

Supporting Information for:

The Effect of Resonance-Assisted Hydrogen Bond on the Second-Order Nonlinear Optical properties of Pyridine Hydrazone Photoswitches : A Quantum Chemistry Investigation

Douniazed Hannachi*^{a, b}, Nouredine Khelfaoui^a, Meriem Zaidi^{a, c}, Diha Yahiaoui^a, Salima Lakehal^d, Christophe Morell^e, Henry Chermette*^e

^aLaboratoire d'Électrochimie, d'Ingénierie Moléculaire et de Catalyse Redox (LEIMCR), Département d'Enseignement de Base en Technologie, Faculté de Technologie, Université Ferhat Abbas, Sétif-1, Algérie.

^bDépartement de Chimie, Faculté des Sciences, Université Ferhat Abbas, Setif-1, Algérie.

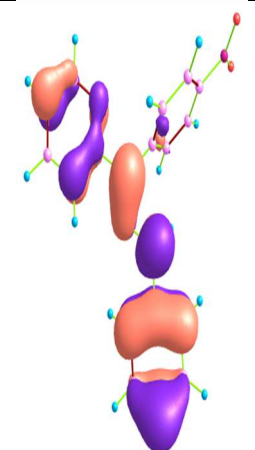
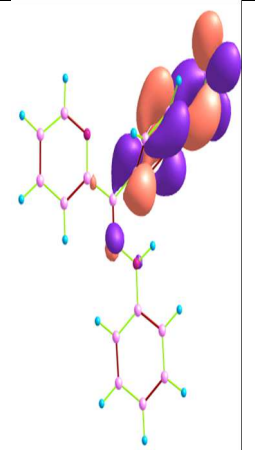
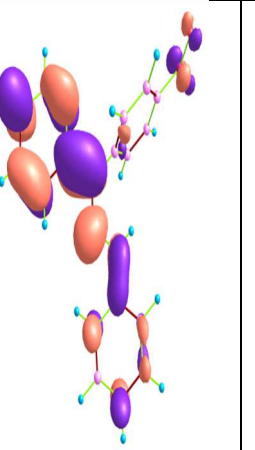
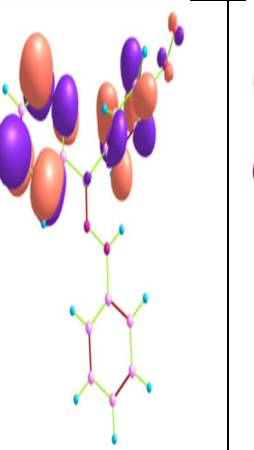
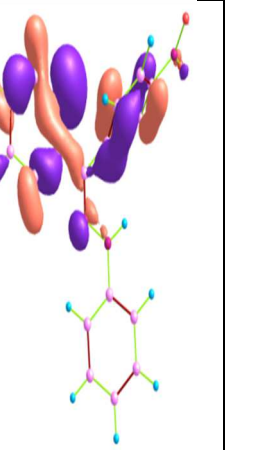
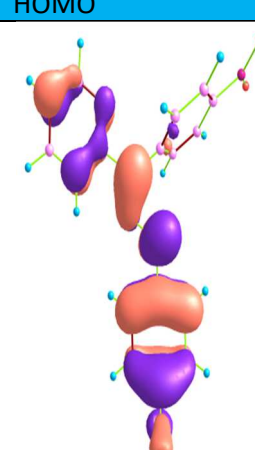
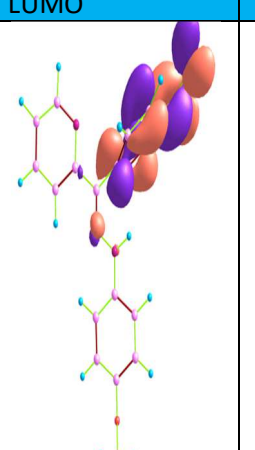
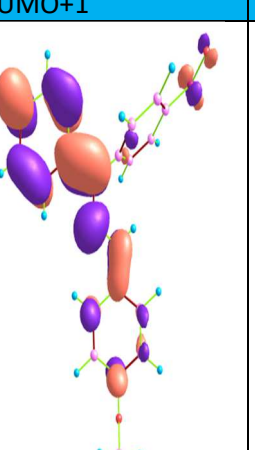
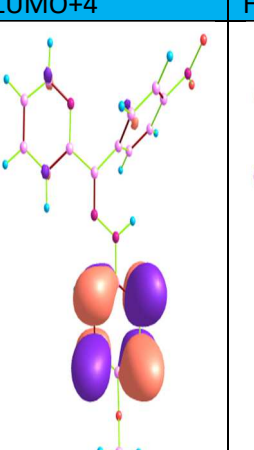
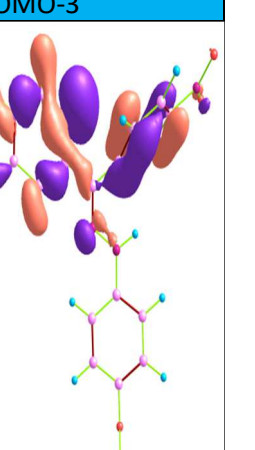
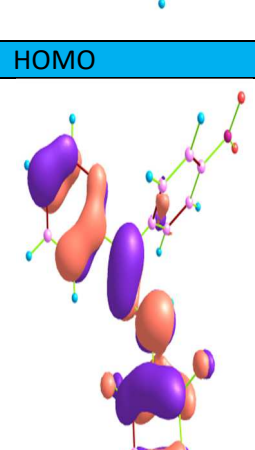
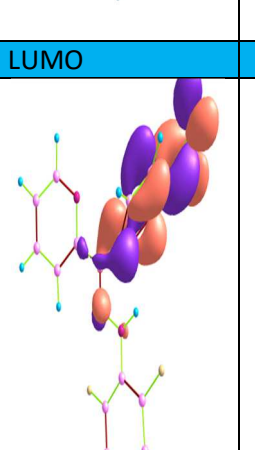
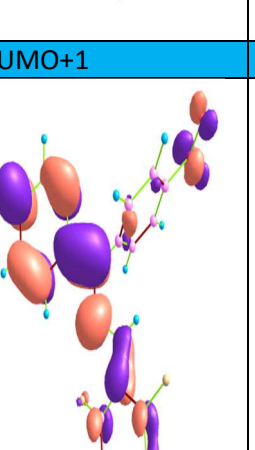
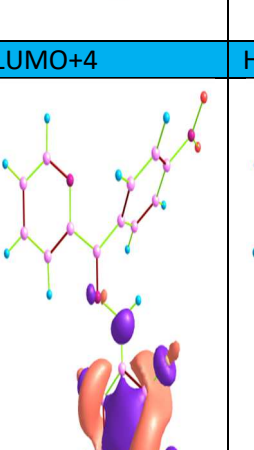
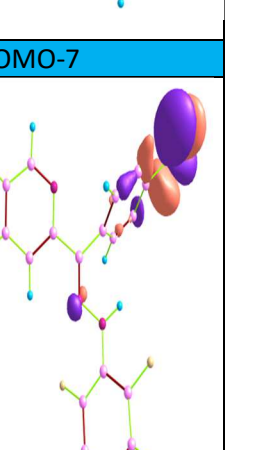
^cLaboratoire de Chimie, Ingénierie Moléculaire et Nanostructures (LCIMN), Université Ferhat Abbas Sétif 1, Sétif 19000, Algérie.

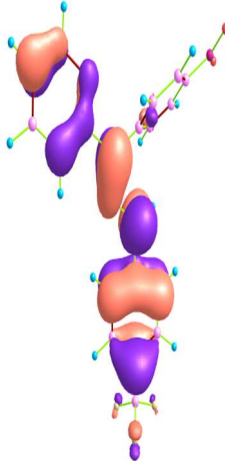
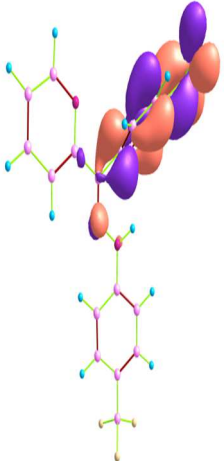
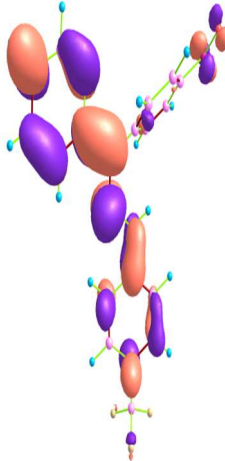
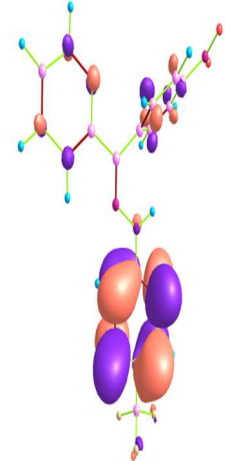
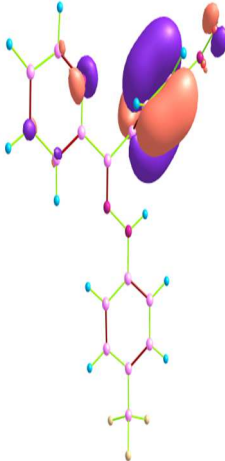
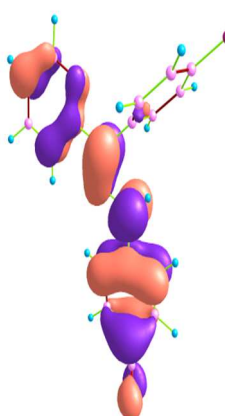
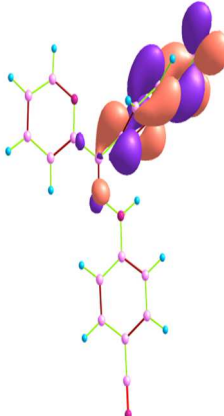
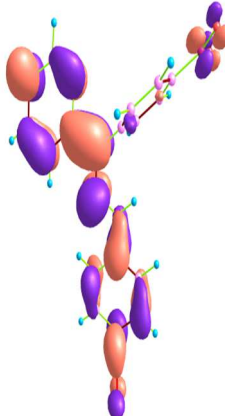
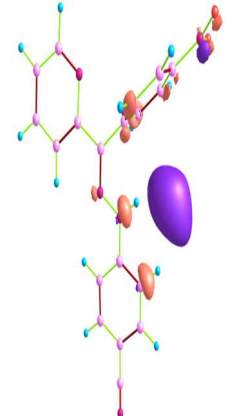
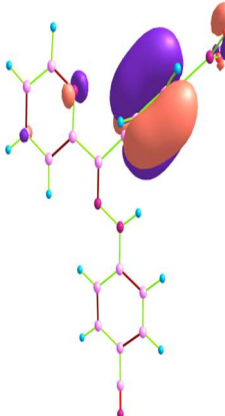
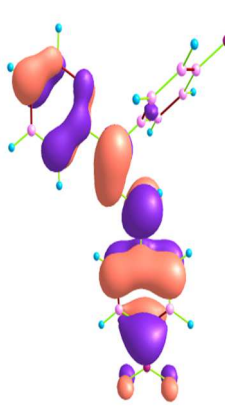
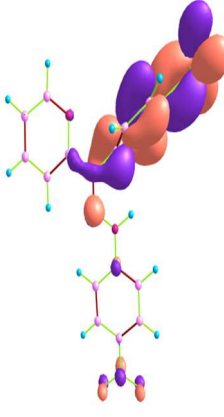
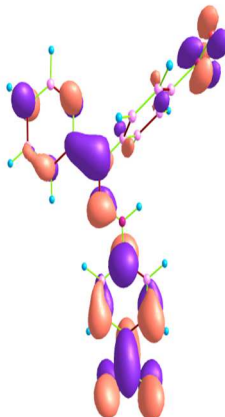
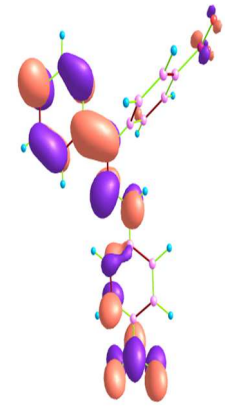
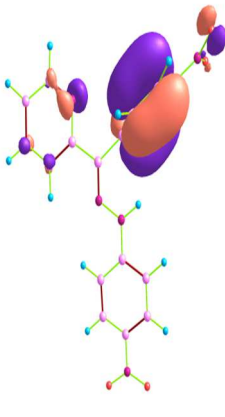
^dInstitut des Science de la Terre et de l'Univers, Université de Batna-2, Algérie.

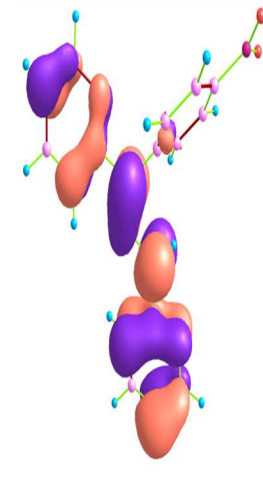
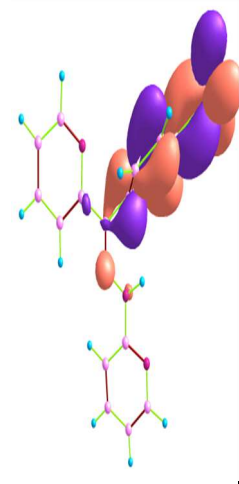
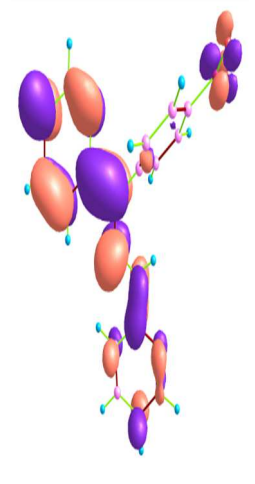
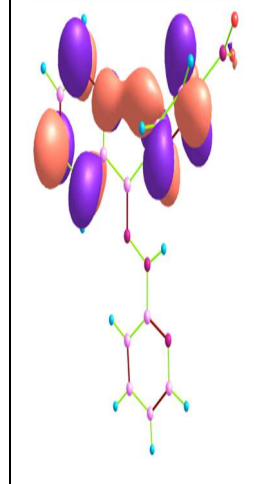
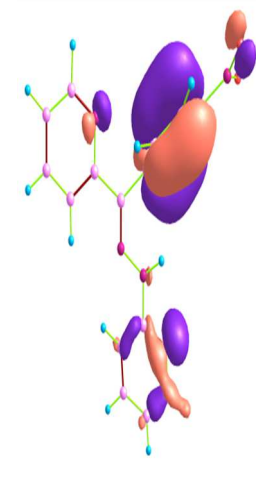
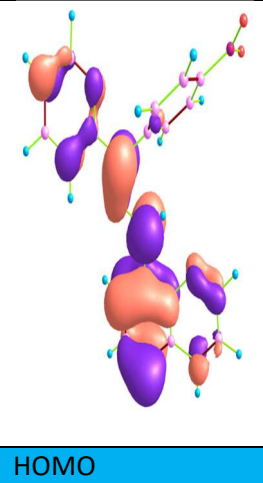
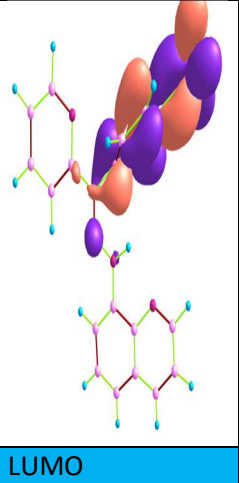
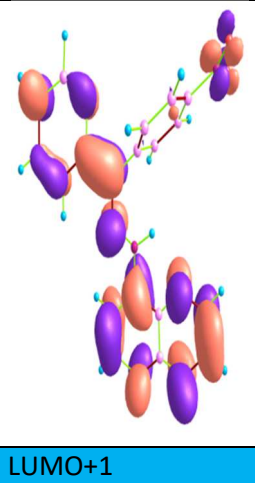
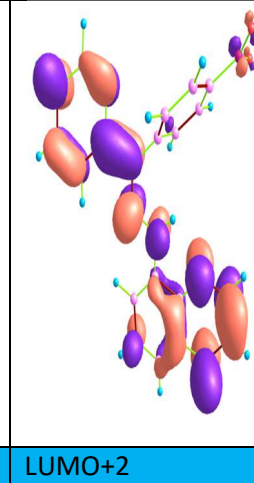
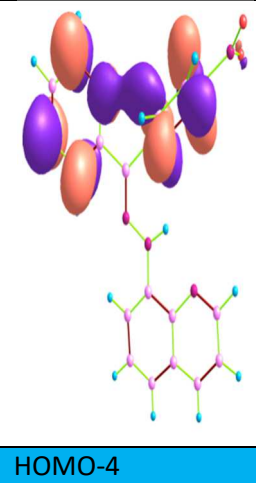
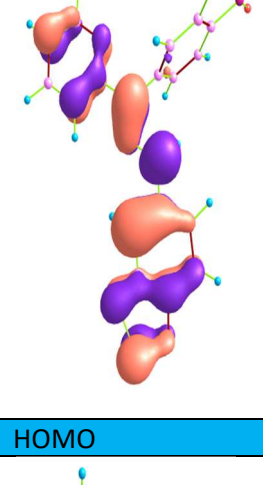
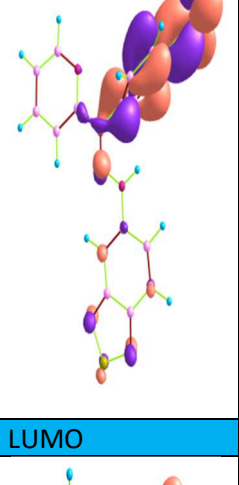
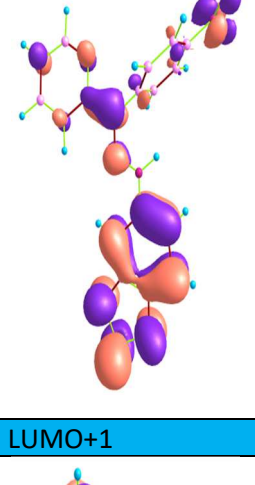
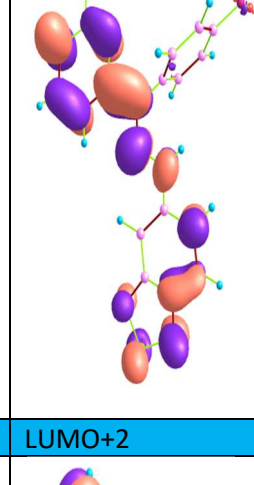
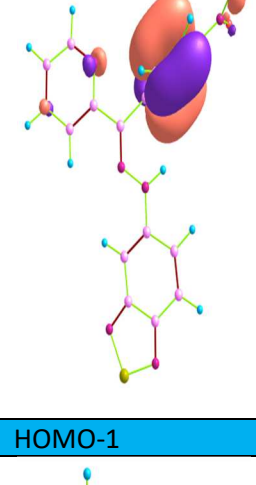
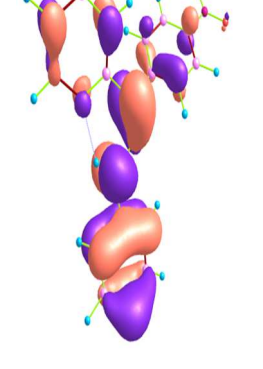
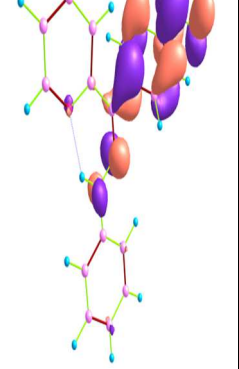
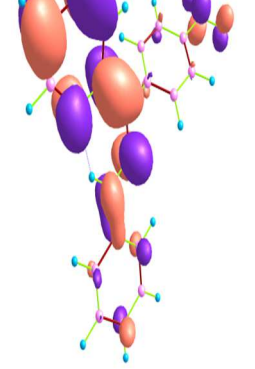
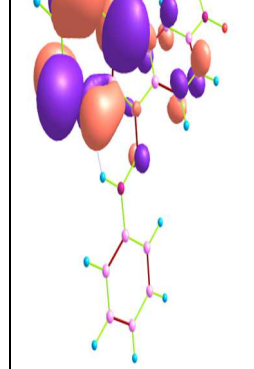
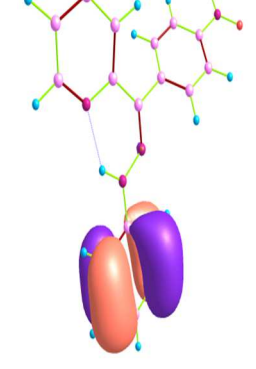
^eUniversité de Lyon, Université Claude Bernard Lyon 1, Institut des Sciences Analytiques, UMR CNRS 5280, 69622 Villeurbanne Cedex, France

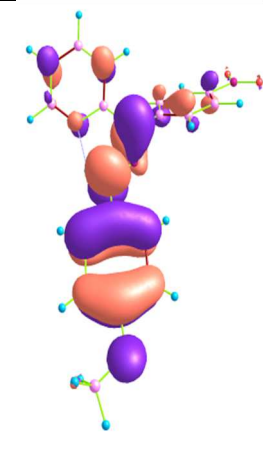
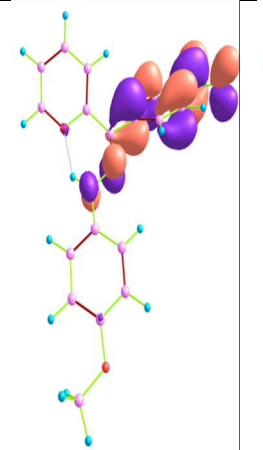
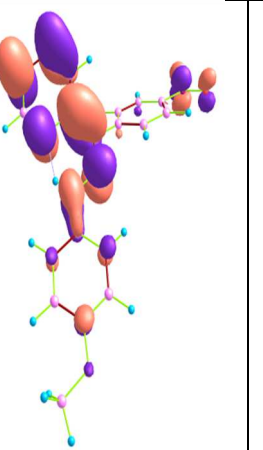
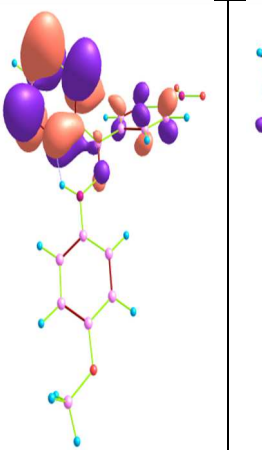
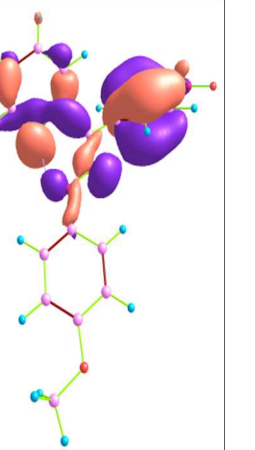
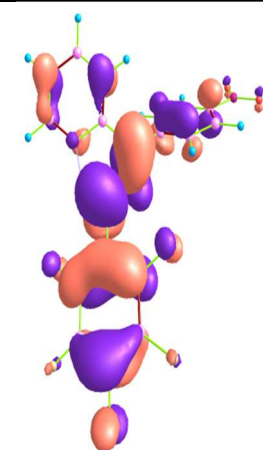
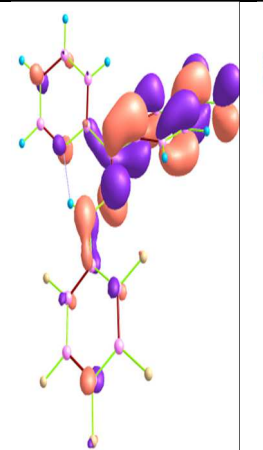
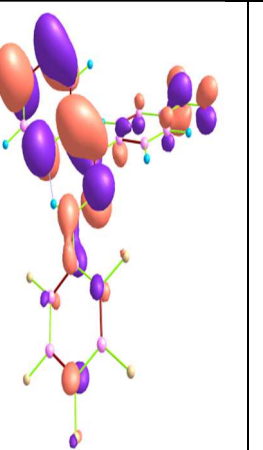
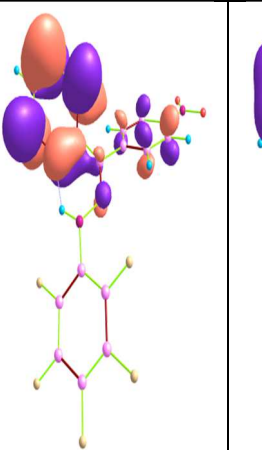
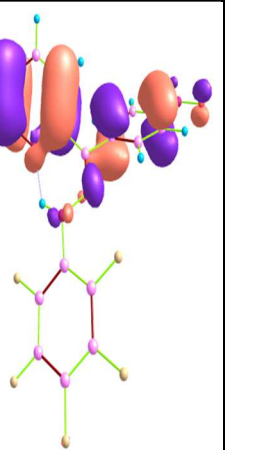
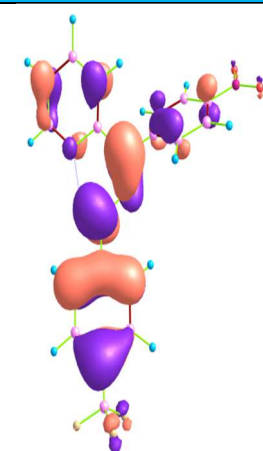
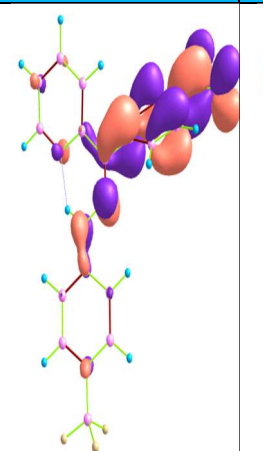
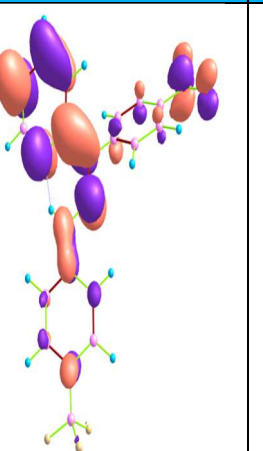
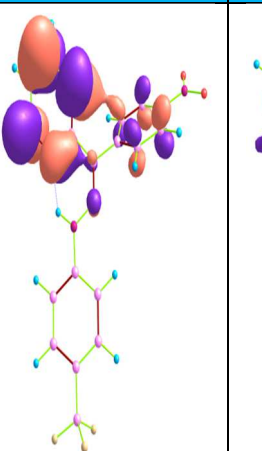
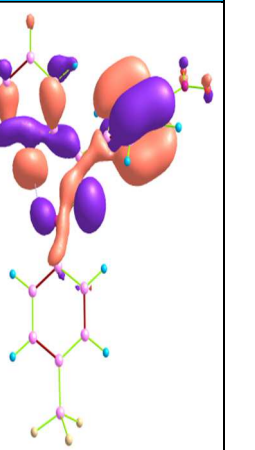
Table of contents

