7\ x10^1$	$5.7\ x10^1$
***p*-Nitroaniline**	$1.4\ x10^3$	$1.4x10^3$	$1.3x10^3$	$1.3x10^3$
4-Nitrostilbene	$4.2x10^3$	$4.3x10^3$	$4.1x10^3$	$4.1x10^3$
4-(*N*,*N*-dimethylamino) stilbene	$5.1x10^3$	$5.1x10^3$	$5.0x10^3$	$5.0x10^3$
4-[*N*,*N*-dimethylamino]-4′-Nitro stilbene	$1.5x10^4$	$1.5x10^4$	$1.5x10^4$	$1.5x10^4$
4-Amine-4′-nitro stilbene	$1.1x10^4$	$1.1x10^4$	$1.1x10^4$	$1.0x10^4$

4-Bromo-4′ -nitro stilbene	$5.4x10^3$	$5.5x10^3$	$5.3x10^3$	$5.2x10^3$
4-Alkoxy-4′ -nitro stilbene	$8.4x10^3$	$8.4x10^3$	$8.2x10^3$	$8.1x10^3$

Table S11: Static first hyperpolarizability β_o (*au*) values of the designed supramolecular complexes at ***ω*B97XD/6-311++G(2d, 2p)** and **CAM-B3LYP/6-31+G(d, p)**

Complexes	β_o **(*ω*B97XD/6-311++G(2d, 2p)**	β_o **(CAM-B3LYP/6-31+G(d, p)**
IA	8.5×10^3	9.3×10^3
IB	1.1×10^4	1.2×10^4
IC	1.1×10^4	1.3×10^4
ID	1.3×10^4	1.5×10^4
IE	1.1×10^3	1.6×10^3
IF	4.3×10^3	5.1×10^3
IIA	6.8×10^3	8.0×10^3
IIB	9.0×10^3	1.1×10^4
IIC	9.4×10^3	1.1×10^4
IID	1.1×10^4	1.3×10^4
IIE	2.6×10^3	6.0×10^1
IIF	2.8×10^3	3.6×10^3
IIIA	3.8×10^3	4.3×10^3
IIIB	5.2×10^3	5.7×10^3
IIIC	5.1×10^3	5.6×10^3
IIID	6.7×10^3	7.3×10^3
IIIE	3.2×10^3	3.3×10^3
IIIF	1.6×10^3	1.9×10^3

Table S12: First hyperpolarizability β_o (*au*) values of *trans* and *cis* supramolecular complexes

Complexes	β_o
IA	8.5×10^3
iA	7.0×10^3
IB	1.1×10^4
iB	7.2×10^3
IC	1.1×10^4
iC	7.5×10^3
ID	1.3×10^4
iD	7.6×10^3
IIA	6.8×10^3
iiA	5.7×10^3
IID	1.1×10^4
iiD	6.1×10^3
IIIA	3.8×10^3
iiiA	4.0×10^3
IIID	6.7×10^3
iiiD	4.1×10^3