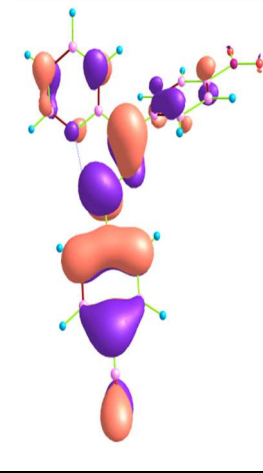
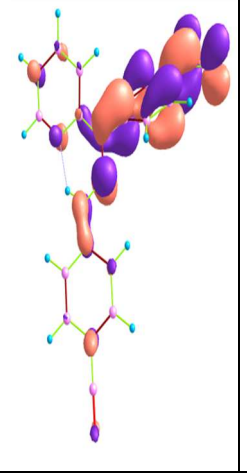
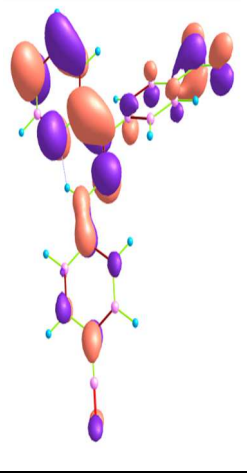
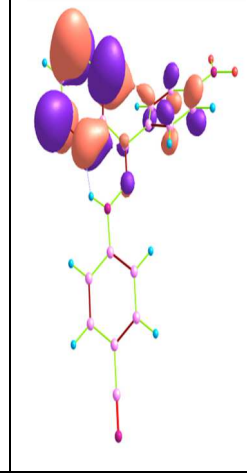
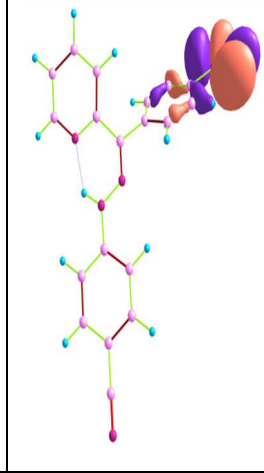
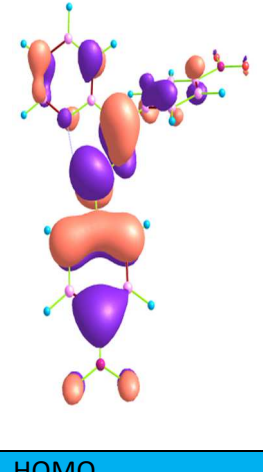
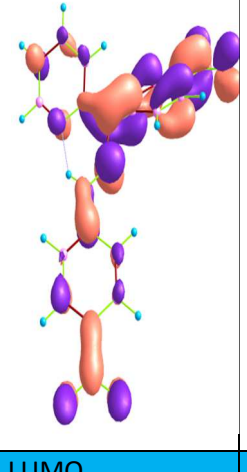
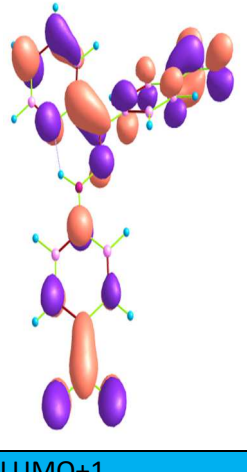
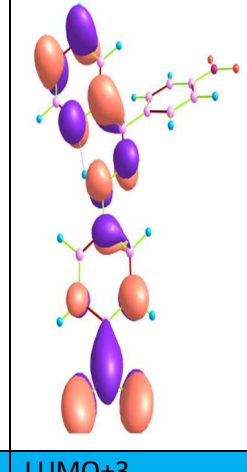
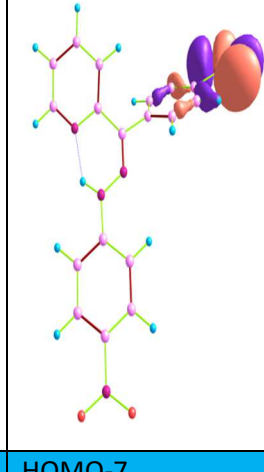
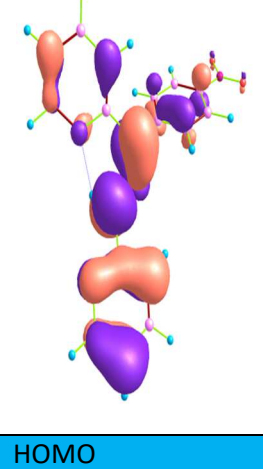
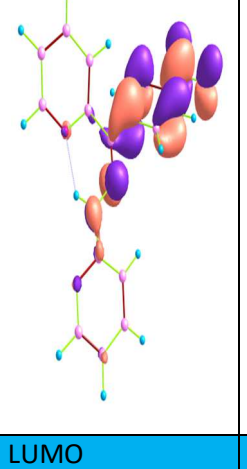
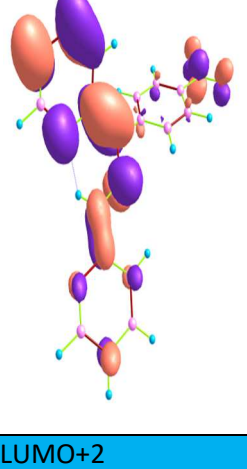
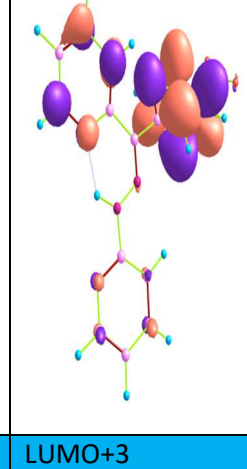
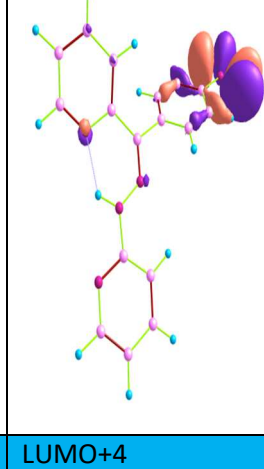
Figure S1. Molecular orbitals of the studied compounds	S13
Figure S2. Electron density difference maps of title compounds from the ground state to the crucial excited state $S_0 \rightarrow S_n$ plotted using isovalues of 0.008 au	S23
Figure S3. Calculated UV – vis absorption spectra of title compounds	S25
Figure S4. Relationship between I_{Ψ}^{2w} and polarization angle Ψ of Z and E isomers (green static, red $\lambda=1340$ nm, blue $\lambda=1064$ nm)	S29
Table S1. QTAIM calculated values of electron density (ρ), Laplacian ($\nabla^2(\rho)$), total electron energy density (H), kinetic electron energy density (G), and potential electron energy density (V) at bond critical points (au) for the Zi (i=1 to 18) compounds. RCP: ring critical point in N1-N2-C3-C4-N6-H; BCP: critical point in intramolecular H-bond N1-H...N6.	S30
Table S2. Dihedral angles (φ) of Z and E isomers	S31
Table S3. Vertical transition energy ($\Delta E_{0 \rightarrow n}$, eV) and wavelength ($\Delta \lambda_{0 \rightarrow n}$, nm), oscillator strengths ($f_{0 \rightarrow n}$, dimensionless), charge transfer distances (q^{CT}), charge transfer distance (d^{CT} , Å), and dipole moment variation ($\Delta \mu_{0 \rightarrow n}$, D) associated to the $S_0 \rightarrow S_n$ transition, as calculated at the ω B97XD/6-311+g(d) of the studied Ei and Zi (i=1 to 18) compounds	S32
Table S4. Second harmonic generation ($\beta_{SHG}^\lambda \equiv \beta(-2\omega; \omega, \omega)$, a.u.), electrooptic Pockels effect ($\beta_{EOPE}^\lambda \equiv \beta(-\omega; \omega, 0)$, a.u.), dynamic hyper-Rayleigh scattering (β_{HRS}^λ , a. u.) and depolarization ratio DR^λ of Ei and Zi (i=1 to 18) compounds ($\lambda = 695, 1064$ and 1340 nm)	S35
Table S5. Static and dynamic β_{ji} values of Ei and Zi (i=1 to 18) compounds	S36
Table S6. The frequency dispersion factor between static and dynamic ($\beta_{HRS}^\lambda / \beta_{HRS}^\infty$)	S37
The optimized cartesian coordinates and energy of all structures	S38

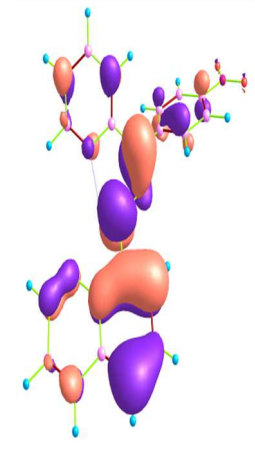
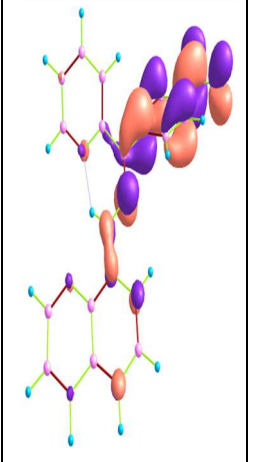
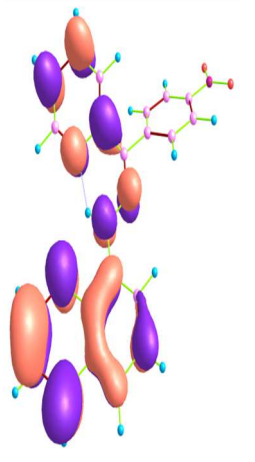
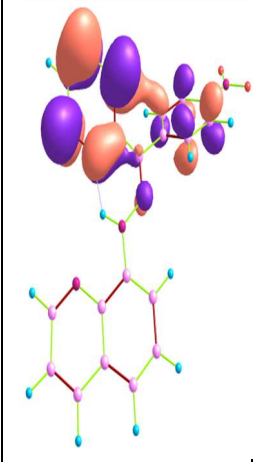
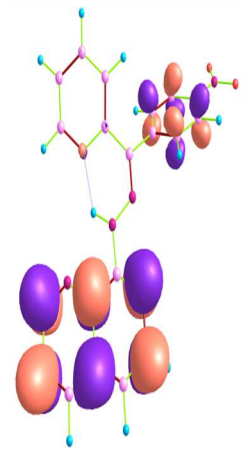
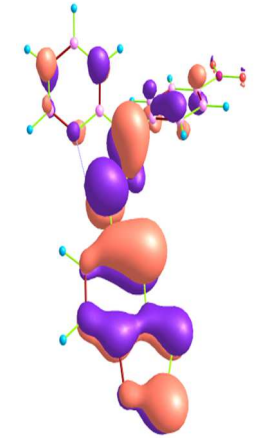
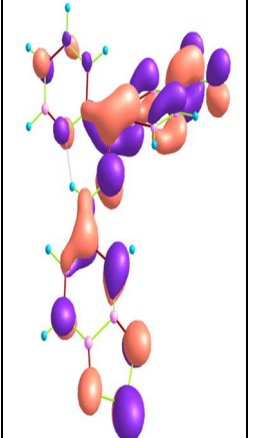
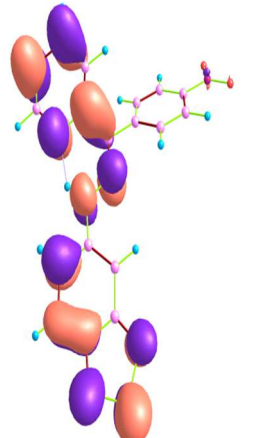
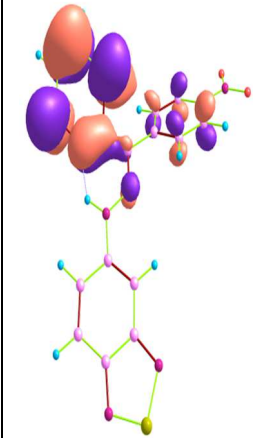
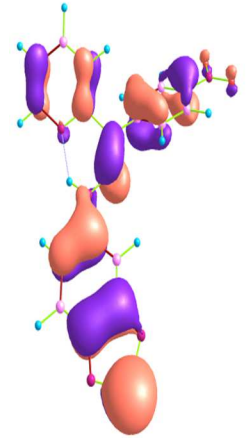
	HOMO	LUMO	LUMO+1	LUMO+3	HOMO-3
E1					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-3
E2					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-7
E3					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-4

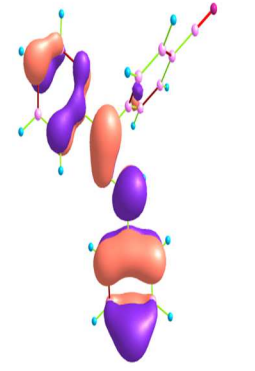
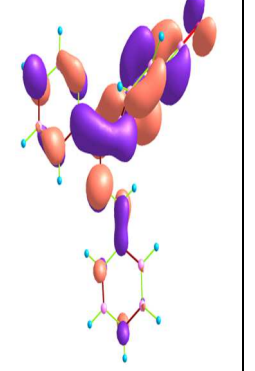
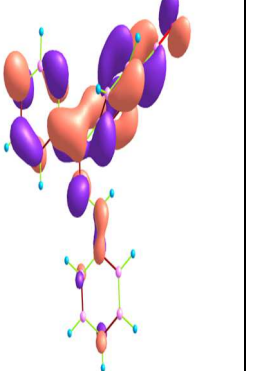
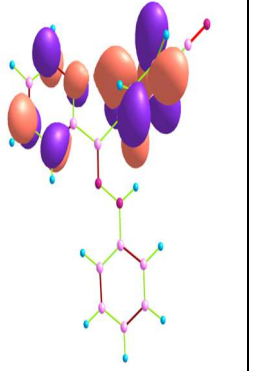
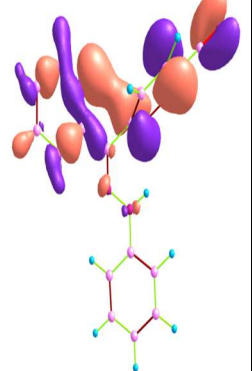
E4					
	HOMO	LUMO	LUMO+1	LUMO+6	HOMO-4
E5					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4
E6					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4

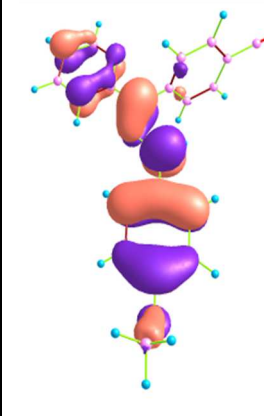
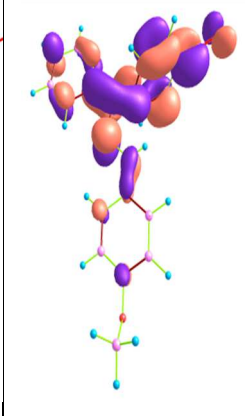
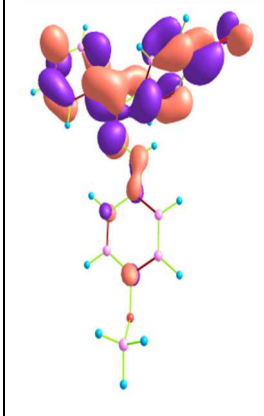
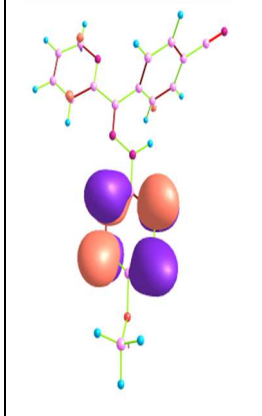
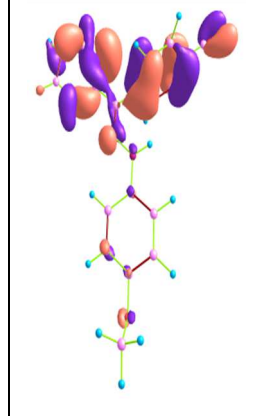
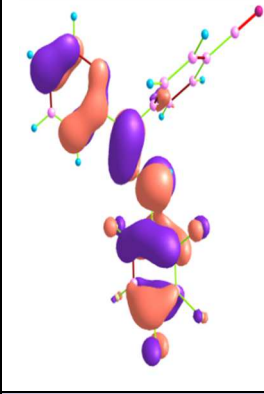
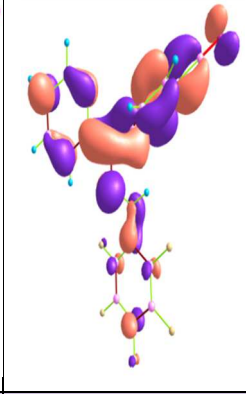
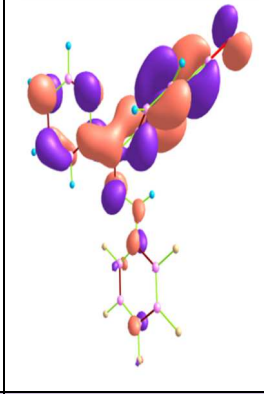
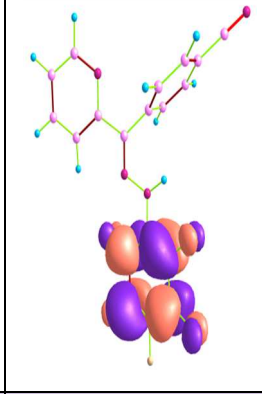
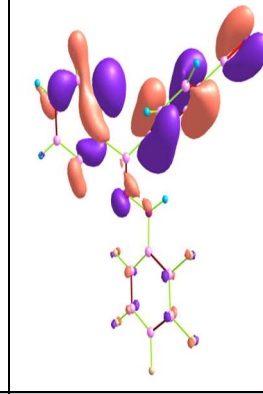
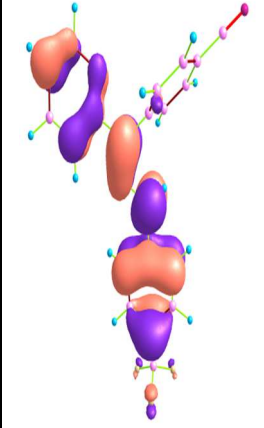
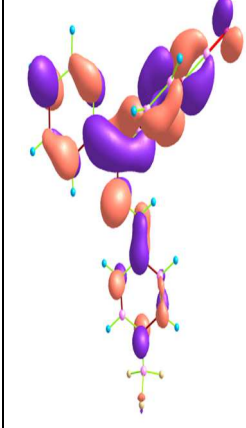
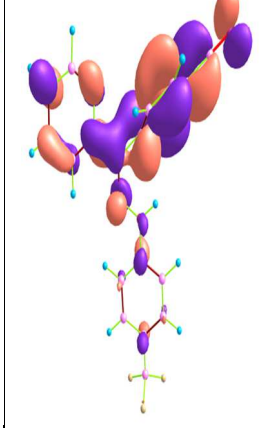
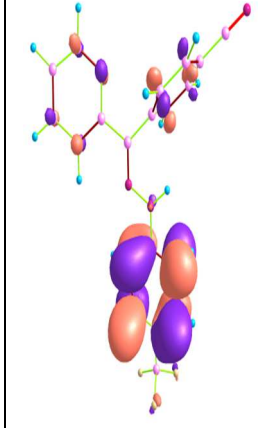
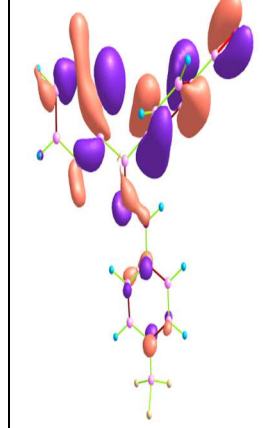
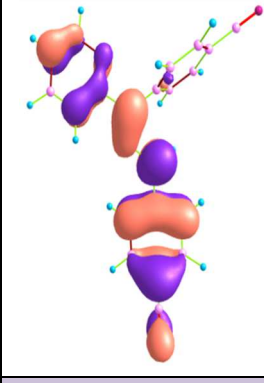
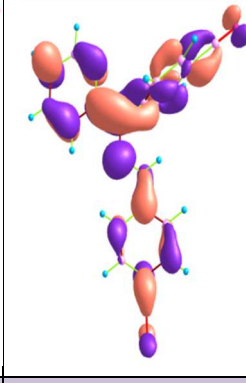
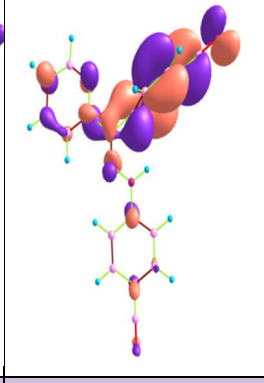
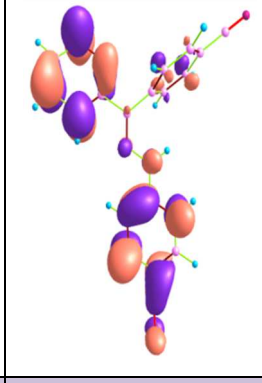
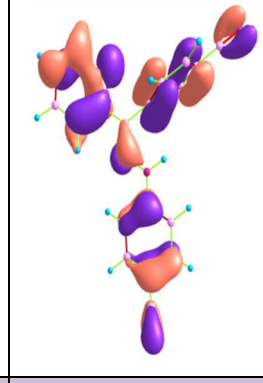
E7					
	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
E8					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4
E9					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-1
Z1					

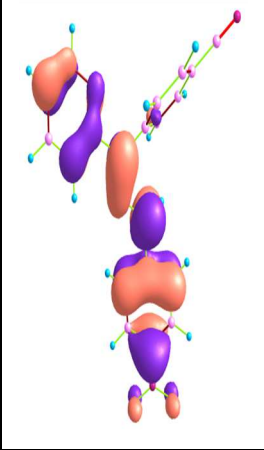
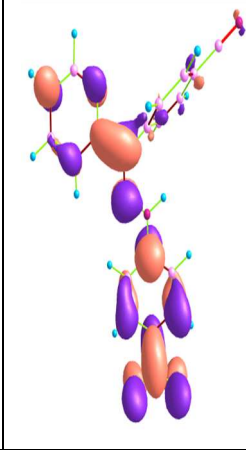
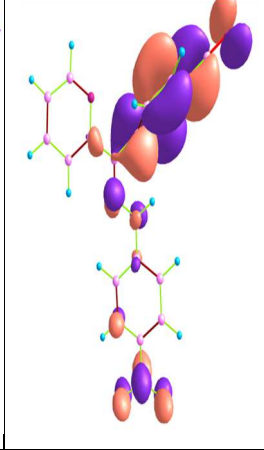
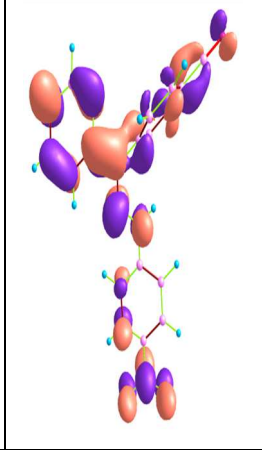
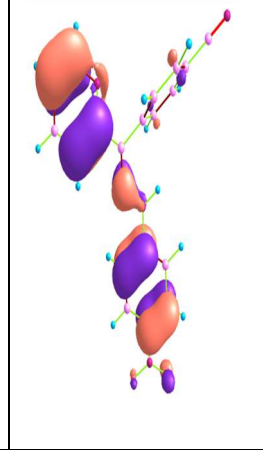
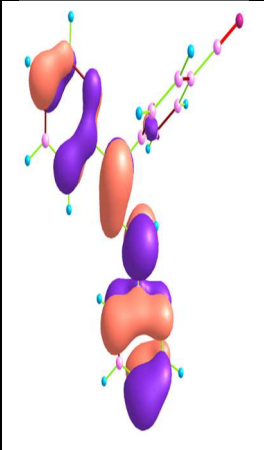
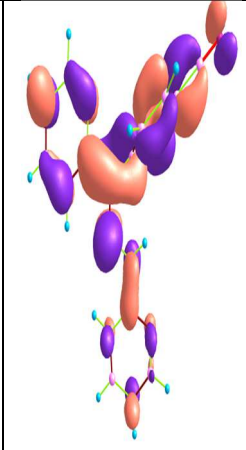
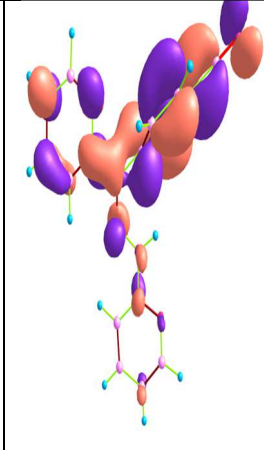
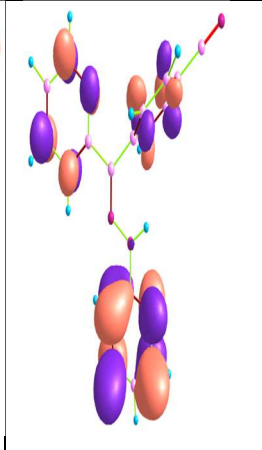
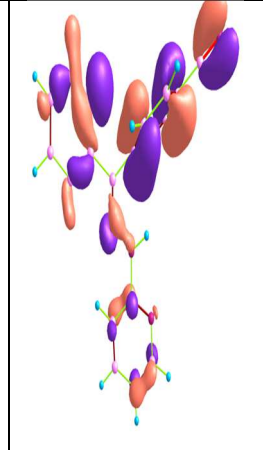
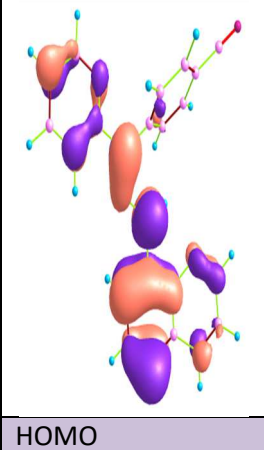
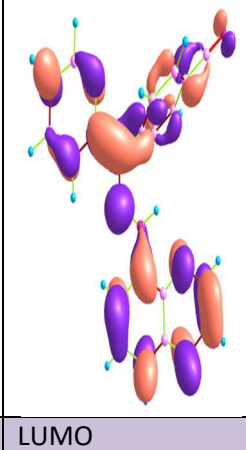
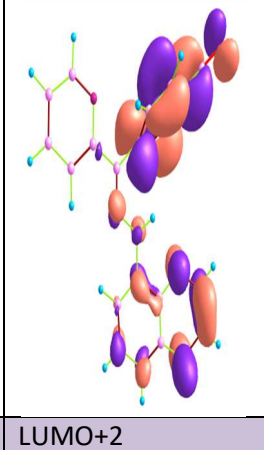
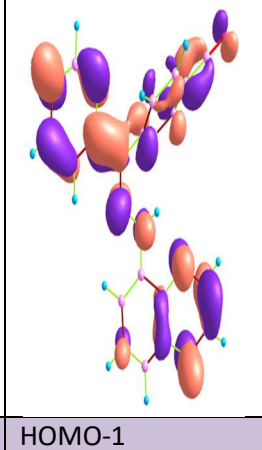
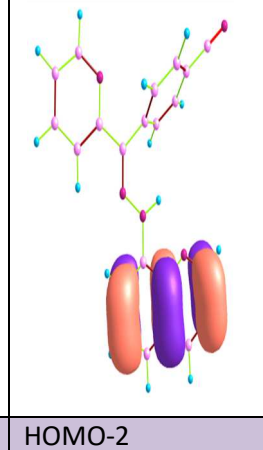
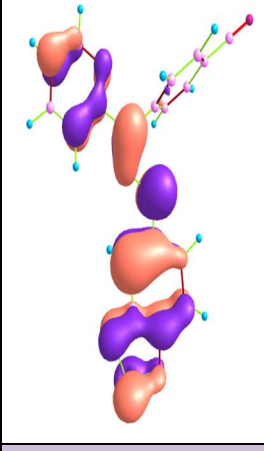
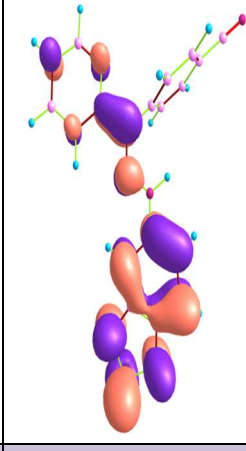
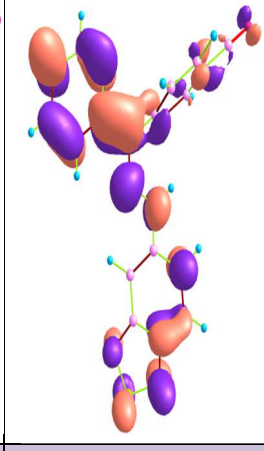
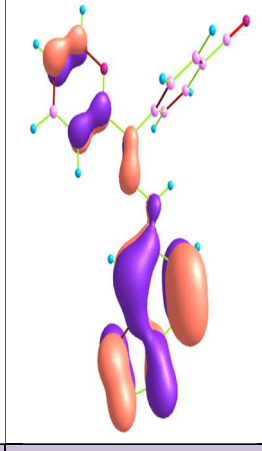
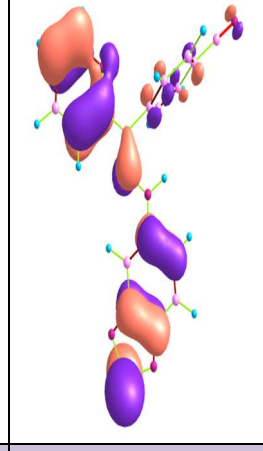
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4
Z2					
Molecule	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-5
Z3					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-3
Z4					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-6

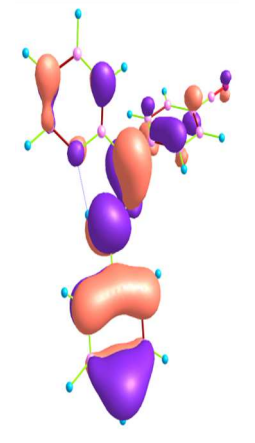
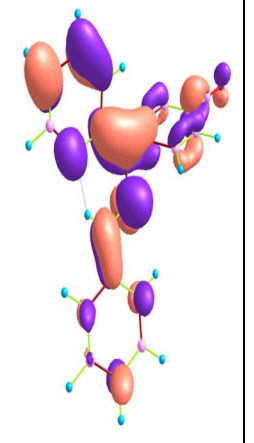
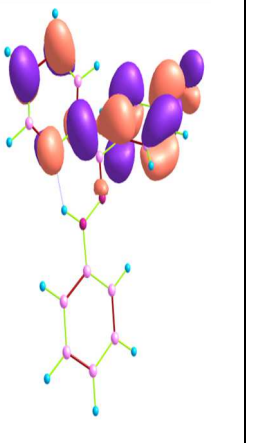
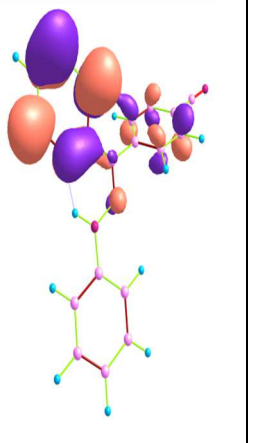
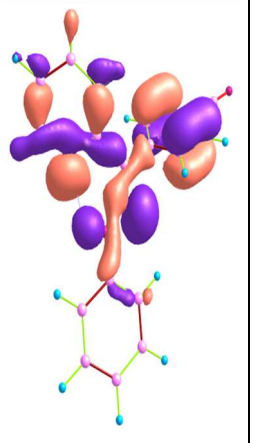
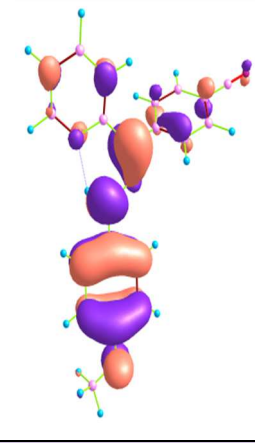
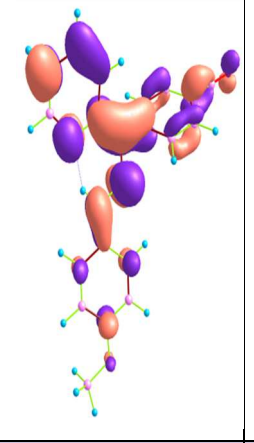
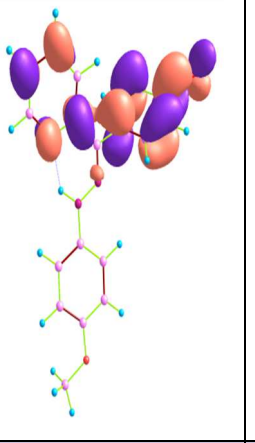
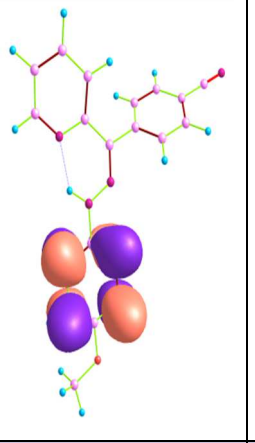
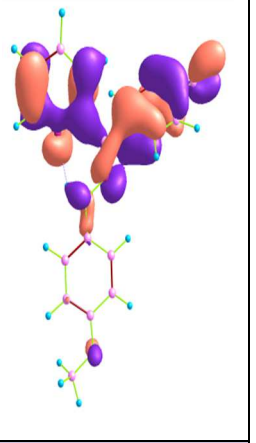
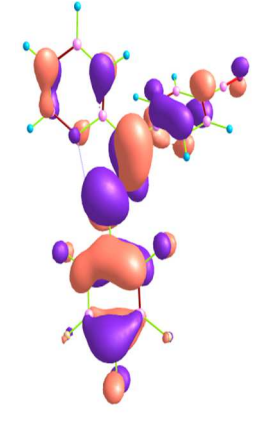
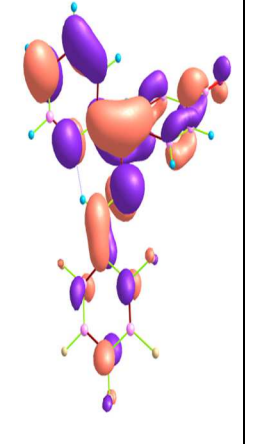
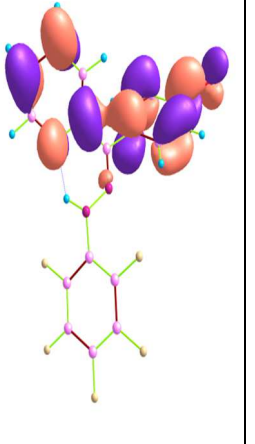
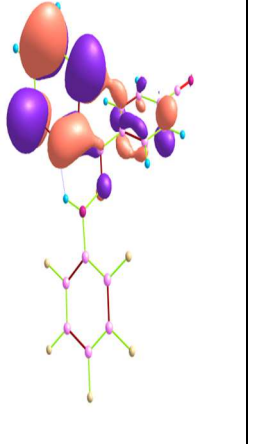
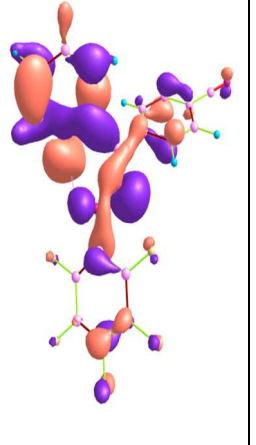
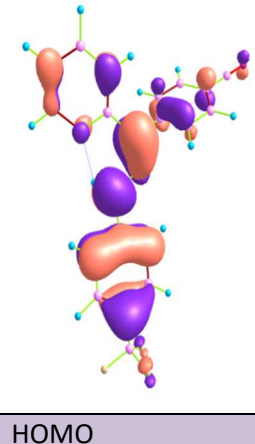
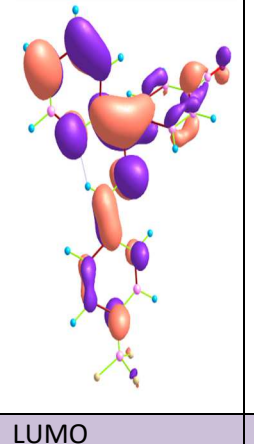
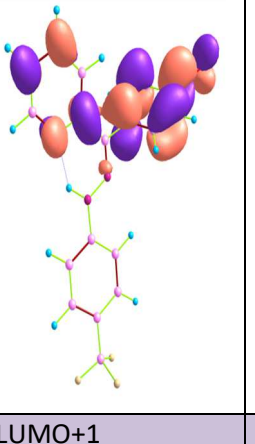
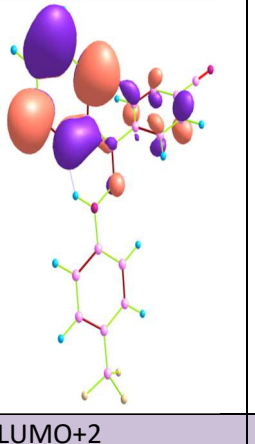
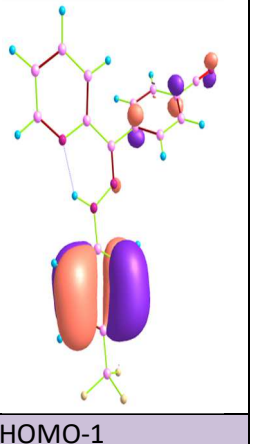
Z5					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-7
Z6					
	HOMO	LUMO	LUMO+1	LUMO+3	HOMO-7
Z7					
	HOMO	LUMO	LUMO+2	LUMO+3	LUMO+4

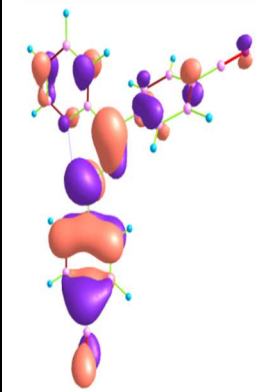
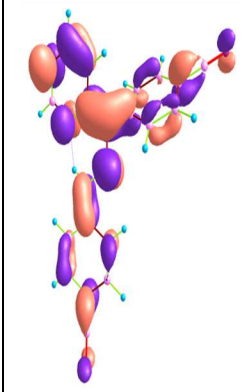
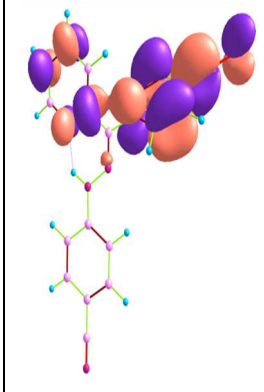
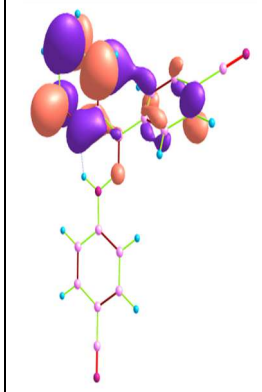
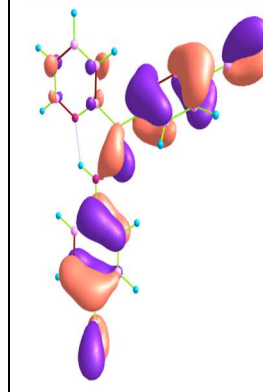
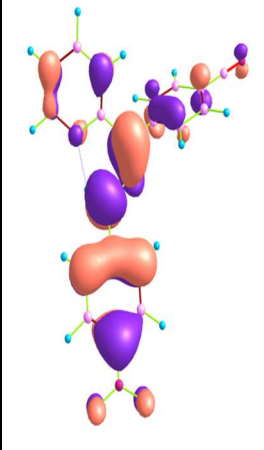
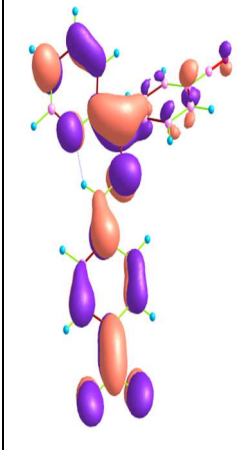
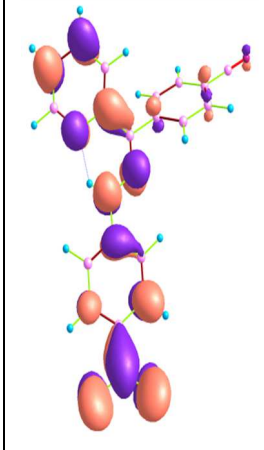
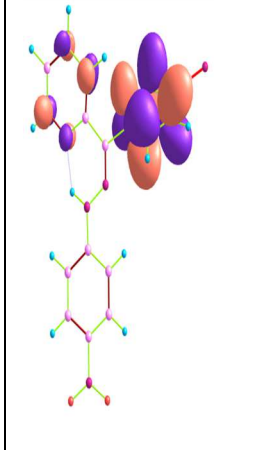
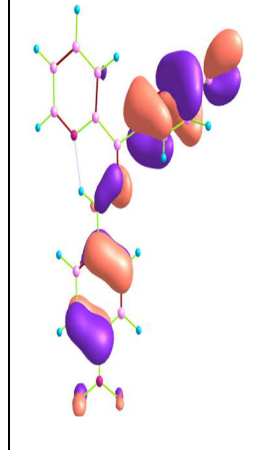
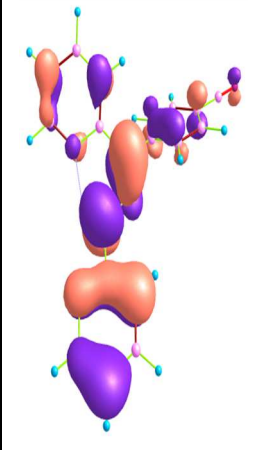
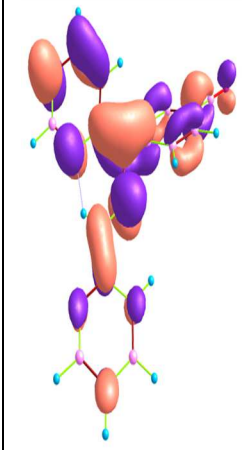
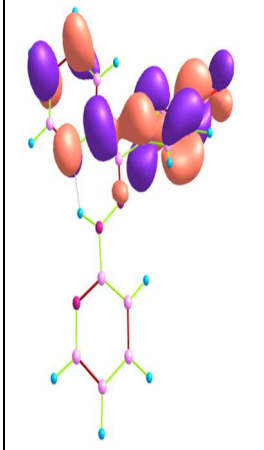
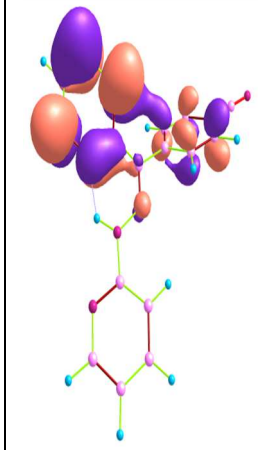
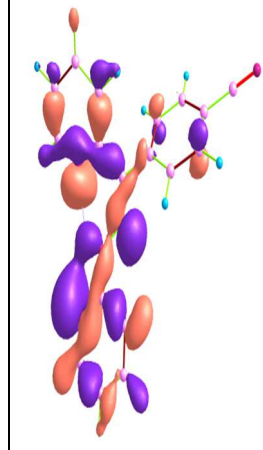
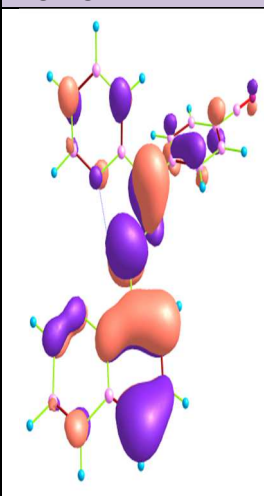
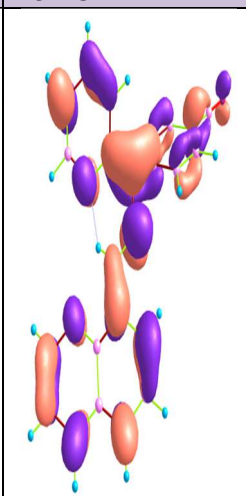
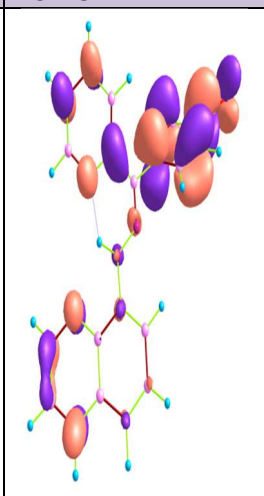
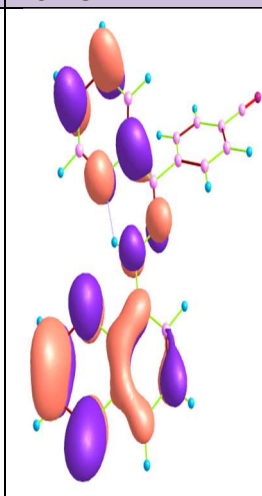
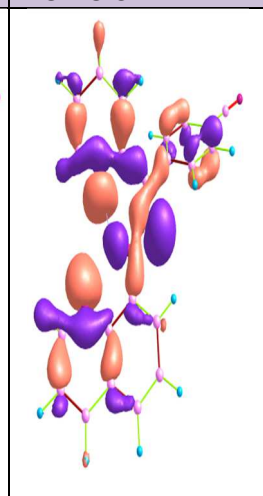
Z8					
	HOMO	LUMO	LUMO+2	LUMO+3	HOMO-2
Z9					

Molecule	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4
E10					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-3

E11					
	HOMO	LUMO	LUMO+1	LUMO+5	HOMO-1
E12					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-1
E13					
	HOMO	LUMO	LUMO+1	LUMO+3	HOMO-1
E14					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-2

E15					
	HOMO	LUMO	LUMO+1	LUMO+3	HOMO-1
E16					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-2
E17					
	HOMO	LUMO	LUMO+2	HOMO-1	HOMO-2
E18					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-3

Z10					
	HOMO	LUMO	LUMO+1	LUMO+5	HOMO-4
Z11					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-4
Z12					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-2
Z13					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-1

Z14					
	HOMO	LUMO	LUMO+1	LUMO+4	HOMO-1
Z15					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-2
Z16					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-3
Z17					
	HOMO	LUMO	LUMO+1	LUMO+2	HOMO-2

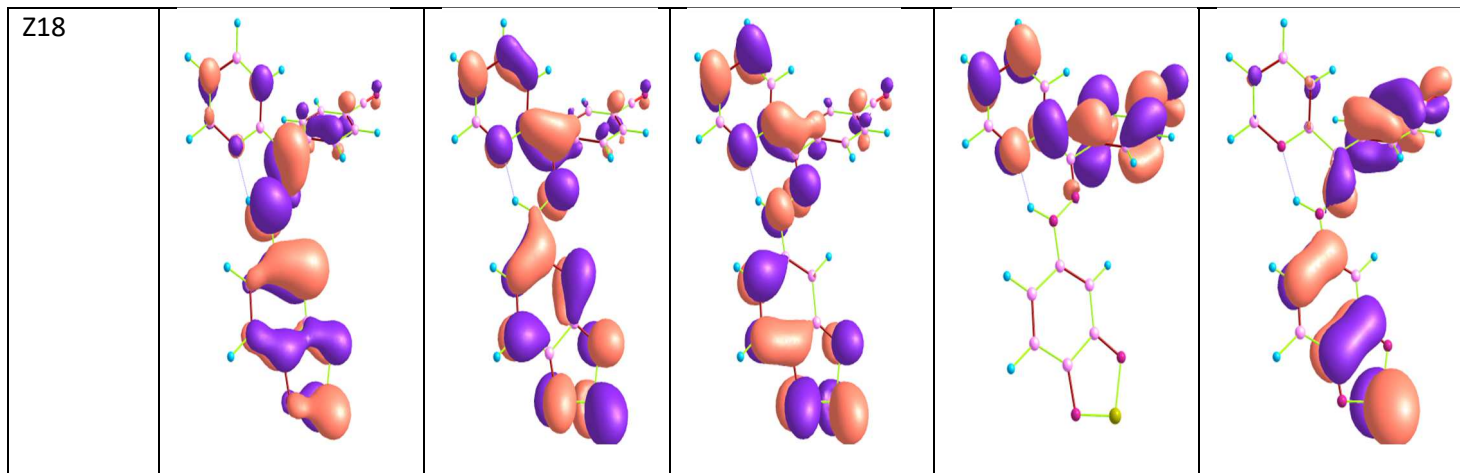
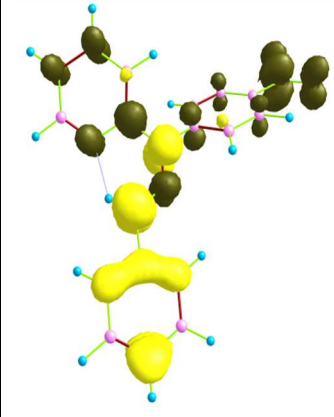
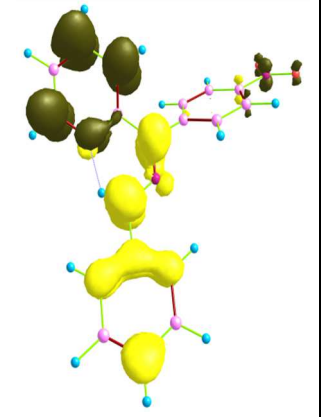
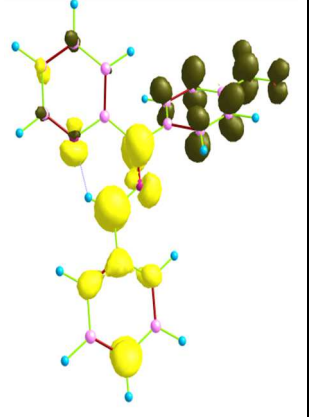
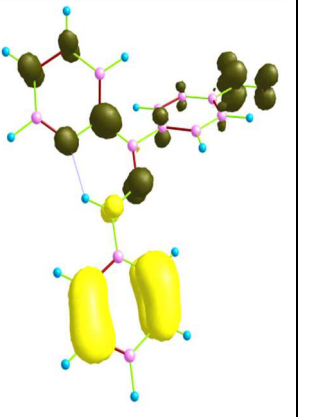
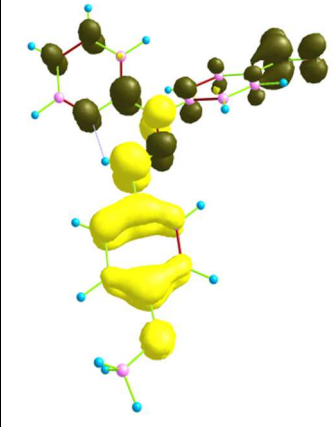
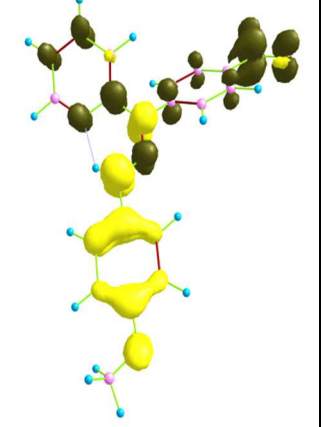
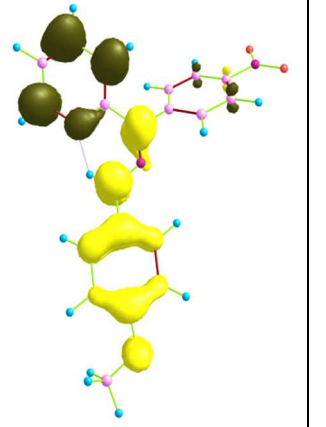
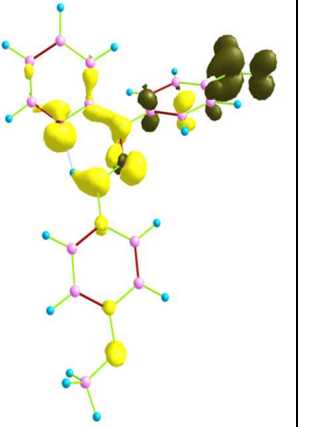
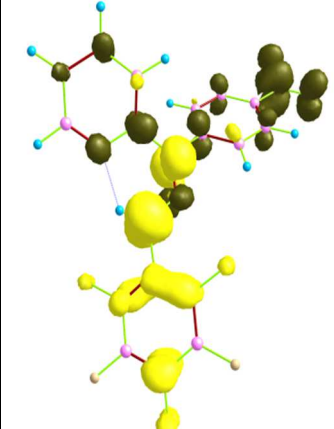
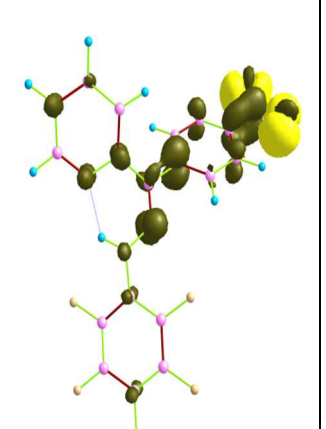
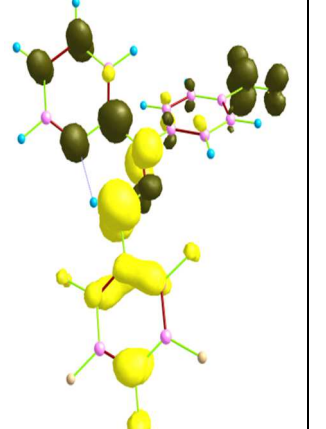
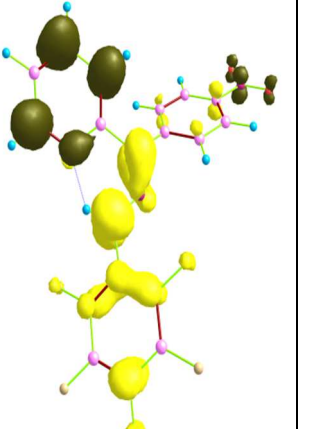


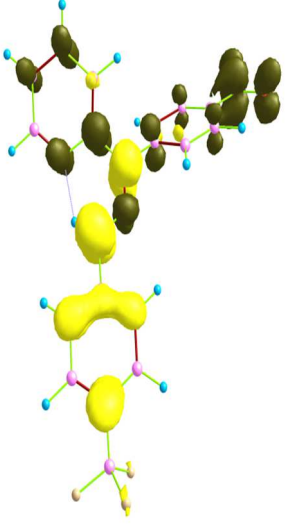
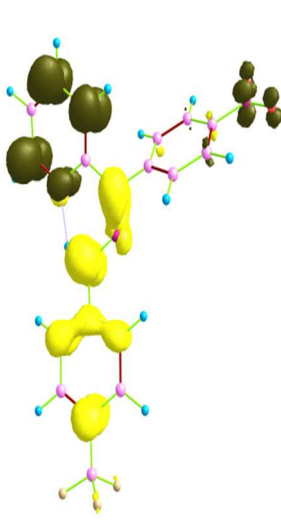
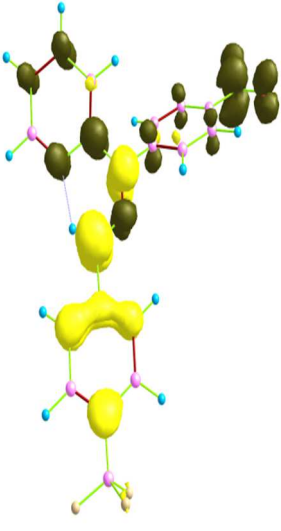
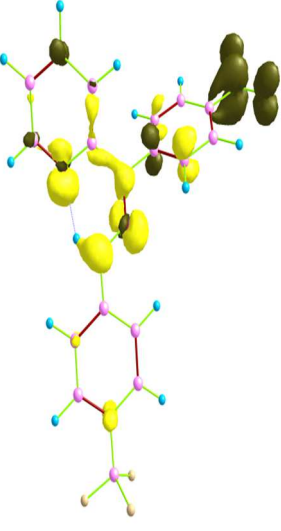
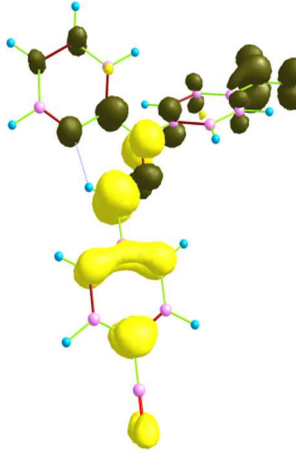
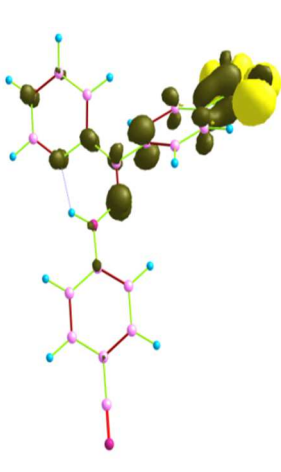
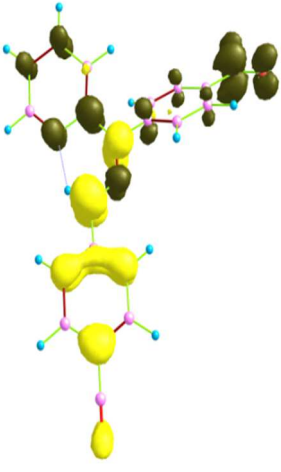
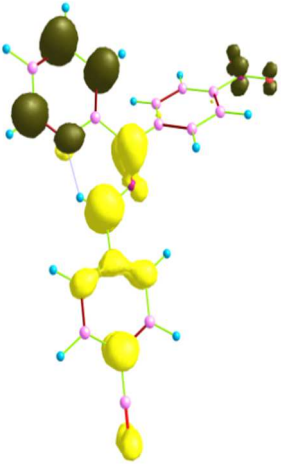
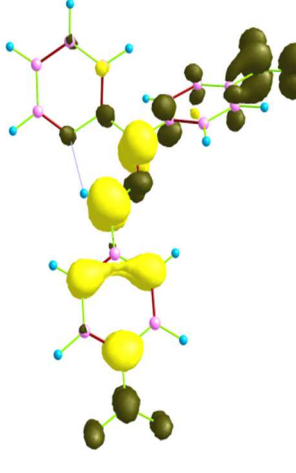
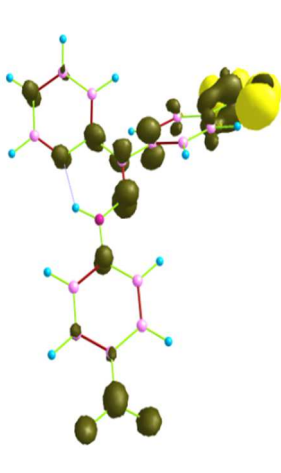
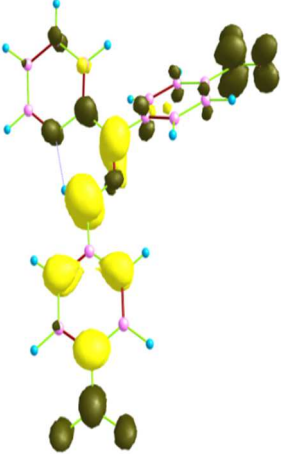
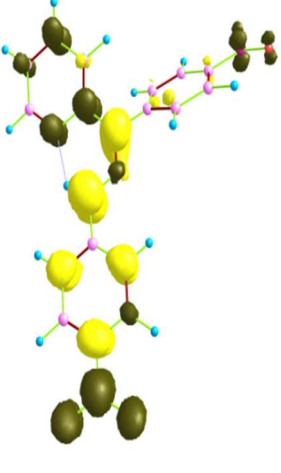
Figure S1. Molecular orbitals of the studied compounds

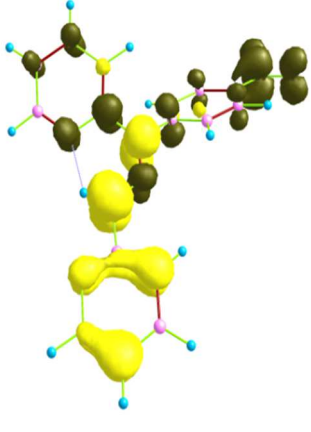
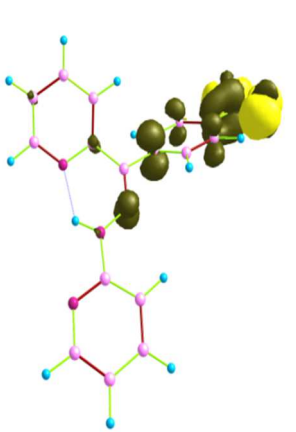
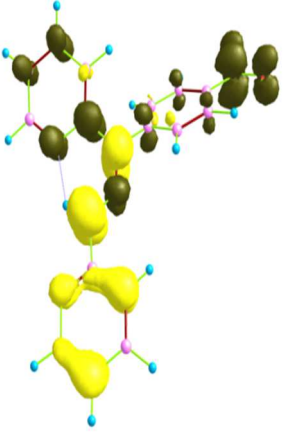
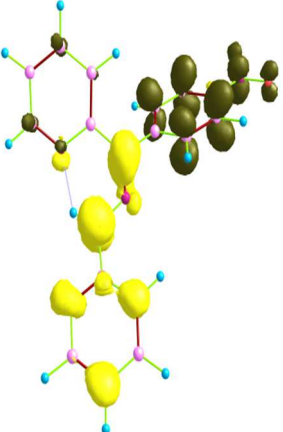
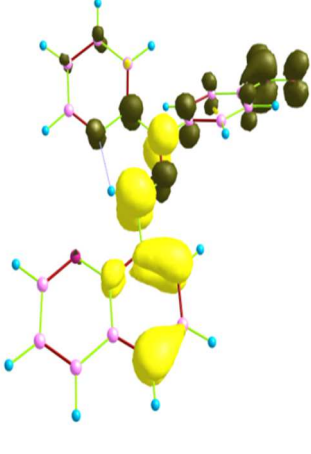
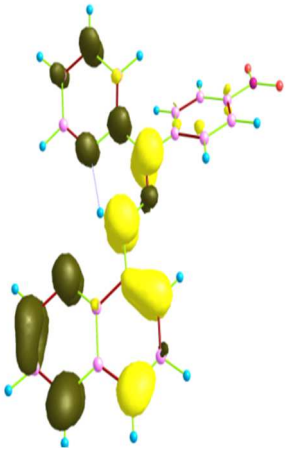
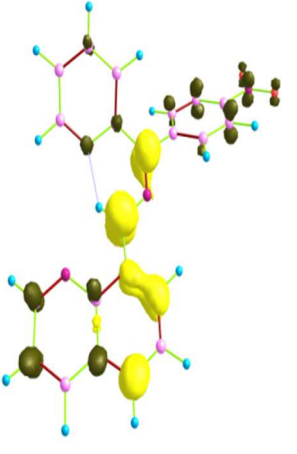
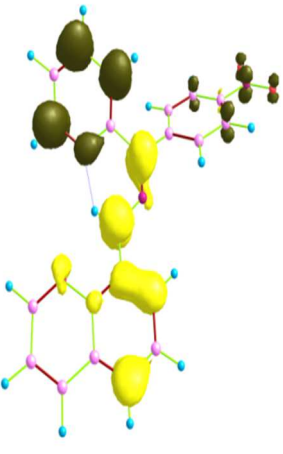
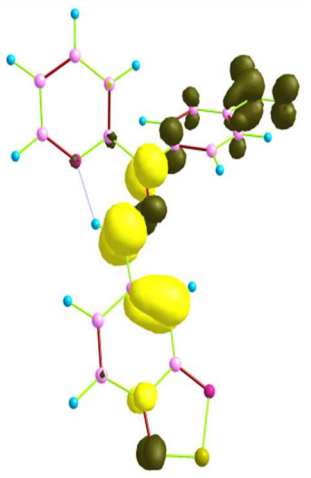
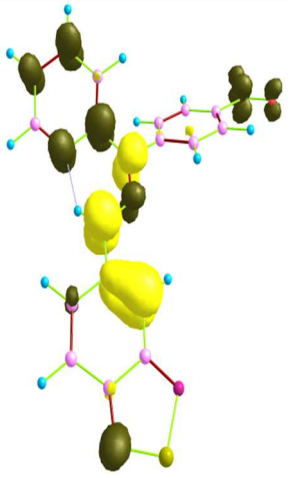
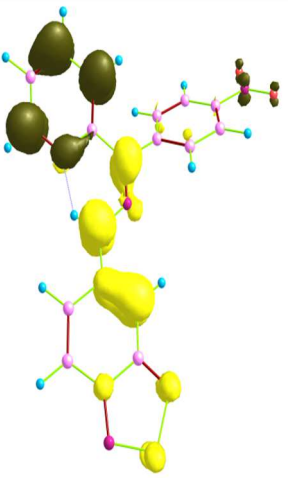
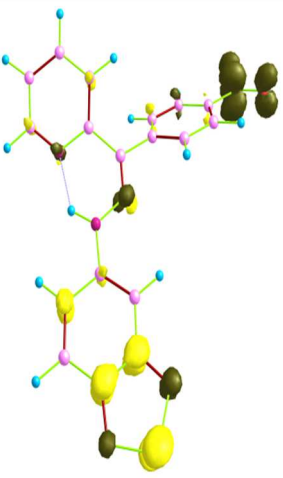
	S0→S1	S0→S3	S0→S8	S0→S15
E1				
	S0→S1	S0→S3	S0→S5	S0→S15
E2				
	S0→S1	S0→S2	S0→S4	S0→S9
E3				
	S0→S1	S0→S3	S0→S6	S0→S7

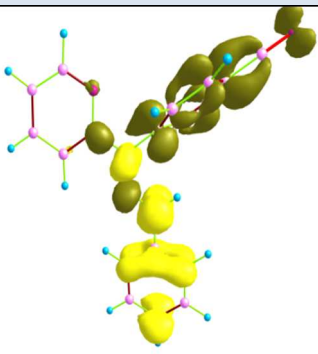
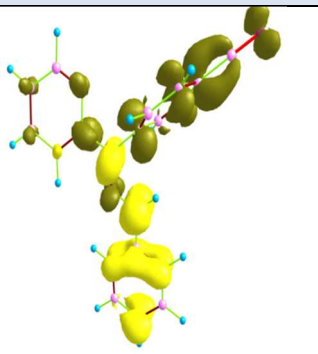
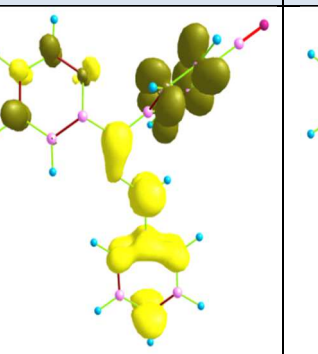
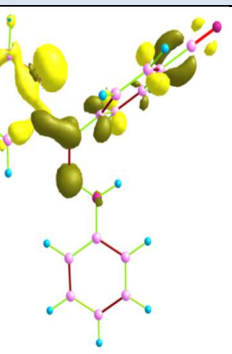
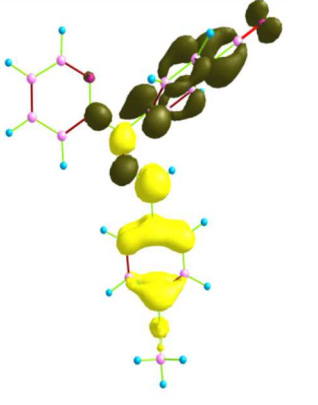
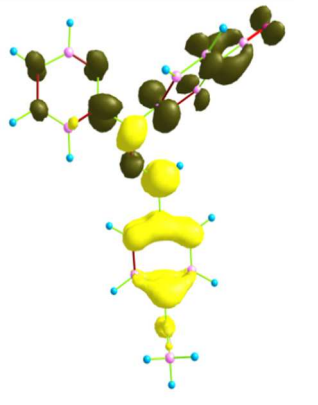
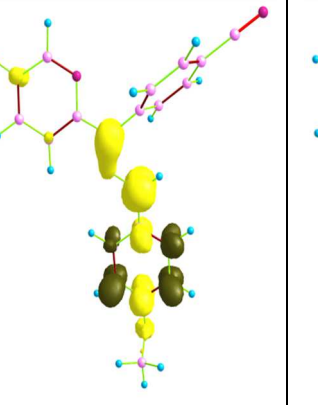
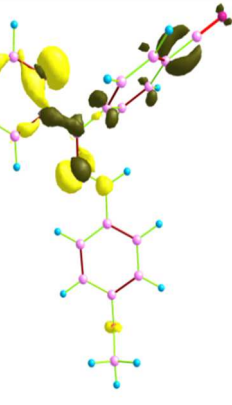
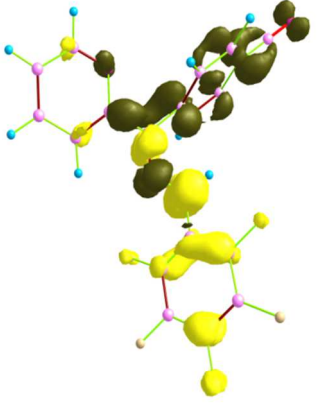
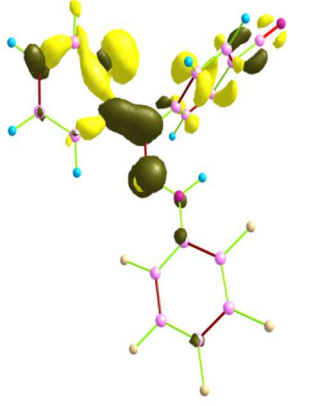
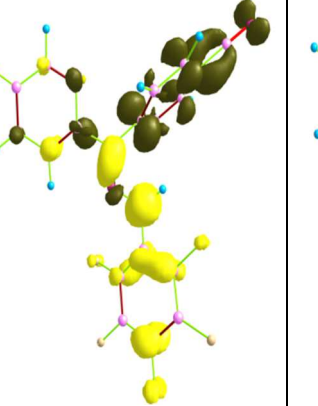
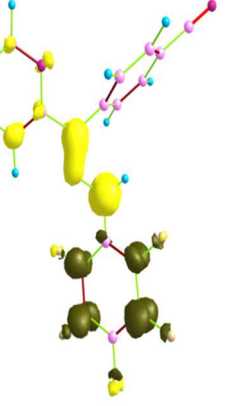
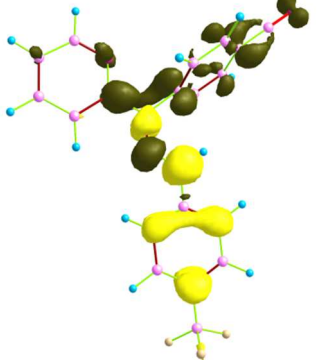
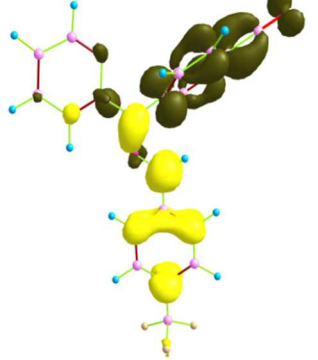
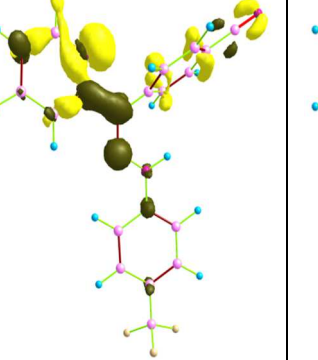
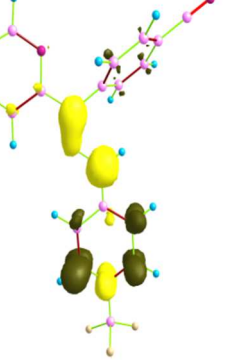
E4				
	S0→S1	S0→S3	S0→S7	S0→S14
E5				
	S0→S1	S0→S4	S0→S7	S0→S10
E6				
	S0→S1	S0→S3	S0→S7	S0→S8

E7				
	S0→S1	S0→S2	S0→S3	S0→S10
E8				
	S0→S1	S0→S3	S0→S4	S0→S9
E9				
	S0→S1	S0→S6	S0→S10	S0→S16

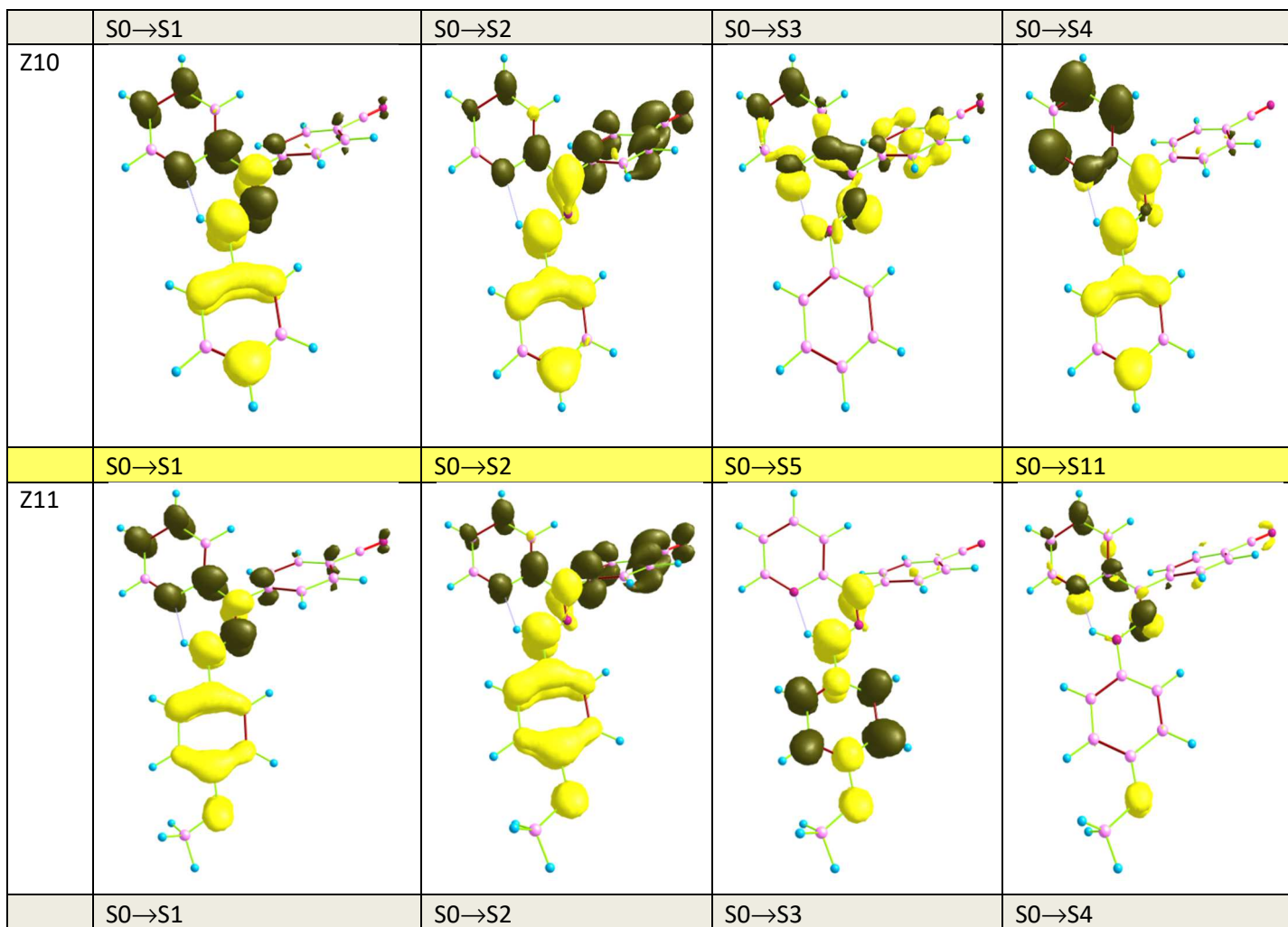
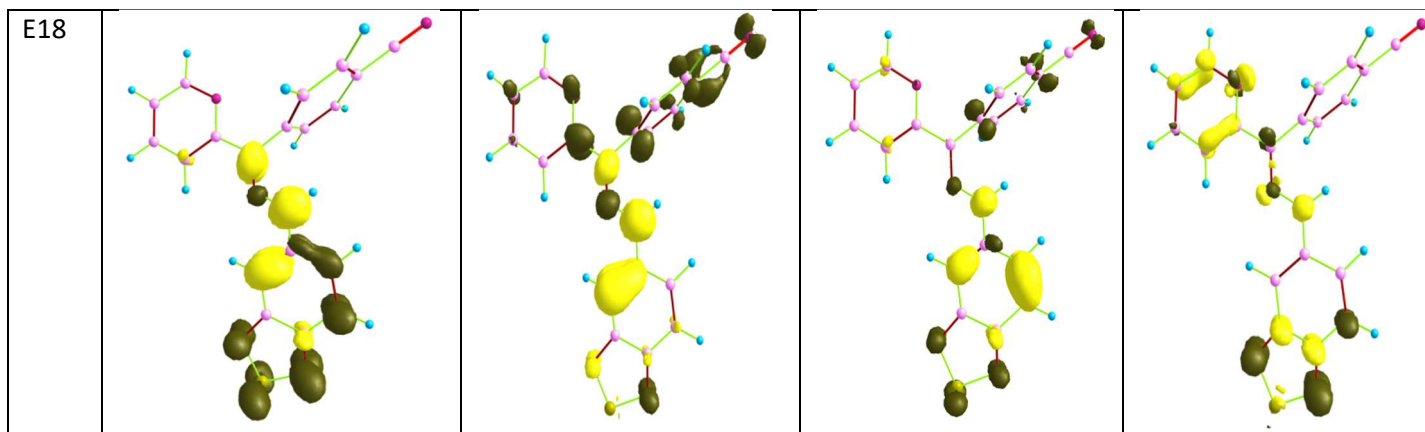
Z1				
	S0→S1	S0→S2	S0→S4	S0→S8
Z2				
	S0→S1	S0→S2	S0→S3	S0→S7
Z3				
	S0→S1	S0→S6	S0→S3	S0→S7

Z4				
	S0→S1	S0→S2	S0→S3	S0→S6
Z5				
	S0→S1	S0→S2	S0→S4	S0→S8
Z6				
	S0→S1	S0→S2	S0→S3	S0→S11

Z7				
	S0→S1	S0→S4	S0→S5	S0→S8
Z8				
	S0→S1	S0→S3	S0→S8	S0→S11
Z9				

	S0→S1	S0→S2	S0→S5	S0→S16
E10				
	S0→S1	S0→S2	S0→S3	S0→S10
E11				
	S0→S1	S0→S2	S0→S3	S0→S4
E12				
	S0→S1	S0→S2	S0→S3	S0→S4
E13				
	S0→S1	S0→S2	S0→S8	S0→S13

E14				
	S0→S1	S0→S4	S0→S7	S0→S15
E15				
	S0→S1	S0→S2	S0→S3	S0→S4
E16				
	S0→S1	S0→S2	S0→S4	S0→S13
E17				
	S0→S1	S0→S2	S0→S3	S0→S12



Z12				
	S0→S1	S0→S3	S0→S4	S0→S14
Z13				
	S0→S1	S0→S3	S0→S7	S0→S9
Z14				
	S0→S1	S0→S4	S0→S12	S0→S15
Z15				
	S0→S1	S0→S2	S0→S3	S0→S4

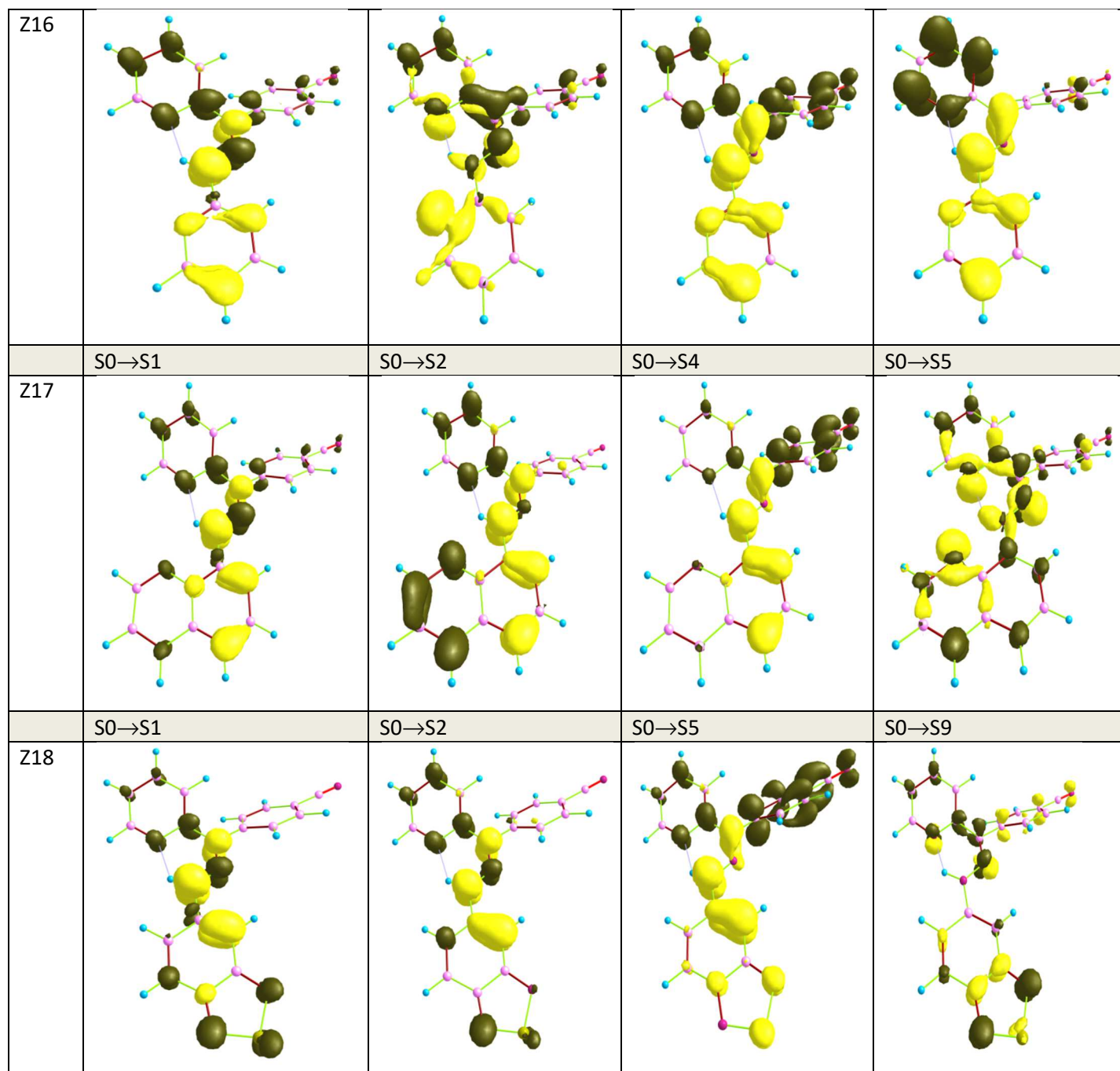
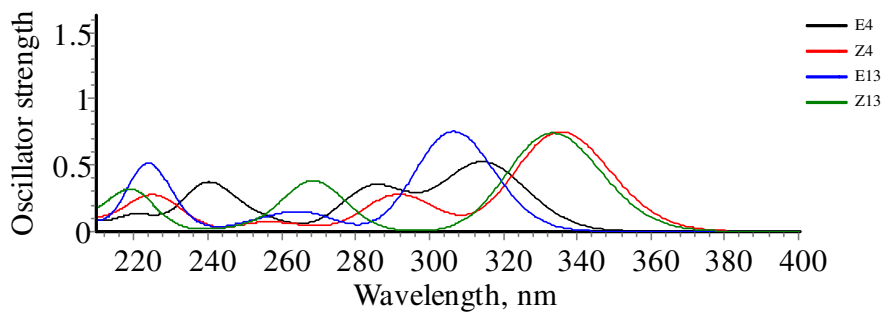
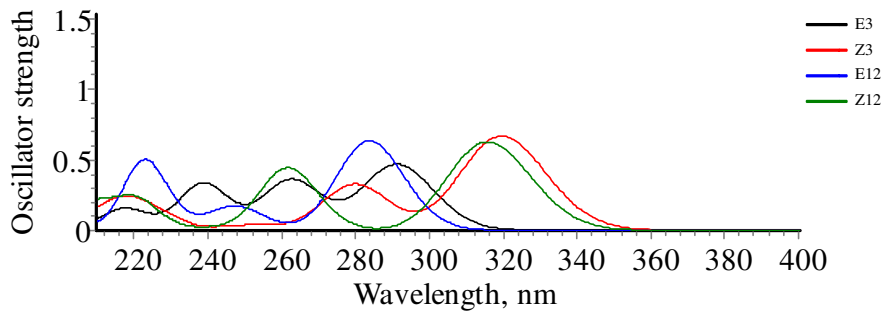
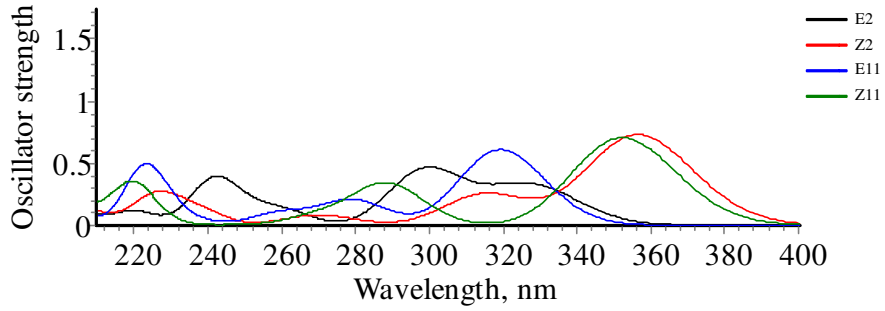
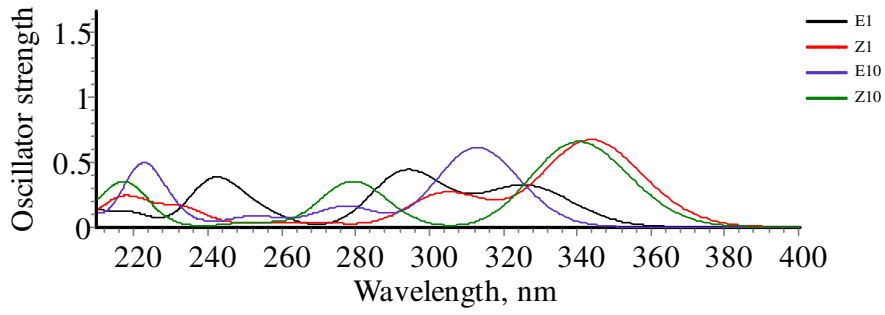
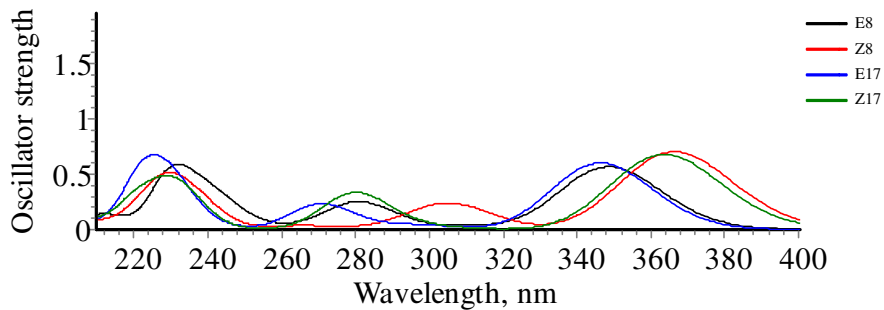
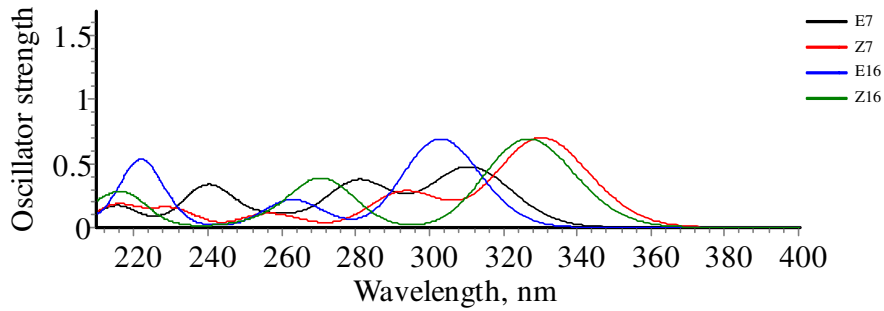
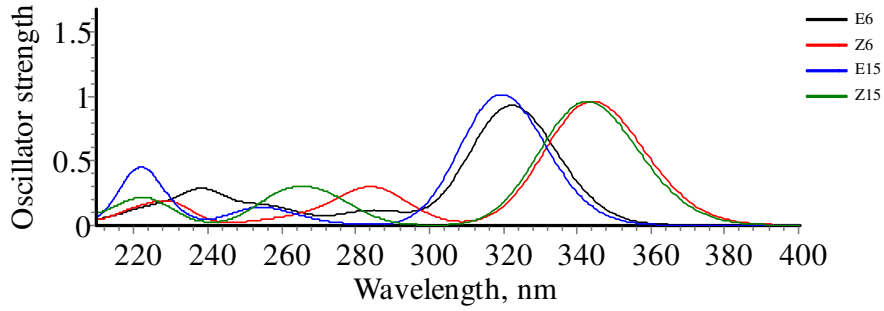
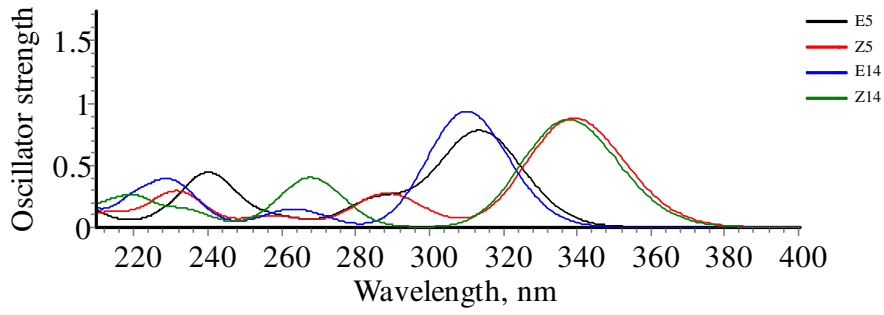


Figure S2. Electron density difference maps of title compounds from the ground state to the crucial excited state $S_0 \rightarrow S_n$ plotted using isovalues of 0.008 au





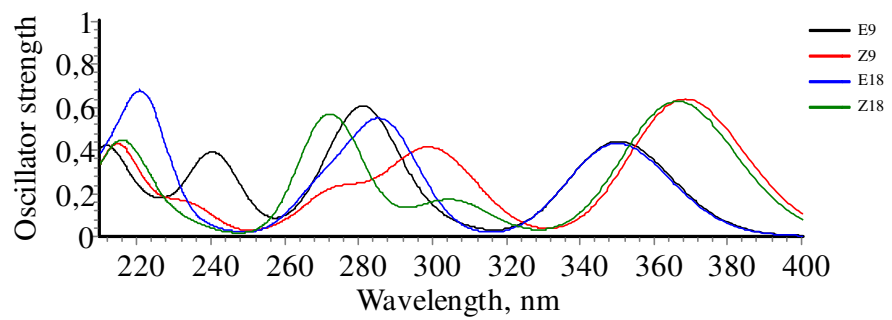
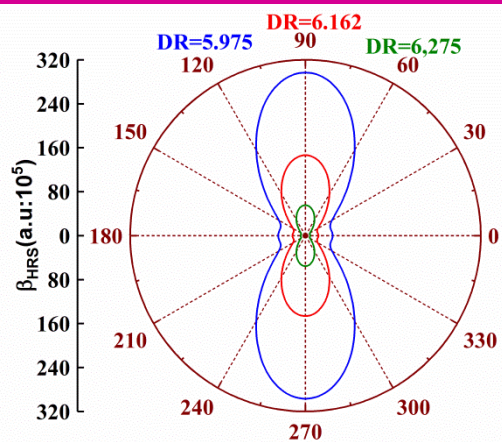
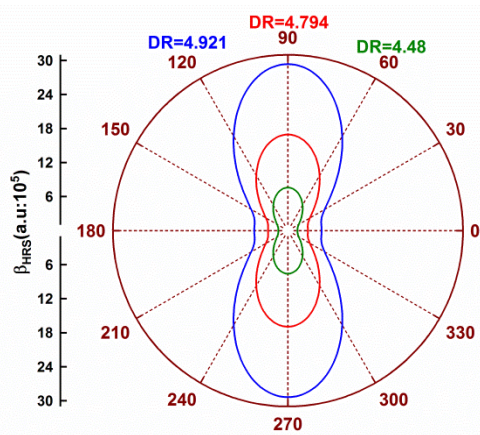


Figure S3. Calculated UV – vis absorption spectra of title compounds

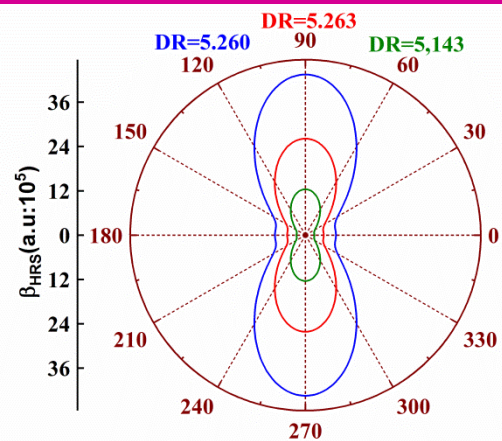
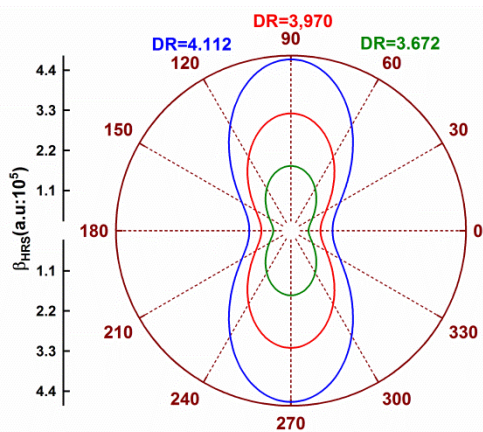
E-isomer

Z-Isomer

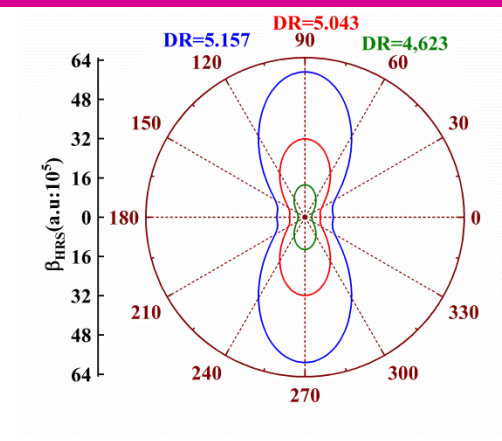
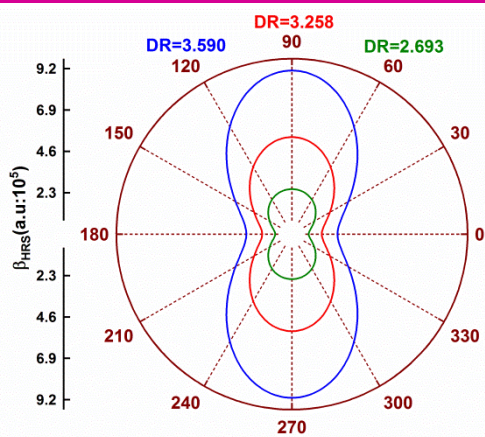
2



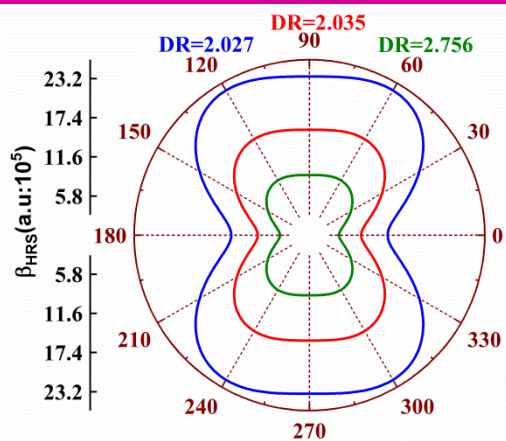
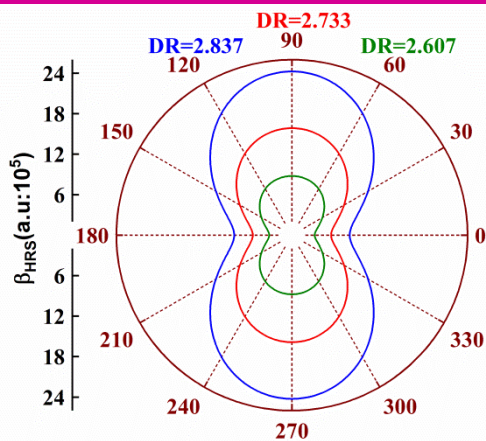
3



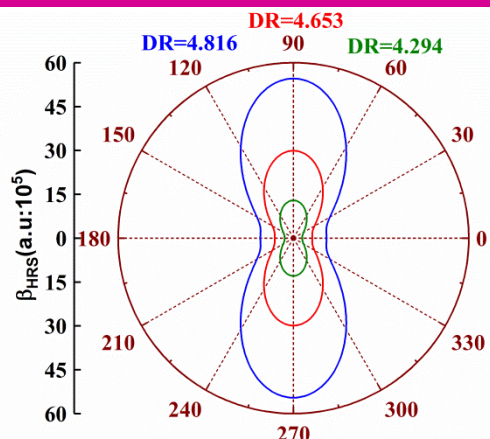
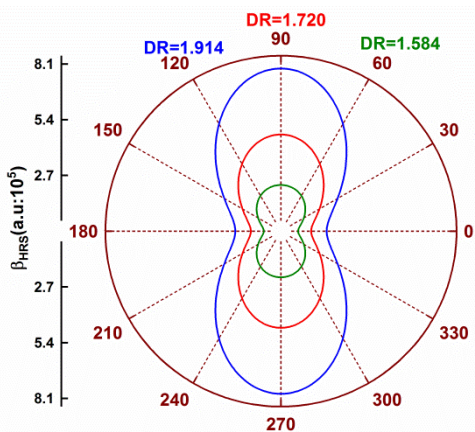
4



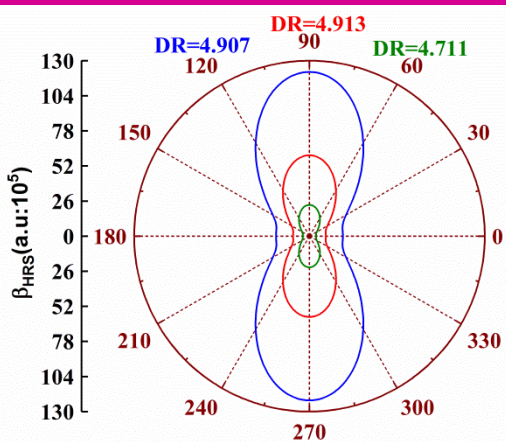
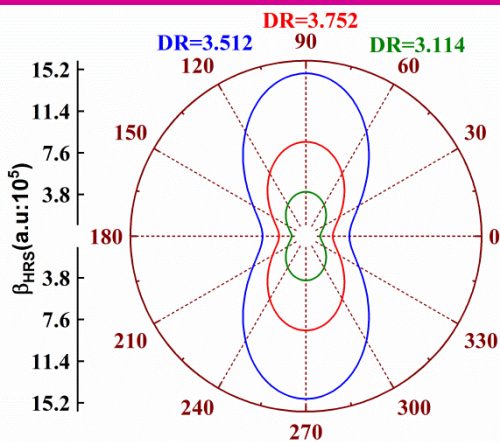
6



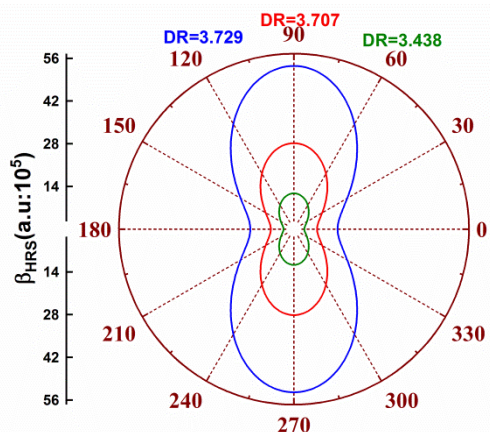
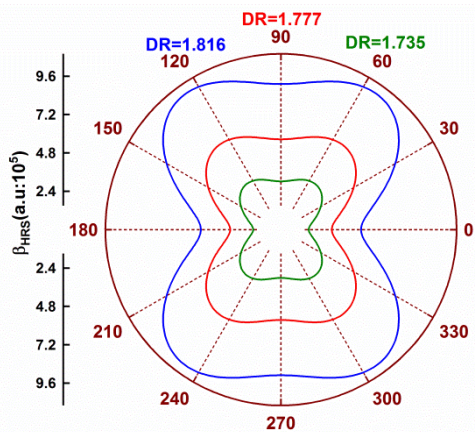
7



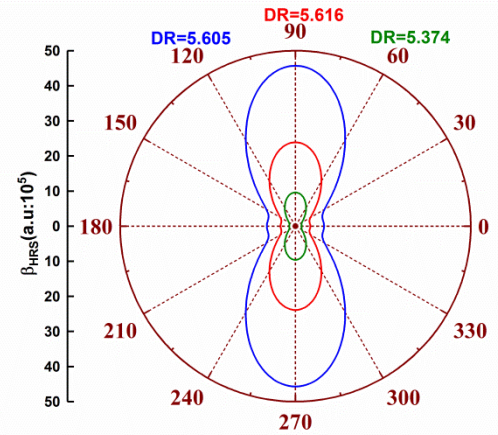
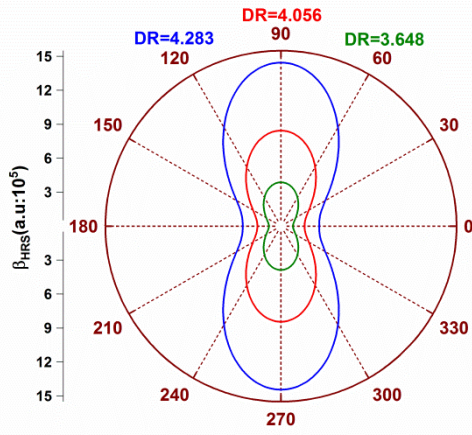
8



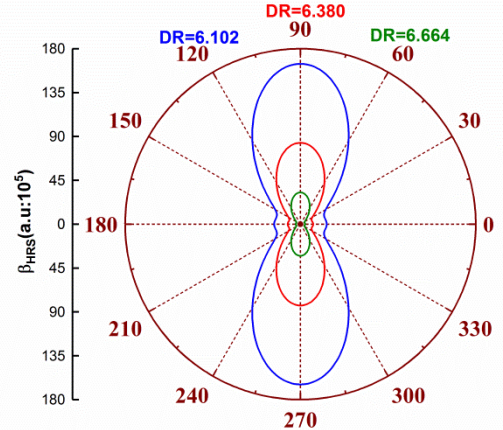
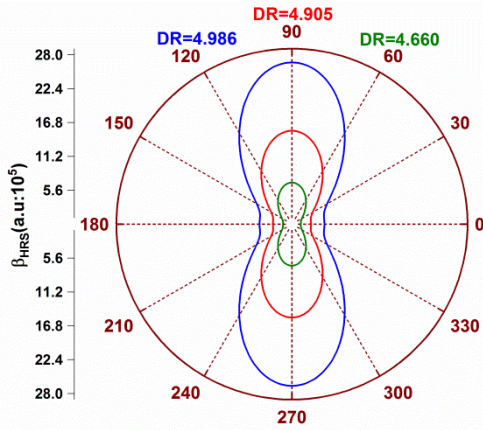
9



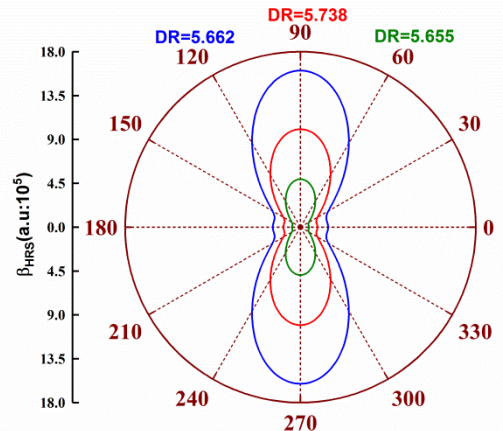
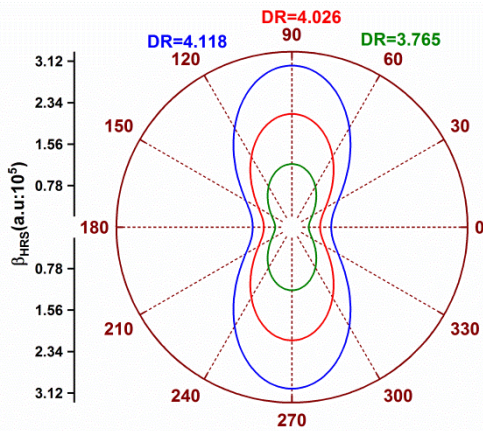
10



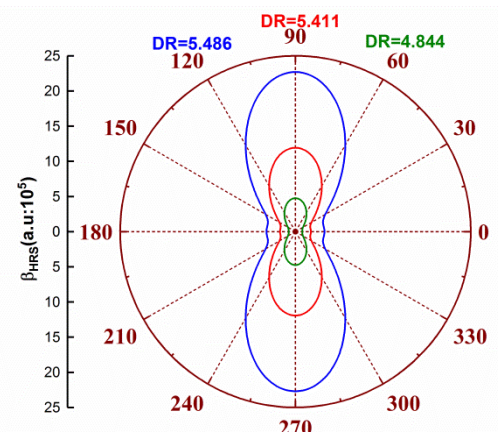
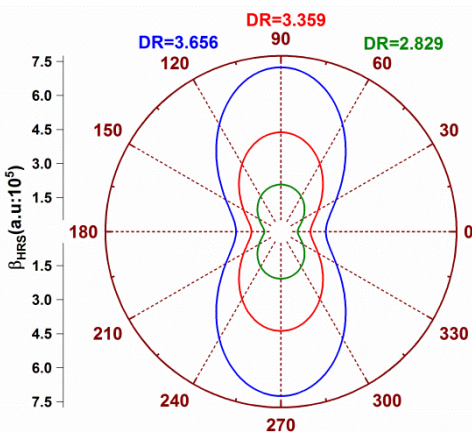
11



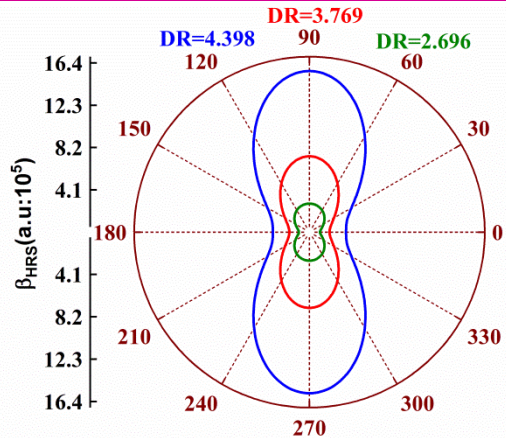
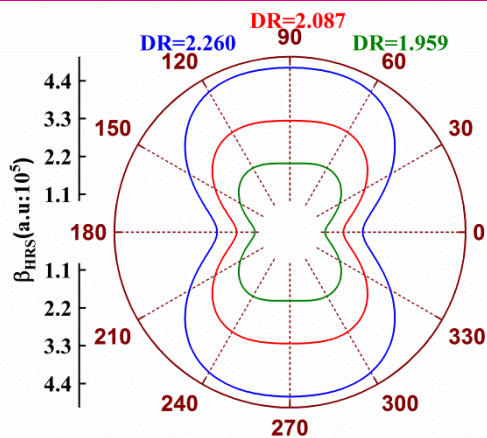
12



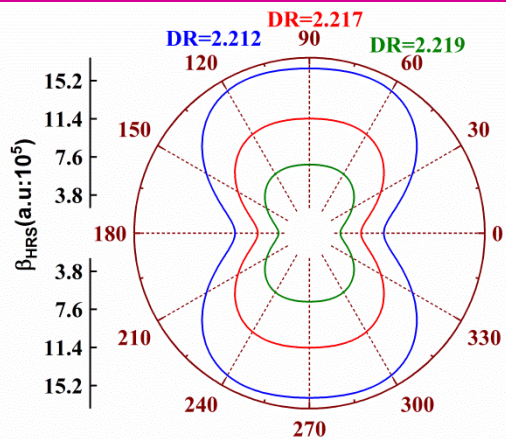
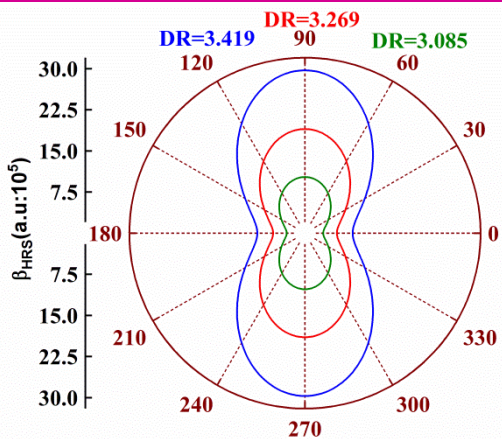
13



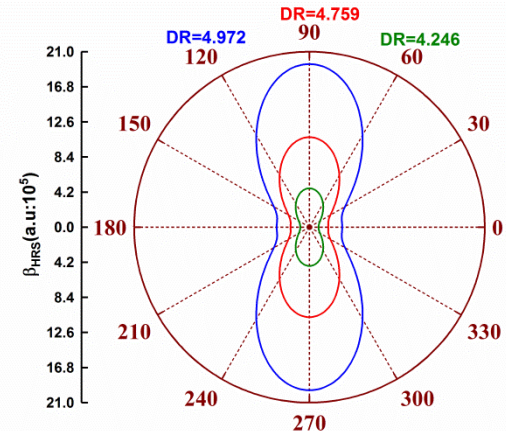
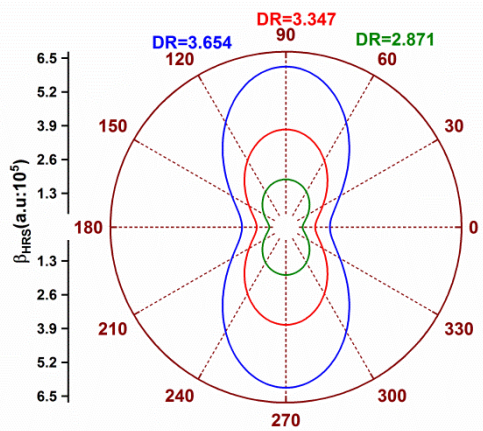
14



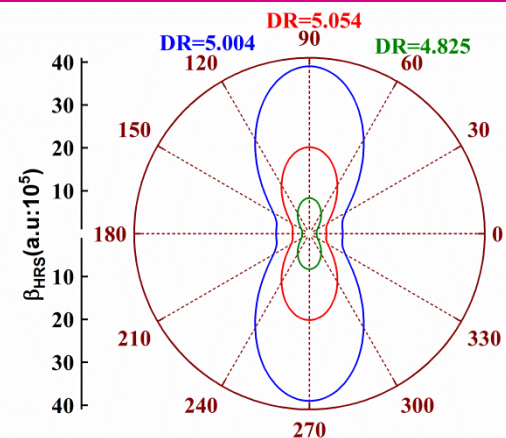
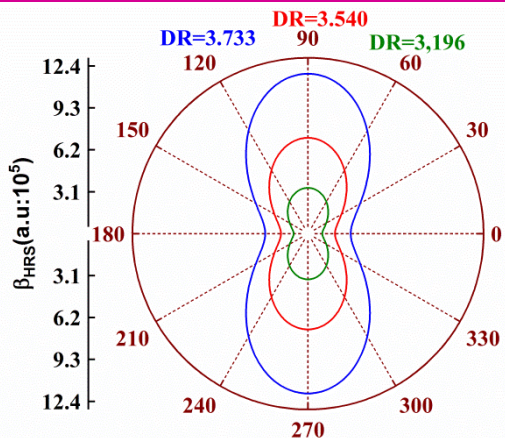
15



16



17



18

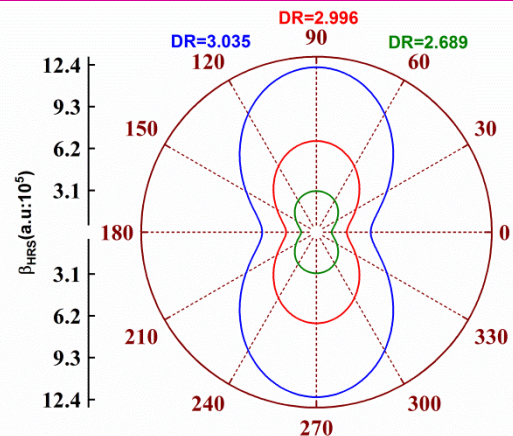
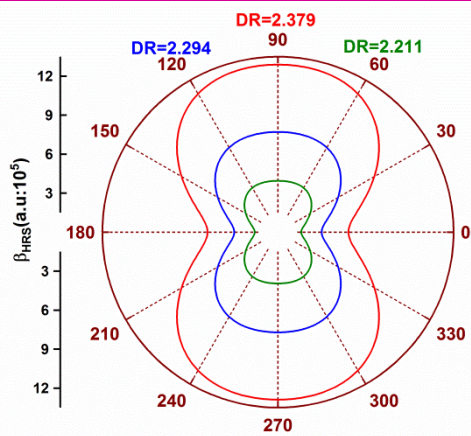


Figure S4. Relationship between $I_{\Psi\Psi}^{2w}$ and polarization angle Ψ of Z and E isomers (green static, red $\lambda=1340\text{nm}$, blue $\lambda=1064\text{nm}$)

Table S1. QTAIM calculated values of electron density (ρ), Laplacian ($\nabla^2(\rho)$), total electron energy density (H), kinetic electron energy density (G), and potential electron energy density (V) at bond critical points (au) for the Zi (i=1 to 18) compounds. **RCP:** ring critical point in N1-N2-C3-C4-N6-H; **BCP:** critical point in intramolecular H-bond N1-H...N6.

		ρ	∇	G	V	H			ρ	∇	G	V	H
Z1	RCP	0.015	0.099	0.019	-0.014	0.005	Z10	RCP	0.015	0.100	0.019	-0.014	0.005
	BCP	0.034	0.106	0.028	-0.029	-0.001		BCP	0.034	0.108	0.028	-0.030	-0.001
Z2	RCP	0.015	0.099	0.019	-0.014	0.005	Z11	RCP	0.015	0.099	0.019	-0.014	0.005
	BCP	0.034	0.107	0.028	-0.029	-0.001		BCP	0.034	0.107	0.028	-0.029	-0.001
Z3	RCP	0.016	0.101	0.020	-0.014	0.005	Z12	RCP	0.016	0.100	0.019	-0.014	0.005
	BCP	0.034	0.107	0.028	-0.029	-0.001		BCP	0.033	0.106	0.027	-0.029	-0.001
Z4	RCP	0.015	0.099	0.019	-0.014	0.005	Z13	RCP	0.015	0.100	0.019	-0.014	0.005
	BCP	0.034	0.107	0.028	-0.029	-0.001		BCP	0.035	0.109	0.029	-0.030	-0.001
Z5	RCP	0.015	0.099	0.019	-0.014	0.005	Z14	RCP	0.015	0.100	0.019	-0.014	0.005
	BCP	0.034	0.107	0.028	-0.030	0.001		BCP	0.034	0.107	0.028	-0.030	-0.001
Z6	RCP	0.015	0.100	0.019	-0.014	0.005	Z15	RCP	0.015	0.100	0.019	-0.014	0.005
	BCP	0.035	0.108	0.029	-0.030	-0.001		BCP	0.035	0.108	0.028	-0.030	-0.001
Z7	RCP	0.015	0.096	0.019	-0.013	-0.005	Z16	RCP	0.015	0.097	0.019	-0.013	0.005
	BCP	0.031	0.102	0.026	-0.026	-0.0004		BCP	0.031	0.103	0.026	-0.027	-0.0005
Z8	RCP	0.012	0.098	0.019	-0.014	0.005	Z17	RCP	0.015	0.098	0.019	-0.014	0.005
	BCP	0.032	0.104	0.026	-0.027	-0.0005		BCP	0.031	0.103	0.026	-0.027	-0.0003
Z9	RCP	0.016	0.100	0.019	-0.014	0.005	Z18	RCP	0.015	0.099	0.019	-0.014	0.005
	BCP	0.034	0.107	0.028	-0.029	-0.001		BCP	0.034	0.107	0.028	-0.029	-0.001

Table S2. Dihedral angles (φ) of Z and E isomers

Zi	φ_2	φ_1	φ'_2	φ'_1	φ_3	Ei	φ_2	φ_1	φ'_2	φ'_1
Z1	-43.81	-18.94	-177.88	3.64	130.50	E1	69.78	-174.47	1.03	-178.75
Z2	-42.30	-18.70	-177.95	4.11	130.30	E2	72.94	179.91	0.92	-179.03
Z3	-38.63	-25.01	-179.96	1.81	129.90	E3	69.92	175.36	-0.64	179.08
Z4	-45.89	-18.96	-175.20	3.25	130.72	E4	70.08	-173.64	1.52	-178.61
Z5	-46.95	-17.72	-178.33	3.42	130.70	E5	74.13	-175.16	1.53	-179.00
Z6	-46.89	-18.58	-178.24	3.17	131.13	E6	71.13	-174.14	1.56	-178.72
Z7	-43.62	-20.57	-178.18	3.28	127.69	E7	68.19	-173.24	1.45	-178.61
Z8	-42.57	-20.59	-177.98	3.70	127.52	E8	67.09	-172.88	1.56	-178.46
Z9	-41.07	-21.45	-178.33	3.62	130.77	E9	75.98	-175.55	1.23	-178.99
Z10	-45.81	-17.53	-178.51	3.79	130.61	E10	72.71	-175.80	1.42	-178.96
Z11	-44.21	-18.78	-177.85	3.69	130.56	E11	69.18	-172.95	1.38	-178.55
Z12	-38.28	-25.52	179.89	1.70	129.44	E12	71.71	174.29	-0.95	179.31
Z13	-45.89	-18.96	-178.20	3.25	130.70	E13	70.08	-173.64	1.52	-178.61
Z14	-46.71	-19.25	-178.29	3.11	130.93	E14	74.83	-173.69	1.12	-178.93
Z15	-47.43	-18.01	-178.76	2.97	130.91	E15	74.14	-173.45	1.16	-178.82
Z16	-44.42	-19.94	-178.60	3.42	127.82	E16	71.01	-174.92	1.51	-178.94
Z17	-42.11	-22.04	-177.73	3.68	127.51	E17	66.94	-173.00	1.57	-178.42
Z18	-44.01	-19.11	-178.95	3.31	130.48	E18	79.84	-176.62	1.13	-179.19

φ_3 : N1HN6

φ_2 : N2C3C5C7

φ_1 : N2C3C4N6

φ'_2 : N1N2C3C5

φ'_1 : N1N2C3C4

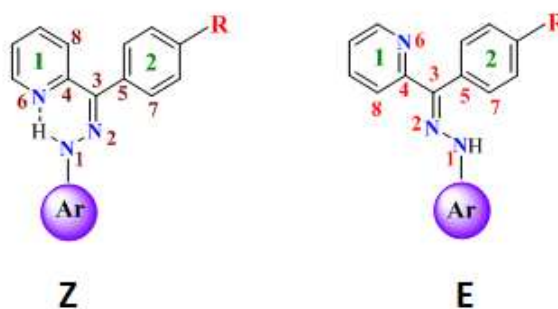


Table S3. Vertical transition energy ($\Delta E_{0 \rightarrow n}$, eV) and wavelength ($\Delta \lambda_{0 \rightarrow n}$, nm), oscillator strengths ($f_{0 \rightarrow n}$, dimensionless), charge transfer distances (q^{CT}), charge transfer distance (d^{CT} , Å), and dipole moment variation ($\Delta \mu_{0 \rightarrow n}$, D) associated to the $S_0 \rightarrow S_n$ transition, as calculated at the ω B97XD/6-311+g(d) of the studied E_i and Z_i ($i=1$ to 18) compounds

NO ₂	Sn	E	λ	f_{os}	%	d^{CT}	q^{CT}	$\Delta \mu_{0 \rightarrow n}$	Transition	MO contributions
E1 3.67*	1	3.798	326	0.316	65	5.690	0.755	20.640	H→L	TC (N1, Ar1, Ring1) To Ring 2
	3	4.217	294	0.435	67	4.202	0.628	12.674	H→L+1	TC Ring Ar1 To Ring 1, IC in Ring 1
	8	4.961	249	0.015	50	4.329	0.623	12.944	H→L+3	TC (N1, N2, Ar1)To Ring2 ,IC in Ring1
	5	5.808	213	0.010	40	5.022	0.656	15.822	H-3→L	TC Ring 1 To Ring 2 , IC in Ring 2
Z1 3.05*	1	3.606	344	0.673	48	5.092	0.710	17.368	H→L	TC Ring Ar1 To Ring2
	6	4.556	272	0.023	74	4.551	0.705	15.419	H→L+1	TC Ring Ar1 To Ring 1, IC in Ring 1
	10	5.337	232	0.054	42	5.029	0.574	13.870	H→L+2	TC (N1,Ar1) To Ring 1, IC in Ring 1
	16	5.801	214	0.102	32	6.237	0.625	18.717	H-1→L	TC Ar1 To Ring 2
E2	1	3.780	328	0.315	65	5.884	0.767	21.671	H→L	TC (N1,Ar2, Ring 1)To Ring 2
	3	4.148	299	0.437	63	4.539	0.647	14.117	H→L+1	TC Ring Ar2 To Ring1, IC in Ring 1
	5	4.770	260	0.105	72	1.637	0.542	4.285	H→L+4	TC(N1,N2 , Ring 1) To Ar2, IC in Ar2
	15	5.817	213	0.012	39	4.652	0.633	14.142	H→3-L	TC Ring 1 To Ring 2, IC in Ring 2
Z2	1	3.477	357	0.727	46	5.477	0.676	17.771	H→L+1	TC Ar2To Ring1
	2	3.921	316	0.230	34	5.738	0.733	20.195	H→L	TC Ar2To Ring2
	4	4.423	280	0.016	79	5.250	0.784	19.775	H→L+2	TC Ar2To Ring1
	8	4.750	261	0.016	34	5.707	0.509	13.958	H-4→L	TC Ring 3To Ring 2, IC in Ring 2
E3	1	4.002	309	0.002	81	2.245	0.753	8.114	H-7→L	IC in Ring 2
	2	4.257	291	0.467	54	5.111	0.666	16.342	H→L	TC (N1, Ar3,Ring 1) To Ring 2
	4	4.709	263	0.321	48	4.168	0.568	11.364	H→L+1	TC Ar3To Ring 1, IC in Ring 1
	9	5.221	237	0.018	48	3.456	0.629	10.447	H→L+4	TC (Ring 1 , N2) To Ar3,IC in Ar3
Z3	1	3.873	319	0.662	58	5.239	0.669	16.830	H→L	TC Ar3To Ring2
	2	4.000	309	0.006	70	4.374	0.808	16.980	H-5→L	IC in Ring 1
	3	4.427	280	0.321	52	4.258	0.619	12.654	H→L+1	TC Ar3To Ring 1, IC in Ring 1
	7	4.948	251	0.027	70	4.156	0.662	13.224	H→L+2	TC (N1, Ar3)To Ring 1
E4	1	3.931	315	0.463	50	4.771	0.666	15.252	H→L	TC(N1 , Ar4, Ring 1)To Ring 2
	3	4.349	285	0.344	52	4.520	0.636	13.805	H→L+1	TC Ar4 To Ring1 ,IC in Ring 1
	6	4.864	255	0.021	44	2.485	0.469	5.598	H-4→L	IC in Ring 2
	7	4.886	254	0.058	48	1.958	0.467	4.390	H→L+4	TC (N1, N2), IC in Ar4
Z4	1	3.693	336	0.752	48	5.130	0.691	17.020	H→L	TC (Ar4, Ring 1)To Ring 2
	3	4.250	292	0.279	44	5.136	0.610	15.054	H→L+1	TC Ar4 To Ring1
	6	4.694	264	0.025	70	4.367	0.671	14.075	H→L+2	TC (N1, Ar4)To Ring 2, IC in Ring 1
	7	4.819	257	0.015	34	4.334	0.472	9.834	H-3→L	TC Ring 1 To Ring 2, IC in Ring 2
E5	1	3.945	314	0.697	50	4.366	0.612	12.832	H→L+1	IC in Ring(Ar5,1)
	3	4.331	286	0.231	52	5.542	0.695	18.509	H→L	TC (N1, Ring (Ar5,1))To Ring 2
	7	4.894	253	0.020	67	2.958	0.568	8.067	H-4→L	IC in Ring 2
	14	5.768	215	0.003	72	2.314	0.868	9.647	H→L+6	TC (N1, N2, Ar5, R1)
Z5	1	3.655	339	0.879	52	5.600	0.688	18.496	H→L	TC Ar5To Ring 2
	2	4.000	309	0.004	65	4.401	0.786	16.608	H-6→L	IC in Ring 2
	3	4.297	288	0.272	46	5.177	0.636	15.819	H→L+1	TC Ar5To Ring1
	6	4.720	263	0.017	60	4.541	0.620	13.523	H-L+2	TC N1, Ar5 To Ring1
E6	1	3.844	322	0.923	52	2.335	0.674	7.557	H→L+1	TC N1, IC in Ring (Ar6,1)
	4	4.348	285	0.115	48	3.629	0.720	12.547	H→L	TC(N1, Ring (Ar6,1))To Ring2
	7	4.707	263	0.050	44	0.935	0.471	2.117	H→L+2	IC in Ring (Ar6,1)
	10	4.888	254	0.035	56	2.338	0.543	6.102	H-4→L	IC in Ring2

Z6	1	3.601	344	0.960	67	4.205	0.665	13.435	H→L	TC Ar6 To Ring 2, IC in Ar6
	2	4.000	309	0.002	50	5.670	0.830	22.603	H-7→L	TC Ring 2To Ar6, IC in Ring 2
	4	4.350	285	0.283	50	3.099	0.633	9.427	H→L+1	TC (N1, Ar6)To Ring 2, IC in Rings
	8	4.598	269	0.062	67	0.953	0.618	2.830	H→L+2	(Ar6, 1) IC in Rings (Ar6,1)
E7 3.85*	1	3.971	312	0.314	42	3.549	0.670	11.426	H→L	TC(N1, Ar7)To Ring 2
	3	4.413	281	0.366	56	4.348	0.619	12.933	H→L+1	TC Ar7 To Ring 1, IC in Ring 1
	7	4.850	256	0.012	40	2.725	0.519	6.787	H-4→L	IC in Ring 2
	8	5.058	245	0.016	50	3.465	0.558	9.280	H→L+2	TC(N1,N2, Ar7)To Ring 2, IC in Ring 1
Z7 3.20*	1	3.751	330	0.696	50	5.250	0.695	17.516	H→L	TC Ring (Ar7, 1) To Ring 2
	2	4.002	309	0.005	74	3.075	0.743	10.977	H-7→L	IC in Ring 2
	3	4.223	294	0.282	48	4.829	0.656	15.224	H→L+1	TC Ar7, To Ring 1, IC in Ring1
	11	5.459	227	0.040	56	4.978	0.589	14.076	H→L+3	TC(N1,N2 , Ar7) To Ring 2
E8	1	3.556	349	0.56	64	3.659	0.663	10.590	H→L+1	TC N1 , IC in Ring(Ar8, 1)
	2	3.961	313	0.026	37	3.303	0.652	10.338	H→L	TC Ring((Ar8,1),N1) To R2
	4	4.349	285	0.107	58	1.860	0.538	4.804	H→L+2	IC in Ring(Ar8,1)
	10	4.957	250	0.017	56	4.248	0.652	13.310	H→L+3	TC (N1, N2 , Ar8) To Ring 2
Z8	1	3.384	366	0.706	48	5.096	0.660	16.146	H→L	TC Ar8 To Ring2
	4	4.170	297	0.057	87	2.493	0.638	7.647	H→L+2	IC in(Ar8, R1)
	5	4.417	281	0.07	50	1.553	0.439	3.278	H→L+4	IC in Ar8, TC(N1,N2)
	8	4.610	269	0.023	70	4.739	0.693	15.769	H→L+3	TC(Ar8 , N1)TO Ring1
E9	1	3.537	351	0.441	72	2.002	0.566	5.440	H→L+1	IC in Ar9 and ring 1
	3	4.128	300	0.054	54	5.575	0.665	17.798	H→L	TC(N1, Ring(Ar9 , 1))To Ring2
	4	4.397	281	0.546	60	3.057	0.503	7.384	H→L+2	IC in (Ar9, Ring1)
	9	4.889	254	0.018	65	2.093	0.571	5.735	H-4→L	IC in Ring2
Z9	1	3.364	369	0.638	74	4.519	0.562	12.204	H→L	TC Ar9 To Ring 2, IC in Ar9
	3	4.058	306	0.202	58	2.373	0.523	5.955	H→L+2	TC Ar9 To Ring 1, IC in Ar9
	8	4.665	266	0.017	67	4.960	0.634	15.099	H→L+3	TC(N1, Ar9) To Ring1
	11	5.241	237	0.095	44	4.758	0.359	8.127	H-2→L	TC Ar9 To Ring2, IC in Ring(Ar9,2)

	Sn	E(ev)	λ	f_{os}	%	d^{CT}	q^{CT}	μ^{CT}	Type	MO contributions
E10	1	3.962	312	0.615	81	4.256	0.672	13.736	H→L	TC Ar1 To Ring 2, IC in Ring 1
	2	4.471	277	0.162	81	4.358	0.698	14.612	H→L+1	TC(Ar1,N1) to Ring 2 ,IC in Ring 1
	5	4.941	250	0.008	64	4.093	0.700	13.765	H→L+2	TC Ring (Ar10,N1,N2) to Ring 2,IC in Ring 1
	16	6.146	201	0.013	42	1.137	0.449	2.454	H-4→L	IC in Ring (2,1)
Z10	1	3.642	340	0.659	92	3.551	0.608	10.370	H→L	TC Ar1To Ring1 ,IC in Ring 1
	2	4.435	279	0.345	84	5.058	0.767	18.636	H→L+1	TC Ring(Ar1,N1)To Ring 2,IC in Ring 1
	3	4.539	273	0.004	46	1.448	0.507	3.529	H-3→L	IC in Ring(2 ,1)
	4	4.554	272	0.010	74	4.555	0.677	14.819	H→L+2	TC(Ar10 ,N1) To Ring1
E11	1	3.883	319	0.609	82	4.562	0.690	15.111	H→L	TC (Ar2, N1 N2) To Ring 2
	2	4.437	279	0.2046	81	4.597	0.706	15.582	H→L+1	TC Ar2 To Ring 2
	3	4.758	260	0.100	67	1.273	0.564	3.452	H→L+4	TC (N1,N2) To Ar2,IC in Ar11
	10	5.540	223	0.363	23	1.256	0.415	2.506	H-3 →L	IC in Ring2
Z11	1	3.519	352	0.704	89	4.509	0.649	14.044	H → L	TC Ar2 to Ring 1
	2	4.294	288	0.327	79	5.682	0.796	21.728	H→L+1	TC (Ar2,N2) To Ring 2
	5	4.587	270	0.082	76	1.636	0.564	4.433	H→L+5	IC in Ar2,TC N2 To Ar2
	11	5.635	220	0.175	36	2.256	0.368	3.988	H-4→L	TC Ring 2 To Ring 1
E12	1	4.370	283	0.634	84	3.651	0.601	10.543	H →L	TC Ar3 to Ring 2
	2	4.783	259	0.004	33	1.522	0.472	3.449	H-1→L	IC in Ring(2 ,1)
	3	4.995	248	0.154	67	4.029	0.608	11.767	H→L+1	TC Ar3 to Ring 2, IC in Ring 1
	4	5.116	242	0.018	36	3.591	0.451	7.782	H→L+5	TC (N1,N2 Ring 1) To Ar3, IC inAr12

Z12	1	3.925	315	0.6271	92	3.078	0.561	8.291	H→L	TC Ar3 to Ring 1 , IC in Ring 1
	2	4.573	271	0.002	46	0.542	0.511	1.332	H-4→L	TC(Ar3,N1 ,N2) To Ring 2
	3	4.735	261	0.437	79	4.248	0.689	14.062	H→L+1	TC from Ar3 to the Rings and IC in the rings
	4	4.881	254	0.008	65	3.905	0.637	11.954	H→L+2	TC (N1, Ar3) to Ring 1
E13	1	4.044	306	0.754	87	3.666	0.611	10.755	H→L	IC in Ring 1,TC Ar13To Ring 2
	2	4.652	266	0.130	84	4.527	0.722	15.692	H→L+1	TC Ar4 to Ring 2
	3	4.806	257	0.002	35	2.388	0.513	5.878	H-1→L	IC in Ring 2, Ring 1
	4	4.877	254	0.059	60	1.827	0.507	4.451	H→L+4	IC in Ar4,TC (N1,N2)
Z13	1	3.718	333	0.743	92	3.242	0.587	9.146	H→L	TC Ar4 To Ring 1,IC in Ring 1
	3	4.611	268	0.361	79	5.045	0.736	17.826	H→L+1	TC (Ar4,N1, N2)To Ring2,IC in Ring 1
	4	4.710	263	0.013	79	4.510	0.725	15.701	H→L+2	TC(Ar4,N1)To Ring 1 ,IC in Ring 1
	14	5.948	208	0.053	56	4.277	0.509	10.465	H-2→L	TC Ar4 To Ring 1,IC in Ring 1
E14	1	3.998	310	0.934	98	3.368	0.566	9.165	H→L	TC Ar5 To Ring 2
	2	4.677	265	0.109	84	4.987	0.765	18.335	H→L+1	TC (Ar5, N1,N2) To Ring 2
	8	5.342	232	0.218	32	0.774	0.409	1.522	H→L+3	IC In(Ar5, Ring 1)
	13	5.835	212	0.032	32	0.369	0.377	0.667	H-1→L	TC Ring 1 To Ring 2 ,IC in Ring 2
Z14	1	3.671	337	0.867	92	3.374	0.578	9.365	H→L	TC Ar5 To Ring 1
	3	4.617	268	0.360	74	5.310	0.719	18.344	H→L+1	TC (Ar5, N1,N2) To Ring 2,IC in Ring 1
	7	5.293	234	0.129	56	2.208	0.441	4.673	H→L+3	IC in Ar5
	9	5.568	222	0.047	52	2.829	0.417	5.662	H-1→L	TC(Ar5, Ring2)To Ring1
E15	1	3.879	319	1.013	89	2.666	0.599	7.676	H→L	IC in Ring(Ar6,1) and TC(N1)
	4	4.628	267	0.023	64	3.126	0.691	10.378	H→L+1	TC Ring(Ar6,1) To Ring 2
	7	4.899	253	0.113	46	0.604	0.481	1.395	H→L+2	IC in Ring 1,TC Ar6 to Ring 2
	15	5.820	213	0.015	32	2.322	0.462	5.159	H-2→L	IC in Ring (Ar6,1) TC N1
Z15	1	3.617	342	0.958	92	0.390	0.558	1.046	H→L	IC in Ring(Ar6,1)
	4	4.555	272	0.149	50	1.312	0.498	3.141	H→L+1	IC in Ring(Ar6,1) , TC Ring 2
	12	5.577	222	0.022	36	3.674	0.398	7.030	H-1→L	TC Ring 2 To Ring 1, IC in Ar6
	15	5.758	215	0.042	40	3.871	0.446	8.286	H→L+4	TC (Ar6,N1 ,N2)To Ring 2, IC in Ring1
E16	1	4.092	302	0.690	89	3.749	0.589	10.600	H→L	IC in Ring 1, TC Ar7 to Ring 2
	2	4.702	263	0.189	79	4.377	0.649	13.646	H→L+1	IC in Ring 1, TC Ar7 to Ring 2
	3	4.789	258	0.028	60	0.633	0.541	1.645	H→L+3	TC(N1,N2) , IC in (Ar7, Ring1)
	4	4.810	257	0.004	32	1.828	0.435	3.820	H-1→L	IC in Ring(2 , 1)
Z16	1	3.794	326	0.689	89	3.449	0.574	9.507	H→L	TC Ar7 to Ring1, IC in Ring2
	2	4.526	273	0.012	42	2.926	0.556	7.812	H-2→L	TC Ar7 to Ring 2 , IC in Ring 1
	3	4.571	271	0.356	81	4.820	0.709	16.407	H→L+1	TC(Ar7,N1,N2)to Ring 2,IC in Ring 1
	4	4.729	262	0.007	76	4.129	0.680	13.497	H→L+2	TC(Ar7,N1,N2)to Ring 1,IC in Ring 1
E17	1	3.580	346	0.604	92	1.803	0.542	4.694	H→L	IC in (Ar8, Ring 1)
	2	4.177	296	0.043	67	3.761	0.689	12.442	H→L+1	TC Ring 1 To Ring 2,IC in Ar8
	4	4.583	270	0.227	62	2.911	0.627	8.773	H→L+2	TC Ar8 to Ring 1,IC in Ring 1
	13	5.518	224	0.028	48	1.804	0.329	2.854	H-1→L	TC Ar8 to Ring 1,IC in Ar17
Z17	1	3.409	363	0.6803	92	2.480	0.552	6.575	H→L	TC Ar8 to Ring 2, IC in Ar17
	2	4.148	298	0.028	84	2.400	0.639	7.362	H→L+2	TC Ar8 to Ring 1 ,IC in Ar17
	4	4.426	280	0.299	64	4.405	0.627	13.275	H→L+1	TC (Ar8 ,N1,N2) to Ring 2
	5	4.475	277	0.006	56	0.531	0.634	1.617	H-3→L	IC in (Ring 1, Ar8)
E18	1	3.540	350	0.430	92	3.120	0.509	7.629	H→L	TC N1, IC in(Ar9, Ring 1)
	2	4.321	286	0.507	48	3.843	0.556	10.249	H→L+2	IC in Ring 1,TC Ar9 to Ring 1
	3	4.577	270	0.155	58	1.661	0.413	3.298	H-1→L	TC N1, IC in (Ar9, Ring1)
	12	5.514	224	0.196	46	2.278	0.368	4.028	H-2→L	TC Ring 1 to Ar9,IC in Ar9
Z18	1	3.383	366	0.626	92	0.740	0.502	1.783	H→L	IC in Ar9
	2	4.068	304	0.169	79	0.805	0.520	2.012	H→L+1	IC in(Ar9, Ring 1)
	5	4.579	270	0.324	72	5.238	0.726	18.272	H→L+2	TC (Ar9, N1,N2) to Ring2,IC in Ring 1
	9	5.298	233	0.043	46	1.804	0.405	3.510	H-2→L	TC Ring 2 To Ring 1, IC in Ar9

*The experimental values were derived from λ_{\max} values obtained by measurements in toluene¹.

$\Delta\mu_{0 \rightarrow n}$: is equal to the difference between the dipole moments calculated for the ground and excited states is calculated by using this $(\Delta\mu_{0 \rightarrow n} = q^{CT} \times d^{CT})^2$

Table S4. Second harmonic generation ($\beta_{SHG}^\lambda \equiv \beta(-2\omega; \omega, \omega)$, a.u.), electrooptic Pockels effect ($\beta_{EOPE}^\lambda \equiv \beta(-\omega; \omega, 0)$, a.u.), dynamic hyper-Rayleigh scattering (β_{HRS}^λ , a. u.) and depolarization ratio DR^λ of E_i and Z_i (i=1 to 18) compounds ($\lambda = 695, 1064$ and 1340 nm)

	$\beta_{SHG}^{\lambda=695}$	$\beta_{EOPE}^{\lambda=695}$	$\beta_{HRS}^{\lambda=695}$	DR^{695}		$\beta_{SHG}^{\lambda=695}$	$\beta_{EOPE}^{\lambda=695}$	$\beta_{HRS}^{\lambda=695}$	DR^{695}		$\beta_{SHG}^{\lambda=695}$	$\beta_{EOPE}^{\lambda=695}$	$\beta_{HRS}^{\lambda=695}$	DR^{695}		$\beta_{SHG}^{\lambda=695}$	$\beta_{EOPE}^{\lambda=695}$	$\beta_{HRS}^{\lambda=695}$	DR^{695}
E1	25075	2851	10110	4.057	Z1	337631	7093	142527	2.799	E10	16246	2583	6706	4.613	Z10	128929	4798	53105	3.640
E2	31810	3828	12826	4.363	Z2	186223	12101	83184	2.316	E11	25820	3662	10518	4.663	Z11	286677	9137	120302	3.606
E3	5303	1545	2148	4.571	Z3	29683	4811	11983	4.036	E12	3885	1252	1622	4.447	Z12	16610	3019	6616	4.171
E4	13900	1944	5631	4.160	Z4	84890	5402	34862	3.326	E13	10502	1743	4392	4.390	Z13	52331	3382	21375	3.896
E5	10702	771	4575	3.572	Z5	120788	4346	50083	3.134	E14	8784	1034	3929	3.643	Z14	80569	2545	33158	3.650
E6	15368	2888	7521	3.546	Z6	65892	2154	45757	0.612	E15	19273	3477	8750	4.020	Z15	14518	2003	18306	0.720
E7	11730	1802	4749	4.198	Z7	57049	5115	23460	3.454	E16	8837	1610	3695	4.447	Z16	31400	3104	12705	3.842
E8	183181	2532	83555	1.776	Z8	33853	7461	18530	1.020	E17	161806	2266	70219	2.403	Z17	24526	4349	11930	1.573
E9	90612	1028	40594	4.087	Z9	6955	4742	8620	0.174	E18	124164	1781	54949	4.220	Z18	7393	2191	4304	0.769
	$\beta_{SHG}^{\lambda=1064}$	$\beta_{EOPE}^{\lambda=1064}$	$\beta_{HRS}^{\lambda=1064}$	DR^{1064}		$\beta_{SHG}^{\lambda=1064}$	$\beta_{EOPE}^{\lambda=1064}$	$\beta_{HRS}^{\lambda=1064}$	DR^{1064}		$\beta_{SHG}^{\lambda=1064}$	$\beta_{EOPE}^{\lambda=1064}$	$\beta_{HRS}^{\lambda=1064}$	DR^{1064}		$\beta_{SHG}^{\lambda=1064}$	$\beta_{EOPE}^{\lambda=1064}$	$\beta_{HRS}^{\lambda=1064}$	DR^{1064}
E1	3438	2027	1469	4.350	Z1	8736	4921	3505	5.299	E10	3077	1876	1334	4.283	Z10	5894	3342	2320	5.605
E2	4562	2795	1879	4.921	Z2	15113	8299	5885	5.975	E11	4353	2684	1791	4.986	Z11	11289	6376	4374	6.102
E3	1751	1228	763	4.112	Z3	5646	3611	2274	5.260	E12	1405	1016	614	4.118	Z12	3502	2322	1374	5.662
E4	2346	1378	1078	3.590	Z4	6591	3796	2658	5.157	E13	2077	1267	960	3.656	Z13	4157	2348	1637	5.486
E5	1042	440	847	1.914	Z5	5473	2878	2288	4.506	E14	1240	785	830	2.260	Z14	3325	1561	1384	4.398
E6	3325	2250	1811	2.837	Z6	2440	1732	1873	2.027	E15	4024	2680	1959	3.419	Z15	2216	1662	1544	2.212
E7	2175	1269	1004	3.562	Z7	6208	3613	2566	4.816	E16	1915	1170	886	3.654	Z16	3770	2189	1531	4.972
E8	3066	1806	1370	3.752	Z8	9379	5066	3826	4.907	E17	2697	1662	1224	3.733	Z17	5394	3018	2163	5.004
E9	1239	769	1188	1.816	Z9	5863	3273	2603	3.729	E18	2124	1334	1353	2.379	Z18	2712	1498	1274	3.035
	$\beta_{SHG}^{\lambda=1340}$	$\beta_{EOPE}^{\lambda=1340}$	$\beta_{HRS}^{\lambda=1340}$	DR^{1340}		$\beta_{SHG}^{\lambda=1340}$	$\beta_{EOPE}^{\lambda=1340}$	$\beta_{HRS}^{\lambda=1340}$	DR^{1340}		$\beta_{SHG}^{\lambda=1340}$	$\beta_{EOPE}^{\lambda=1340}$	$\beta_{HRS}^{\lambda=1340}$	DR^{1340}		$\beta_{SHG}^{\lambda=1340}$	$\beta_{EOPE}^{\lambda=1340}$	$\beta_{HRS}^{\lambda=1340}$	DR^{1340}
E1	2531	1858	1116	4.065	Z1	6239	4490	2530	5.242	E10	2310	1730	1025	4.056	Z10	4226	3054	1677	5.616
E2	3429	2582	1430	4.794	Z2	19593	7564	4123	6.162	E11	3284	2482	1362	4.905	Z11	8046	5837	3106	6.380
E3	1426	1159	634	3.970	Z3	4351	3360	1763	5.263	E12	1163	964	515	4.026	Z12	2752	2176	1086	5.738
E4	1725	1262	839	3.258	Z4	4773	3474	1954	5.043	E13	1559	1168	753	3.359	Z13	2975	2144	1188	5.411
E5	633	387	696	1.720	Z5	3762	2594	1641	4.136	E14	932	742	692	2.087	Z14	2148	1378	963	3.769
E6	2646	2114	1471	2.733	Z6	1996	1639	1526	2.035	E15	3174	2510	1574	3.269	Z15	1881	1583	1287	2.217
E7	1596	1158	783	3.211	Z7	4529	3310	1906	4.653	E16	1441	1078	698	3.347	Z16	2747	2005	1141	4.759
E8	2250	1658	1050	3.512	Z8	6511	4604	2684	4.913	E17	2034	1537	952	3.540	Z17	3824	2758	1553	5.054
E9	926	719	939	1.777	Z9	4164	2983	1890	3.707	E18	1607	1245	1052	2.294	Z18	1917	1363	948	2.996

Table S5. Static and dynamic β_{ji} values of Ei and Zi (i=1 to 18) compounds

	static				695				1064				1340				
	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$			
E1	1245	1545	17611	18700	2626	2562	1945	2061	Z1	3026	2477	204135	340680	6668	5027	4798	3672
E2	1740	1637	22956	22311	3499	2918	2642	2280	Z2	5034	2904	101060	220963	11547	7251	8149	4856
E3	793	948	3908	3584	1337	1397	1095	1193	Z3	2296	1805	20831	22257	4318	3289	3348	2548
E4	815	1431	9903	10204	1782	2189	1321	1823	Z4	2308	2087	55484	74690	5018	3929	3665	2958
E5	241	1733	7544	9326	781	2471	485	2132	Z5	1705	2214	77130	111609	4142	3868	2880	2988
E6	1494	2742	12359	15413	2618	4293	2071	3567	Z6	1185	3267	-	195299	1915	5319	1569	4325
E7	771	1353	8381	8539	1654	2051	1223	1719	Z7	2245	2225	38061	48976	4747	4072	3486	3126
E8	1120	1635	64585	252138	2311	2695	1718	2168	Z8	3075	2714	-	68901	7119	5959	4995	4175
E9	495	2103	70911	74630	974	3551	726	2835	Z9	1990	2576	-	44210	4378	5143	3171	3751
	static				695				1064				1340				
	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$	$\beta_{j=1}$	$\beta_{j=3}$			
E10	1169	1410	12233	11093	2373	2360	1786	1897	Z10	2038	1506	88339	106782	4481	3112	3240	2244
E11	1670	1495	19256	17221	3348	2743	2534	2123	Z11	3886	1996	199264	243547	8625	5228	6188	3462
E12	654	759	2923	2775	1076	1122	895	959	Z12	1472	1009	11648	11962	2661	1820	2110	1413
E13	764	1258	7879	7599	1600	1925	1205	1604	Z13	1402	1194	36628	40830	3145	2255	2273	1663
E14	529	1584	6538	7895	982	2233	739	1937	Z14	857	1504	55225	66545	2484	2390	1628	1888
E15	1776	2620	15185	16305	3162	4119	2482	3412	Z15	1153	2704	-	75130	1781	4200	1488	3497
E16	725	1171	6658	6319	1477	1778	1115	1490	Z16	1342	1348	21643	24533	2859	2352	2103	1832
E17	1037	1466	88609	182899	2059	2415	1564	1955	Z17	1851	1584	4907	37924	4048	3301	2915	2346
E18	872	2059	97161	98367	1690	3543	1265	2808	Z18	898	1581	-	17373	1925	2898	1421	2176

Table S6. The frequency dispersion factor between static and dynamic ($\beta_{HRS}^\lambda/\beta_{HRS}^\infty$)

Dynamic/static		Dynamic/static		Dynamic/static		Dynamic/static	
$\lambda = 695 \text{ nm}$							
E1	13.373	Z1	88.088	E10	9.552	Z10	49.77
E2	13.318	Z2	32.801	E11	11.53	Z11	62.235
E3	4.531	Z3	9.846	E12	4.191	Z12	8.705
E4	9.625	Z4	27.580	E13	8.302	Z13	28.236
E5	8.379	Z5	47.472	E14	7.169	Z14	53.915
E6	6.831	Z6	39.719	E15	7.517	Z15	18.37
E7	8.587	Z7	18.604	E16	7.434	Z16	16.783
E8	114.458	Z8	11.069	E17	105.43	Z17	11.930
E9	58.917	Z9	7.008	E18	72.58	Z18	6.662
$\lambda = 1064 \text{ nm}$							
E1	4.35	Z1	2.166	E10	1.90	Z10	2.174
E2	4.92	Z2	2.320	E11	1.963	Z11	2.262
E3	4.112	Z3	1.868	E12	1.586	Z12	1.807
E4	3.59	Z4	2.102	E13	1.814	Z13	2.162
E5	1.914	Z5	2.168	E14	1.514	Z14	2.250
E6	2.837	Z6	1.625	E15	1.682	Z15	1.550
E7	3.562	Z7	2.034	E16	1.782	Z16	2.022
E8	3.752	Z8	2.285	E17	1.837	Z17	2.163
E9	1.816	Z9	2.116	E18	1.787	Z18	1.972
$\lambda = 1340 \text{ nm}$							
E1	4.065	Z1	1.563	E10	1.460	Z10	1.571
E2	4.794	Z2	1.625	E11	1.493	Z11	1.606
E3	3.970	Z3	1.448	E12	1.330	Z12	1.428
E4	3.258	Z4	1.545	E13	1.423	Z13	1.569
E5	1.72	Z5	1.555	E14	1.262	Z14	1.565
E6	2.733	Z6	1.324	E15	1.352	Z15	1.292
E7	3.211	Z7	1.511	E16	1.404	Z16	1.507
E8	3.512	Z8	1.603	E17	1.429	Z17	1.55
E9	1.777	Z9	1.536	E18	1.389	Z18	1.467

The optimized cartesian coordinates and energy of all structures

E1

C	0.23519500	1.02422400	0.03496000
N	1.42711300	0.54333000	0.03678100
N	1.62234300	-0.77241400	0.01017900
H	0.83202200	-1.39924600	-0.07850700
C	2.90830800	-1.31327600	-0.02688600
C	3.04425300	-2.69724100	-0.15665400
C	4.04694600	-0.51307900	0.07139300
C	4.30641000	-3.27132300	-0.18991800
C	5.30319200	-1.10265700	0.03436900
H	3.93799500	0.55845400	0.17784900
C	5.44584600	-2.47959100	-0.09619600
H	4.39810000	-4.34750600	-0.29367300
H	6.18328700	-0.47205200	0.11025200
H	6.43129800	-2.93095700	-0.12433800
C	-0.98990500	0.17264400	0.02634500
C	-1.78637500	0.09142200	-1.11597900
C	-1.32975300	-0.57485200	1.15471200
C	-2.90812100	-0.72167900	-1.13709300
H	-1.53109300	0.67921100	-1.99034900
C	-2.45164600	-1.39105200	1.15110500
H	-0.71707300	-0.50774200	2.04763600
C	-3.22134800	-1.45063500	0.00043900
H	-3.53844500	-0.79294400	-2.01381700
H	-2.73330200	-1.96923700	2.02140900
C	0.08304000	2.49768900	0.03706300
C	1.19009900	3.34644700	-0.07273000

N	-1.16555900	2.95731700	0.15061300
C	0.98038000	4.71292100	-0.05384100
H	2.18217600	2.92472300	-0.17243100
C	-1.35077900	4.27603500	0.16575800
C	-0.31858100	5.19721200	0.06917400
H	1.81877900	5.39693000	-0.13653400
H	-2.38139500	4.60742000	0.26183600
H	-0.52663500	6.26084700	0.08786700
N	-4.41486700	-2.31718300	-0.01429000
O	-4.65757800	-2.95884900	0.98847200
O	-5.08268900	-2.33860900	-1.02884600
H	2.16024200	-3.32484100	-0.23332300
Z1			
C	0.13551200	0.60376000	-0.01443000
N	1.06232000	-0.30094100	0.00153000
N	2.34587000	-0.00615800	0.04216100
H	2.61428800	0.96399000	0.18621100
C	3.30508800	-1.02197300	0.05517100
C	4.64925100	-0.65751200	0.15715600
C	2.95791600	-2.37012700	-0.03529900
C	5.63464400	-1.63379300	0.17000100
C	3.95500500	-3.33549100	-0.02171100
H	1.91387900	-2.64678600	-0.10932700
C	5.29586300	-2.97948500	0.07988700
H	6.67561200	-1.33843700	0.25259000
H	3.67742500	-4.38238000	-0.09190500
H	6.06724100	-3.74151100	0.08983600
C	-1.24516800	0.04924100	-0.01061800
C	-1.57016800	-1.03359500	-0.83203000

C	-2.22379600	0.56137400	0.84743200
C	-2.83787500	-1.59128100	-0.80632200
H	-0.81473900	-1.43724200	-1.49579400
C	-3.49555200	0.01403500	0.88702700
H	-1.98265100	1.38669200	1.50886500
C	-3.78530600	-1.05584100	0.05371000
H	-3.10015700	-2.42525500	-1.44434400
H	-4.25304800	0.39632400	1.55860400
C	0.33704200	2.07038000	-0.06671700
C	-0.67992900	2.92312500	-0.52089200
N	1.54057900	2.55461000	0.28393700
C	-0.44683900	4.28502300	-0.57981000
H	-1.63304100	2.51687300	-0.83469800
C	1.75070800	3.86849700	0.22541700
C	0.79231900	4.77907900	-0.18829000
H	-1.22275400	4.95596100	-0.93305500
H	2.74081700	4.20230400	0.52317100
H	1.01505800	5.83917600	-0.21508600
N	-5.13596900	-1.63879600	0.08304900
O	-5.94677800	-1.14869400	0.84529000
O	-5.36318900	-2.57574300	-0.65728800
H	4.91993000	0.39229400	0.22808600
E2			
C	0.71910700	1.16177900	-0.06379400
N	-0.55565900	1.00856700	-0.12905900
N	-1.08358400	-0.21182200	-0.14964700
H	-0.48502700	-1.02270800	-0.05236300
C	-2.46762700	-0.40220900	-0.16711200
C	-2.96425900	-1.70351100	-0.07794700

C	-3.35632500	0.66602500	-0.28546100
C	-4.33175000	-1.93359800	-0.10066300
C	-4.72278700	0.42685800	-0.30721800
H	-2.97038300	1.67399200	-0.36763500
C	-5.21729600	-0.86890200	-0.21373200
H	-4.72201800	-2.94401800	-0.04022800
H	-5.42020000	1.25161600	-0.41243900
C	1.67374500	0.01540000	-0.02813700
C	2.31556000	-0.34038300	1.15802000
C	1.90306300	-0.73271400	-1.18349800
C	3.17694900	-1.42539600	1.19584300
H	2.14748800	0.24476600	2.05488700
C	2.76491000	-1.81960900	-1.16339800
H	1.40881100	-0.45569200	-2.10871700
C	3.38694300	-2.14733000	0.03063000
H	3.68508100	-1.71088300	2.10746900
H	2.95964000	-2.40349200	-2.05337900
C	1.25365500	2.54182500	-0.02175800
C	0.40750300	3.65609600	-0.05375100
N	2.58271700	2.65169100	0.04748900
C	0.97285800	4.91716800	-0.01427800
H	-0.66443900	3.51517700	-0.10942800
C	3.11133100	3.87346700	0.08711100
C	2.35744900	5.03712100	0.05867300
H	0.34227100	5.80007000	-0.03882300
H	4.19571100	3.91818800	0.14471700
H	2.84096300	6.00658200	0.09290900
N	4.30210100	-3.30401800	0.06255800
O	4.44814000	-3.93473700	-0.96548100

O	4.85328300	-3.55718400	1.11505300
H	-2.27870200	-2.54248400	0.00635200
O	-6.56970400	-1.10212200	-0.27014400
C	-7.21840200	-1.01969000	0.98457400
H	-8.27665400	-1.20767800	0.80546300
H	-6.82735600	-1.77091100	1.68129700
H	-7.09570900	-0.02549400	1.43047800
ZZ			
C	0.69573000	0.81721000	-0.00393000
N	-0.42203000	0.15851200	-0.01751600
N	-1.59764200	0.74329200	-0.05731400
H	-1.63311800	1.75030900	-0.19586300
C	-2.77037500	-0.02361600	-0.04586000
C	-3.99449600	0.62252000	-0.16189400
C	-2.74475300	-1.41447400	0.08655900
C	-5.18642900	-0.09725900	-0.14720000
C	-3.92657000	-2.12949300	0.10114400
H	-1.79354400	-1.92422400	0.17216300
C	-5.15817900	-1.48194900	-0.01394500
H	-6.12125900	0.44113900	-0.24167600
H	-3.91621400	-3.20901000	0.20332900
C	1.90222200	-0.05239800	-0.00642100
C	1.94177200	-1.19663400	0.79612700
C	2.99131200	0.22070800	-0.84107700
C	3.03647100	-2.04454100	0.77516000
H	1.09895600	-1.41741100	1.44034900
C	4.09449900	-0.61642100	-0.87319400
H	2.96924200	1.08953700	-1.49025100
C	4.10202100	-1.73888500	-0.05894200

H	3.07648700	-2.92916000	1.39747800
H	4.93509600	-0.41646200	-1.52480800
C	0.84427400	2.28806200	0.05588600
C	2.03439800	2.87846600	0.50867200
N	-0.21628700	3.04280200	-0.28028000
C	2.12445300	4.25618100	0.57955200
H	2.86882600	2.26029200	0.81416100
C	-0.11506500	4.36932400	-0.20837800
C	1.03085800	5.02871300	0.20339400
H	3.03708200	4.72427600	0.93314200
H	-1.00332700	4.92624100	-0.49357300
H	1.06003600	6.11126100	0.24144900
N	5.27227100	-2.62936000	-0.08129900
O	6.20160600	-2.32400900	-0.80395600
O	5.24371000	-3.61871200	0.62473200
H	-4.03008900	1.70320100	-0.26687800
O	-6.25823500	-2.28097200	0.01523700
C	-7.52106700	-1.67336200	-0.11118200
H	-7.62263600	-1.15466800	-1.07151700
H	-8.25155200	-2.47898700	-0.06223700
H	-7.71128500	-0.96642100	0.70466300
E3			
C	-1.00292500	1.22185800	0.01014200
N	0.26359800	1.06589100	0.11345000
N	0.76044900	-0.18086500	0.30502700
H	0.17483200	-0.97176600	0.06138000
C	2.13007600	-0.36542600	0.15167100
C	2.60151400	-1.52500900	-0.46134200
C	3.08265800	0.53378300	0.63291800

C	3.95144800	-1.79068200	-0.60273700
C	4.43838600	0.28930000	0.47453300
C	4.88007300	-0.87242500	-0.13932000
C	-1.97941100	0.09593200	0.07501500
C	-2.65947700	-0.32209800	-1.06843000
C	-2.19353000	-0.56281500	1.28599200
C	-3.54420000	-1.38722300	-1.00919300
H	-2.50474300	0.19742800	-2.00672600
C	-3.08206600	-1.62518000	1.36233400
H	-1.66599400	-0.23759800	2.17620600
C	-3.74065100	-2.01945800	0.20897200
H	-4.08129000	-1.72459500	-1.88580800
H	-3.26672300	-2.14200900	2.29487400
C	-1.50543700	2.60756300	-0.17823300
C	-0.63789600	3.70266800	-0.13408200
N	-2.81837500	2.73188900	-0.37877600
C	-1.16808000	4.96870100	-0.30760200
H	0.41943000	3.54608700	0.03825500
C	-3.31296700	3.95679600	-0.54598800
C	-2.53595400	5.10589800	-0.51937400
H	-0.52280600	5.84043200	-0.27607800
H	-4.38582000	4.01736600	-0.70696500
H	-2.99200100	6.07937700	-0.65800400
N	-4.68529900	-3.15147300	0.28025600
O	-4.83312000	-3.69272400	1.35746700
O	-5.25630300	-3.47259500	-0.74227100
F	1.71119800	-2.40859200	-0.92907100
F	4.35477800	-2.90707600	-1.19494800
F	6.17918300	-1.10598400	-0.27582000

F	5.32236000	1.16423200	0.93761100
F	2.71787200	1.63371400	1.28333500
Z3			
C	-0.99193800	0.84337200	-0.09004000
N	0.09384000	0.14982100	-0.07695400
N	1.29407800	0.73548300	-0.17538500
H	1.35276900	1.72816000	0.04273400
C	2.43182600	-0.05022600	-0.07837700
C	3.57573300	0.49496700	0.50550100
C	2.53248200	-1.35079600	-0.57722900
C	4.76208100	-0.20721500	0.60695100
C	3.71163700	-2.07200000	-0.45947900
C	4.83104200	-1.50662300	0.12954700
C	-2.23233400	0.03032700	0.02983300
C	-2.31978300	-1.20162400	-0.62397400
C	-3.30168100	0.45399000	0.82425200
C	-3.45200100	-1.98967000	-0.50174600
H	-1.48548100	-1.53899500	-1.22703300
C	-4.43983400	-0.32494600	0.95849000
H	-3.24100500	1.39623000	1.35801700
C	-4.49914300	-1.53577600	0.28641700
H	-3.53236000	-2.94209200	-1.00902800
H	-5.26854300	-0.00945600	1.57860000
C	-1.08970300	2.31924000	-0.24731000
C	-2.22962700	2.91321900	-0.79924900
N	-0.02652600	3.05256900	0.11678800
C	-2.26680800	4.28971100	-0.94878100
H	-3.06656200	2.30383900	-1.11611700
C	-0.07513700	4.37477400	-0.02573000

C	-1.17297700	5.04431600	-0.54513700
H	-3.13977500	4.76707800	-1.38080200
H	0.81227100	4.91711600	0.28700100
H	-1.16179000	6.12348400	-0.64215300
N	-5.71069900	-2.36401500	0.41391300
O	-6.61496800	-1.93767500	1.10554200
O	-5.73498700	-3.42308100	-0.18091900
F	1.51554600	-1.92456100	-1.21346900
F	3.77614900	-3.30787800	-0.94005000
F	5.95942800	-2.19887500	0.22880900
F	5.82376700	0.35184600	1.17461200
F	3.51758200	1.74318400	0.98339000
E4			
C	1.38503300	1.17341800	-0.01618300
N	0.10268100	1.10925500	-0.01514900
N	-0.50704100	-0.07858300	0.02091400
H	0.04063800	-0.92680200	0.09706200
C	-1.89129800	-0.17467400	0.01493600
C	-2.47516600	-1.43981900	0.12737100
C	-2.70723300	0.95284100	-0.11036300
C	-3.85212800	-1.57554600	0.11583700
C	-4.08313200	0.80560200	-0.11995300
H	-2.25525400	1.93096400	-0.20574900
C	-4.66539100	-0.45408400	-0.01007600
H	-4.29290300	-2.56167600	0.20212100
H	-4.70950500	1.68478600	-0.22183800
C	2.26297300	-0.03306300	-0.01176800
C	2.98509600	-0.38026400	1.12976800
C	2.33783300	-0.84209200	-1.14628800

C	3.77256300	-1.52056700	1.14513200
H	2.93885700	0.25385700	2.00785900
C	3.12447100	-1.98481800	-1.14776600
H	1.78553500	-0.56866500	-2.03926700
C	3.82674400	-2.30491800	0.00279800
H	4.34113800	-1.80297700	2.02148400
H	3.20001600	-2.61872000	-2.02155200
C	2.01231700	2.51640300	-0.02529400
C	1.24761200	3.68074000	0.09718900
N	3.34048100	2.53774100	-0.15897300
C	1.89507900	4.90252200	0.06789400
H	0.17380700	3.60993800	0.21474300
C	3.94934300	3.72165200	-0.18390100
C	3.27846200	4.93116800	-0.07730800
H	1.33054200	5.82445600	0.16071100
H	5.02982700	3.69519400	-0.29664900
H	3.82460500	5.86703000	-0.10441700
N	4.66214600	-3.52146400	0.01202400
O	4.67247200	-4.20394400	-0.99278200
O	5.28644200	-3.76716500	1.02431800
H	-1.84896500	-2.32202500	0.22303400
C	-6.15681200	-0.58660900	0.03134900
F	-6.76711500	0.29846600	-0.77774200
F	-6.57102200	-1.81133000	-0.33638500
F	-6.65027400	-0.37074600	1.26948400
Z4			
C	1.33500600	0.87866900	0.01506600
N	0.14941800	0.36433200	0.00374600
N	-0.94594200	1.10737600	-0.02890100

H	-0.84535800	2.10878400	-0.17523100
C	-2.19866300	0.50625900	-0.03749800
C	-3.32679100	1.32595500	-0.11635400
C	-2.35596000	-0.88104800	0.03579700
C	-4.59521200	0.76950900	-0.12145800
C	-3.62631400	-1.42660600	0.02929500
H	-1.48042900	-1.51463600	0.08895400
C	-4.75256100	-0.60904000	-0.04882800
H	-5.46266300	1.41552400	-0.18349200
H	-3.74283700	-2.50373000	0.08442200
C	2.43053300	-0.12951700	0.00988300
C	2.37542100	-1.23282200	0.86436600
C	3.50291600	-0.01548700	-0.87960900
C	3.36694900	-2.20056100	0.83993300
H	1.54453900	-1.32669200	1.55373700
C	4.49996100	-0.97617000	-0.91972300
H	3.54984400	0.82493200	-1.56396500
C	4.41766900	-2.05553400	-0.05313500
H	3.33676200	-3.05448400	1.50399800
H	5.32550500	-0.90348300	-1.61546500
C	1.67372800	2.32239800	0.06225900
C	2.93052600	2.75154300	0.50978600
N	0.72326000	3.20472200	-0.28867100
C	3.20250100	4.10716300	0.56538700
H	3.67562900	2.03072500	0.82103200
C	0.99954200	4.50615000	-0.23594200
C	2.22290400	5.01171400	0.17444700
H	4.16835400	4.45512400	0.91603400
H	0.19614500	5.17334600	-0.53483400

H	2.39530500	6.08117300	0.19857700
N	5.47813300	-3.07724000	-0.08332500
O	6.38737300	-2.92277600	-0.87514800
O	5.38188800	-4.01308000	0.68568600
H	-3.20948800	2.40371000	-0.17458100
C	-6.11214400	-1.23731400	-0.03129000
F	-7.09488700	-0.34638000	-0.24089400
F	-6.37526200	-1.83781800	1.14827600
F	-6.23868700	-2.19239600	-0.97379500
E5			
C	-0.57547100	1.16105100	-0.00882500
N	0.69912600	1.01072100	-0.01936700
N	1.22031400	-0.22072300	-0.05827400
H	0.60911600	-1.02585400	-0.11764600
C	2.59048700	-0.41975700	-0.04911000
C	3.07743100	-1.72831900	-0.15317600
C	3.48908400	0.64522100	0.06740300
C	4.43737800	-1.96847700	-0.14074100
C	4.84911700	0.39793600	0.07783100
H	3.11019500	1.65488500	0.15274700
C	5.33926200	-0.90688300	-0.02561200
H	4.80845200	-2.98365800	-0.22312000
H	5.54510400	1.22422200	0.16902000
C	-1.53084500	0.01438000	-0.00459600
C	-2.22014900	-0.34009000	-1.16374200
C	-1.71012500	-0.73271100	1.15993200
C	-3.08027900	-1.42723700	-1.16596200
H	-2.08983100	0.24474600	-2.06729700
C	-2.57053500	-1.82068400	1.17461200

H	-1.18067100	-0.45354300	2.06477200
C	-3.23975700	-2.14939600	0.00679500
H	-3.62493100	-1.71448100	-2.05577300
H	-2.72834000	-2.40476300	2.07176300
C	-1.11596000	2.54093600	0.01178900
C	-0.27811500	3.65675300	-0.07473900
N	-2.44240900	2.64171800	0.12353000
C	-0.84954500	4.91584300	-0.03203300
H	0.79136700	3.52155600	-0.17414000
C	-2.97742600	3.86029000	0.16120500
C	-2.23061200	5.02756700	0.09038500
H	-0.22671900	5.80209600	-0.09485200
H	-4.05921500	3.90013700	0.25527100
H	-2.71856700	5.99460300	0.12836900
N	-4.15267400	-3.30948800	0.01175100
O	-4.25409600	-3.93975000	1.04495100
O	-4.74441300	-3.56341600	-1.01779400
H	2.38483400	-2.55969900	-0.24539900
C	6.74824200	-1.15377400	-0.01184900
N	7.88338300	-1.35234500	-0.00026500
Z5			
C	-0.51887800	0.80082600	-0.00545300
N	0.59127300	0.14079200	0.00697900
N	1.77397800	0.73902900	0.03778700
H	1.80127700	1.74693300	0.17447900
C	2.93508800	-0.01944000	0.04322000
C	2.90788000	-1.41434600	-0.05190400
C	5.34412800	-0.07150900	0.14512200
C	4.09292500	-2.12575800	-0.04797800

H	1.95635700	-1.92427500	-0.12260100
C	5.32137400	-1.46583000	0.04944500
H	6.29276400	0.44714900	0.22354700
H	4.07065000	-3.20725600	-0.12151800
C	-1.73228800	-0.06350500	-0.00074300
C	-1.81967900	-1.15133100	-0.87183700
C	-2.77439200	0.16856500	0.90148200
C	-2.92283800	-1.98999300	-0.85163800
H	-1.01248000	-1.33666900	-1.57073400
C	-3.88259400	-0.66223200	0.93652600
H	-2.71210200	0.99795300	1.59801600
C	-3.94038500	-1.72967100	0.05346700
H	-3.00413000	-2.83156500	-1.52722400
H	-4.68815900	-0.49909900	1.64044900
C	-0.67483500	2.27541300	-0.05948700
C	-1.87764200	2.85518000	-0.48392000
N	0.38696400	3.03357900	0.26128900
C	-1.97843700	4.23400300	-0.54864300
H	-2.71469100	2.23160200	-0.77068700
C	0.27598300	4.35891600	0.19821100
C	-0.88339700	5.01085800	-0.19119000
H	-2.90120800	4.69754400	-0.88065700
H	1.16447400	4.92136300	0.47051700
H	-0.92055600	6.09324100	-0.22465000
N	-5.11934900	-2.61279300	0.07752900
O	-6.00542200	-2.34853900	0.86629600
O	-5.13588700	-3.55175100	-0.69330100
C	4.16286500	0.64486200	0.14149400
H	4.18808700	1.72758400	0.21671800

C	6.54388600	-2.20898500	0.05192400
N	7.52965000	-2.80608100	0.05381500
E6			
C	0.99327100	1.17275600	-0.00234200
N	-0.28649100	1.07881800	0.00820400
N	-0.86401300	-0.12854700	0.04948100
H	-0.29126100	-0.96108000	0.11479100
C	-2.23962500	-0.26186000	0.04398500
C	-2.78795500	-1.54786000	0.14506600
C	-3.08600500	0.84774100	-0.06572300
C	-4.15706300	-1.72480500	0.13639900
C	-4.45617400	0.66823300	-0.07229800
H	-2.65871600	1.83767000	-0.14896400
C	-4.98273900	-0.61285700	0.02897100
H	-4.59188500	-2.71255100	0.21517200
H	-5.12571800	1.51447700	-0.15697300
C	1.89947700	-0.01281300	-0.00475900
C	2.62148400	-0.35577500	1.13794700
C	2.00020400	-0.80600400	-1.14824700
C	3.43489200	-1.47795400	1.14531200
H	2.55470500	0.26644100	2.02320800
C	2.81339000	-1.92997800	-1.15746300
H	1.44785200	-0.53490300	-2.04190400
C	3.51491600	-2.24702300	-0.00572500
H	4.00396400	-1.75750900	2.02225200
H	2.90992200	-2.55132700	-2.03815300
C	1.59012500	2.53014400	-0.01923600
C	0.79974300	3.67758700	0.09390700
N	2.91742100	2.57854600	-0.15245500

C	1.42074300	4.91312000	0.05607800
H	-0.27245000	3.58497100	0.21064100
C	3.50063200	3.77491700	-0.18583000
C	2.80293500	4.97031200	-0.08850500
H	0.83611200	5.82316000	0.14081400
H	4.58140700	3.77164600	-0.29796100
H	3.32862300	5.91752200	-0.12286900
N	4.37835400	-3.44450700	-0.00470700
O	4.41226700	-4.11313200	-1.01800600
O	4.99950300	-3.68826700	1.00975400
H	-2.13573000	-2.41162400	0.23120700
N	-6.43418900	-0.79561900	0.01928400
O	-7.13048400	0.19868800	-0.06965600
O	-6.86352300	-1.93166500	0.10101800
Z6			
C	-0.93047100	0.84090700	-0.01709000
N	0.21890900	0.25291700	-0.00564100
N	1.35894300	0.93333200	0.02407200
H	1.31417800	1.93993400	0.16669000
C	2.56973600	0.26353900	0.03194100
C	3.74424000	1.02367000	0.11407300
C	2.64827300	-1.13181900	-0.04495400
C	4.97758400	0.40355300	0.11926100
C	3.88378100	-1.75129100	-0.03958800
H	1.73858000	-1.71437800	-0.10128900
C	5.03779500	-0.98210600	0.04064800
H	5.89228600	0.97830300	0.18303800
H	3.96307300	-2.82911700	-0.09769500
C	-2.08892600	-0.09543000	-0.00912600

C	-2.11393500	-1.18940500	-0.87622500
C	-3.14025600	0.07853700	0.89535400
C	-3.16600200	-2.09135300	-0.84992300
H	-1.29902000	-1.32901200	-1.57684000
C	-4.19698600	-0.81618800	0.93702600
H	-3.12517400	0.91282800	1.58860100
C	-4.19411200	-1.88818500	0.05761200
H	-3.19981100	-2.93865500	-1.52243600
H	-5.00870800	-0.69880800	1.64295700
C	-1.18037600	2.30381400	-0.06611700
C	-2.41215100	2.80676500	-0.50425200
N	-0.17518400	3.12683700	0.27559300
C	-2.60179700	4.17676400	-0.56023600
H	-3.20219500	2.13172000	-0.80730200
C	-0.37176100	4.44245300	0.22243200
C	-1.56591500	5.02023200	-0.17917700
H	-3.54757100	4.58233500	-0.90325800
H	0.47338900	5.05967300	0.51330800
H	-1.67405300	6.09804300	-0.20388400
N	-5.31919000	-2.83921400	0.08847400
O	-6.21436700	-2.62720200	0.88261200
O	-5.28490700	-3.77726500	-0.68268200
H	3.68412600	2.10570800	0.17442400
N	6.34333300	-1.64237600	0.04426900
O	6.36596700	-2.85726900	-0.02482500
O	7.33467000	-0.93898700	0.11569100
E7			
C	-0.25846900	1.01286100	-0.02457600
N	-1.44777600	0.52833300	-0.02277400

N	-1.63667100	-0.79034500	0.01537400
H	-0.86621900	-1.44228300	0.11253000
C	-2.91133000	-1.33588700	0.03835400
N	-2.92893300	-2.65974500	0.16012500
C	-4.06402000	-0.54989400	-0.06743900
C	-4.11712200	-3.26201400	0.18429000
C	-5.28275000	-1.20048800	-0.03795300
H	-3.98533600	0.52364300	-0.17181600
C	-5.32395500	-2.58724300	0.09111800
H	-4.09174200	-4.34352500	0.28606700
H	-6.20166700	-0.62860400	-0.11727900
H	-6.26265500	-3.12727400	0.11752300
C	0.97289100	0.17114600	-0.01704800
C	1.79412800	0.12988300	1.10950400
C	1.29683200	-0.60071900	-1.13307600
C	2.92531200	-0.66969100	1.12705200
H	1.55076800	0.73717500	1.97385400
C	2.42874800	-1.40260600	-1.13313800
H	0.66281400	-0.56687900	-2.01280900
C	3.22362700	-1.42278000	0.00132100
H	3.57486500	-0.71192700	1.99149200
H	2.69789000	-2.00110600	-1.99353100
C	-0.11727100	2.48916700	-0.03624300
C	-1.22841900	3.32907400	0.09342800
N	1.12452100	2.95812100	-0.17885600
C	-1.03096200	4.69739200	0.06153600
H	-2.21453500	2.90003200	0.21734300
C	1.29851900	4.27796800	-0.20588200
C	0.26065400	5.19126000	-0.09276000

H	-1.87300300	5.37494300	0.15888100
H	2.32396800	4.61734500	-0.32572600
H	0.45949200	6.25639500	-0.12262500
N	4.42961900	-2.27214600	0.01116000
O	4.66848200	-2.92290100	-0.98648500
O	5.11171300	-2.26985400	1.01647900
Z7			
C	0.15076000	0.58626500	-0.01621200
N	1.06710500	-0.32474600	-0.00051900
N	2.35720100	-0.03902900	0.03358800
H	2.66663100	0.91808800	0.18457500
C	3.30073900	-1.05835000	0.04979100
N	4.55539300	-0.63123900	0.15835100
C	2.94528100	-2.40832900	-0.04528500
C	5.52004000	-1.55001200	0.17681800
C	3.96558500	-3.33981600	-0.02372300
H	1.90473400	-2.69262200	-0.12584200
C	5.28731900	-2.91342600	0.08874600
H	6.53196100	-1.16447300	0.26872300
H	3.73300900	-4.39746300	-0.09488900
H	6.11072200	-3.61727700	0.10857200
C	-1.23659800	0.04730800	-0.01165800
C	-2.20913900	0.57578700	0.84292100
C	-1.57317900	-1.03419000	-0.82966800
C	-3.48700000	0.04260800	0.88450600
H	-1.95904900	1.40273000	1.49891700
C	-2.84740400	-1.57688300	-0.80266000
H	-0.82236400	-1.44808800	-1.49234500
C	-3.78821000	-1.02754900	0.05575100

H	-4.24084500	0.43652500	1.55349100
H	-3.11951300	-2.40981000	-1.43790500
C	0.36433400	2.05371900	-0.06791900
C	-0.63458000	2.90954800	-0.55109000
N	1.56035100	2.52640400	0.31504300
C	-0.38834000	4.27018100	-0.60864700
H	-1.58281900	2.50858400	-0.88649700
C	1.78423800	3.83705100	0.25789200
C	0.84386100	4.75392900	-0.18620300
H	-1.14894300	4.94676900	-0.98374000
H	2.76902400	4.16211000	0.58121600
H	1.07634400	5.81203900	-0.21134700
N	-5.14561100	-1.59568500	0.08776600
O	-5.38197800	-2.53519700	-0.64629400
O	-5.95129800	-1.09156500	0.84595900
E8			
C	-1.15717100	1.24867600	0.02311700
N	0.07438400	1.61811200	0.02504800
N	1.04057800	0.70100700	0.00542900
H	0.84367300	-0.29181100	-0.07020000
C	-1.57947700	-0.18179400	0.03363900
C	-2.18490000	-0.75143400	-1.08609600
C	-1.32946200	-0.97213800	1.15581400
C	-2.53364000	-2.09219600	-1.09327700
H	-2.39120100	-0.13754000	-1.95537400
C	-1.67600500	-2.31479700	1.16643600
H	-0.86140000	-0.53176300	2.02968500
C	-2.27040000	-2.85251700	0.03641300
H	-3.00289200	-2.54961700	-1.95431200

H	-1.49042000	-2.93858400	2.03068400
C	-2.19364200	2.30692100	0.01038200
C	-1.85679300	3.65608300	-0.14583000
N	-3.45539600	1.89467800	0.15721500
C	-2.86978500	4.59704400	-0.13602100
H	-0.81946300	3.93834100	-0.27320700
C	-4.41973600	2.81302800	0.16286600
C	-4.18561200	4.17292200	0.02310700
H	-2.64005000	5.65073700	-0.25654100
H	-5.43101100	2.43460400	0.28685900
H	-5.00929500	4.87748500	0.03494000
N	-2.63501200	-4.28117700	0.03454400
O	-2.37919200	-4.93003900	1.02973100
O	-3.16776800	-4.72604100	-0.96280400
C	2.37250500	1.06267800	0.02174700
C	3.31585200	-0.01085200	-0.05340000
C	2.82153000	2.35964100	0.11248400
C	4.70072500	0.28027100	-0.03424200
C	4.20521700	2.62927400	0.12901700
H	2.10357200	3.16761000	0.17339400
C	3.67586400	-2.26551200	-0.20976000
C	5.58287800	-0.82358100	-0.10993000
C	5.13430000	1.62581400	0.05816300
H	4.53129300	3.66168000	0.20263700
C	5.07689200	-2.09143900	-0.19771800
H	3.25085300	-3.26371500	-0.28045100
H	6.65501500	-0.65017600	-0.09722300
H	6.19713000	1.84426100	0.07411600
H	5.72782100	-2.95633300	-0.25675300

N	2.82361900	-1.27306300	-0.14011200
Z8			
C	0.73898900	0.57118100	0.03631900
N	-0.17286000	-0.34664200	0.02548300
N	-1.46389700	-0.06763600	0.00529500
H	-1.78317800	0.89025900	-0.12778200
C	2.12817700	0.03983500	0.01082400
C	2.47415500	-1.05971600	0.80130000
C	3.09477200	0.59143800	-0.83634100
C	3.74954500	-1.59742400	0.75396800
H	1.72803800	-1.49198200	1.45742300
C	4.37418200	0.06399600	-0.89741900
H	2.83825500	1.43173600	-1.47253200
C	4.68419100	-1.02452800	-0.09612600
H	4.02745000	-2.44485600	1.36713000
H	5.12293000	0.47601300	-1.56126600
C	0.51439000	2.03500100	0.10548100
C	1.50835800	2.89776000	0.58809500
N	-0.69166400	2.49702600	-0.25606700
C	1.24368600	4.25354500	0.66838800
H	2.46600300	2.50524700	0.90654000
C	-0.93455300	3.80248700	-0.17495000
C	-0.00153400	4.72610200	0.27054000
H	1.99969500	4.93548100	1.04328300
H	-1.92950800	4.11528600	-0.47882200
H	-0.24829700	5.78035400	0.31632500
N	6.04248100	-1.58704100	-0.15043100
O	6.84348700	-1.05951600	-0.89798000
O	6.28595100	-2.54620500	0.55574900

C	-2.39260200	-1.09398500	0.02721800
C	-3.76869400	-0.71304200	-0.06054300
C	-2.05885900	-2.42498200	0.13008600
C	-4.76634800	-1.71862600	-0.03687400
C	-3.06565400	-3.41031700	0.15113100
H	-1.01466100	-2.70472700	0.18965700
C	-5.31335500	0.96376300	-0.25245100
C	-6.11069000	-1.28710200	-0.13046300
C	-4.39236000	-3.08009600	0.07168800
H	-2.77252500	-4.45192100	0.23287900
C	-6.38789500	0.04742500	-0.23875000
H	-5.51074400	2.02975000	-0.33947700
H	-6.90768400	-2.02483700	-0.11697700
H	-5.16155400	-3.84538200	0.08839400
H	-7.40687100	0.40987600	-0.31476700
N	-4.05552300	0.60988800	-0.16697900
E9			
C	-1.01807800	1.14939900	-0.00629100
N	0.24205000	0.90608300	-0.02136600
N	0.67343400	-0.35752800	-0.05556100
H	0.00631700	-1.11742300	-0.10197900
C	2.03138100	-0.64759500	-0.05610000
C	2.37455500	-2.04386500	-0.15314100
C	2.99338200	0.31954600	0.03253700
C	3.66249900	-2.46786100	-0.16251100
C	4.35098700	-0.09586900	0.02374400
H	2.74023700	1.36742700	0.11088100
C	4.69592800	-1.49049900	-0.07304000
H	3.91573800	-3.51845500	-0.23769100

C	-2.05409000	0.07512600	0.00177100
C	-2.74025400	-0.25452800	-1.16655400
C	-2.31286500	-0.63270700	1.17562100
C	-3.67698200	-1.27629800	-1.16843200
H	-2.54660600	0.29955700	-2.07817100
C	-3.25037100	-1.65502100	1.19091500
H	-1.78465300	-0.37334700	2.08698900
C	-3.91552300	-1.95971900	0.01407800
H	-4.22005300	-1.54193900	-2.06579500
H	-3.46975400	-2.20714100	2.09531200
C	-1.45669900	2.56445100	0.00866700
C	-0.53960600	3.61592600	-0.08171500
N	-2.77279900	2.76142800	0.11727200
C	-1.01878200	4.91328800	-0.04776200
H	0.51786000	3.40420700	-0.17675100
C	-3.21798600	4.01582900	0.14699300
C	-2.38847300	5.12540700	0.07086900
H	-0.33219100	5.75085300	-0.11370100
H	-4.29413500	4.13468200	0.23903000
H	-2.80614100	6.12514500	0.10201300
N	-4.91037700	-3.04988800	0.02029400
O	-5.08386800	-3.64640200	1.06407600
O	-5.49322500	-3.28548500	-1.01882000
H	1.57113900	-2.77223000	-0.22182800
N	6.00422200	-1.72051400	-0.06759600
N	5.41696400	0.69826100	0.10096400
S	6.72690000	-0.26820000	0.05273100
Z9			
C	-1.07894800	0.92434300	0.01419700

N	0.11921500	0.44061200	0.05055100
N	1.19356600	1.21254800	0.08933000
H	1.06422900	2.20980700	0.23943500
C	2.46221100	0.64404400	0.08857700
C	3.55769200	1.57506400	0.18303400
C	2.67500900	-0.70283800	-0.00506000
C	4.85054700	1.16652100	0.18331500
C	4.01938500	-1.15990600	-0.00803000
H	1.85467300	-1.40421600	-0.06960900
C	5.11607400	-0.23032700	0.08473400
H	5.67133300	1.86997600	0.25457900
C	-2.14952300	-0.10894100	0.01371600
C	-2.00292500	-1.26811600	-0.75290600
C	-3.28964300	0.03317600	0.81077900
C	-2.96960400	-2.25977100	-0.73442500
H	-1.11725400	-1.38731900	-1.36544400
C	-4.26551400	-0.94961000	0.84050300
H	-3.40996900	0.91479500	1.43109200
C	-4.09179100	-2.08292200	0.06114300
H	-2.86512800	-3.15841800	-1.32811100
H	-5.14567500	-0.85106900	1.46212300
C	-1.44449800	2.36119600	-0.06595600
C	-2.68031800	2.76188700	-0.59082200
N	-0.53213100	3.26487700	0.32857200
C	-2.97388500	4.11154900	-0.67664600
H	-3.39258300	2.02401600	-0.93703600
C	-0.82896300	4.56028500	0.24610600
C	-2.03594900	5.03838600	-0.23868200
H	-3.92381400	4.43738100	-1.08678900

H	-0.05641500	5.24569800	0.58275200
H	-2.22626200	6.10410400	-0.28426600
N	-5.12891100	-3.12815400	0.08026000
O	-6.10743100	-2.93900700	0.77649100
O	-4.94632200	-4.11676200	-0.60211700
H	3.32867800	2.63436300	0.25626300
N	4.41917000	-2.42714700	-0.09426200
N	6.31155800	-0.80907200	0.06726200
S	6.04717400	-2.40954600	-0.05771400
E10			
C	-0.29712900	0.83448800	-0.00172300
N	0.98132400	0.70120000	-0.00462500
N	1.52773500	-0.51187800	-0.03293700
H	0.93636200	-1.33118600	-0.09831500
C	2.91196200	-0.68408500	-0.03339900
C	3.42217900	-1.97921900	-0.15008300
C	3.78780700	0.39516800	0.08815100
C	4.79317700	-2.18895300	-0.14626900
C	5.15728600	0.16885200	0.08790300
H	3.38861700	1.39671200	0.18412400
C	5.67198400	-1.11770500	-0.02844300
H	5.17618200	-3.19999000	-0.23942800
H	5.83140300	1.01423800	0.18231100
H	6.74349400	-1.28396600	-0.02644700
C	-1.23526400	-0.32574600	0.00215200
C	-1.93516100	-0.68092400	-1.15039300
C	-1.38966200	-1.09035400	1.15871800
C	-2.77656600	-1.78149800	-1.15206000
H	-1.82598900	-0.08370700	-2.04885900

C	-2.23214600	-2.19150500	1.17005100
H	-0.85184100	-0.81359000	2.05965500
C	-2.92679700	-2.54045700	0.01091400
H	-3.32136000	-2.05499500	-2.04838300
H	-2.35791600	-2.77795200	2.07292700
C	-0.85087600	2.20781200	0.00677100
C	-0.01972100	3.33110000	-0.07050200
N	-2.17976800	2.30270900	0.09738900
C	-0.59909100	4.58601300	-0.04179300
H	1.05191600	3.20124900	-0.15229600
C	-2.72235100	3.51881000	0.12143800
C	-1.98330400	4.69068800	0.05797700
H	0.01959900	5.47583300	-0.09803800
H	-3.80598900	3.55180400	0.19817700
H	-2.47784900	5.65485900	0.08410000
H	2.74351000	-2.82271200	-0.24598700
C	-3.79570700	-3.68160200	0.01344000
N	-4.49127300	-4.59944400	0.01436700

Z10

C	-0.25384500	0.46860000	0.02342800
N	0.76699100	-0.32880900	0.02796300
N	2.01143400	0.10471500	0.05639800
H	2.17299800	1.09965800	0.19024500
C	3.07760400	-0.79742000	0.04593900
C	4.37274500	-0.28395300	0.14276200
C	2.88500100	-2.17475600	-0.06359100
C	5.46310600	-1.14133000	0.13107200
C	3.98607400	-3.02014300	-0.07414100
H	1.87928800	-2.56932600	-0.13372400

C	5.27860300	-2.51517900	0.02177400
H	6.46393200	-0.72920200	0.20953100
H	3.82816900	-4.09051000	-0.15949900
H	6.13140400	-3.18511800	0.01277000
C	-1.56579600	-0.23486800	0.02473600
C	-1.77977000	-1.31857200	-0.82978500
C	-2.58675900	0.13867700	0.90334000
C	-2.98035100	-2.00855500	-0.81660800
H	-0.99033000	-1.61745300	-1.50961300
C	-3.79112600	-0.54482500	0.92724300
H	-2.43090700	0.96445800	1.58987600
C	-3.99495100	-1.62159800	0.06166600
H	-3.14006700	-2.84362000	-1.48928200
H	-4.57216300	-0.25452300	1.62072500
C	-0.21543300	1.94845200	-0.03063500
C	-1.33318600	2.68649200	-0.44856800
N	0.94042000	2.56133700	0.27801200
C	-1.24749800	4.06499000	-0.51976900
H	-2.24899900	2.18175000	-0.72766200
C	1.00855100	3.88946300	0.20674300
C	-0.05425200	4.69050600	-0.17717800
H	-2.10284800	4.64669800	-0.84705800
H	1.96750800	4.32841400	0.46744800
H	0.05589400	5.76767000	-0.21869000
H	4.52354100	0.78842200	0.22933400
C	-5.24261400	-2.32696100	0.07565400
N	-6.24656500	-2.89173500	0.08635600
E11			
C	1.08886800	0.83163600	-0.03364700

N	-0.19642300	0.84370300	-0.07498900
N	-0.87818500	-0.29795300	-0.06925700
H	-0.38791000	-1.17939100	0.01931600
C	-2.27363900	-0.31227100	-0.12147400
C	-2.93110300	-1.53987100	-0.02771200
C	-3.01875900	0.85607800	-0.28024800
C	-4.31549900	-1.59890000	-0.08693200
C	-4.40367800	0.78783300	-0.33784400
H	-2.50976800	1.80718700	-0.36877700
C	-5.05786700	-0.43456700	-0.24103000
H	-4.82926100	-2.55221300	-0.02403300
H	-4.98765800	1.69195100	-0.47629900
C	1.89226900	-0.42507400	-0.00802400
C	2.57017200	-0.81053200	1.14819300
C	1.94410300	-1.24525500	-1.13564900
C	3.28819800	-1.99434200	1.18297300
H	2.54326400	-0.16976100	2.02256500
C	2.66284000	-2.43098600	-1.11383400
H	1.42608900	-0.94547800	-2.04087600
C	3.33541200	-2.80905800	0.04914400
H	3.81624000	-2.29070500	2.08201100
H	2.70899000	-3.06217300	-1.99391500
C	1.79314200	2.13412000	-0.00943200
C	1.09631000	3.34127800	0.11541100
N	3.12364300	2.08150200	-0.11403000
C	1.81444800	4.52290900	0.12002100
H	0.01774600	3.33205900	0.20914800
C	3.80075000	3.22821900	-0.10682400
C	3.20046400	4.47329100	0.00511700

H	1.30213300	5.47460400	0.21669100
H	4.88014800	3.13931600	-0.19726400
H	3.80100600	5.37576100	0.00549000
H	-2.35957400	-2.45667000	0.08921200
O	-6.42684300	-0.50117000	-0.33467500
C	-7.09524100	-0.30619600	0.89698600
H	-8.16232000	-0.39450800	0.69466000
H	-6.79937900	-1.06595000	1.63014700
H	-6.88438100	0.68689700	1.31122000
C	4.07702700	-4.03629900	0.07980500
N	4.66954600	-5.02348900	0.10514800
Z11			
C	1.05953000	0.54972100	0.00399300
N	-0.11369800	-0.00320200	0.00415900
N	-1.22926300	0.69245000	-0.03090500
H	-1.16829600	1.69609700	-0.18294900
C	-2.47072700	0.04414400	-0.02257800
C	-3.62483200	0.81098800	-0.12526200
C	-2.58442000	-1.34382400	0.09156600
C	-4.88291500	0.21455500	-0.11569000
C	-3.83229000	-1.93663500	0.10179900
H	-1.68851300	-1.94733800	0.16467400
C	-4.99335300	-1.16751800	0.00005000
H	-5.75881500	0.84601100	-0.19922200
H	-3.93108600	-3.01292000	0.18959500
C	2.18550700	-0.42252300	-0.00368700
C	2.15818200	-1.54234900	0.83119800
C	3.26451900	-0.26611900	-0.87897800
C	3.17870100	-2.47793800	0.80004500

H	1.32255600	-1.67295400	1.50913100
C	4.28995900	-1.19558700	-0.92038600
H	3.29308900	0.58462500	-1.55191200
C	4.25326400	-2.30719800	-0.07590800
H	3.15172600	-3.33993600	1.45711700
H	5.11472800	-1.07160100	-1.61303800
C	1.34499400	2.00115800	0.04290000
C	2.58951000	2.48138500	0.48004300
N	0.35984800	2.84914500	-0.30035700
C	2.81160000	3.84489800	0.52885600
H	3.36232300	1.78942000	0.78939600
C	0.58899800	4.16064500	-0.25185600
C	1.79540900	4.71309300	0.14430800
H	3.76682400	4.22932100	0.87091200
H	-0.24240700	4.79641100	-0.54365200
H	1.92907200	5.78824500	0.16380600
H	-3.55070000	1.89101000	-0.21590700
O	-6.16761300	-1.85345800	0.02299800
C	-7.36458800	-1.12318400	-0.09384600
H	-7.41565900	-0.58591400	-1.04800200
H	-8.16938100	-1.85509300	-0.05285600
H	-7.48402000	-0.41046000	0.73040500
C	5.31551900	-3.26868500	-0.10830900
N	6.17083700	-4.04002400	-0.13304300
E12			
C	-1.38138000	0.88109900	0.04239100
N	-0.10593600	0.90613600	0.15119700
N	0.55690800	-0.25819800	0.36736900
H	0.08117100	-1.12372800	0.13734900

C	1.93637200	-0.25721200	0.18761900
C	2.54941100	-1.34108400	-0.43789800
C	2.76638100	0.76372900	0.65239100
C	3.92021400	-1.42023600	-0.60552100
C	4.13952100	0.70672400	0.46784500
C	4.72357600	-0.38369300	-0.15777700
C	-2.18807100	-0.37142500	0.12025300
C	-2.75967600	-0.92032500	-1.02666500
C	-2.34436300	-1.01956200	1.34523800
C	-3.47714000	-2.10304600	-0.95492900
H	-2.65057500	-0.41144800	-1.97746100
C	-3.06793600	-2.19919200	1.42905300
H	-1.90006700	-0.59365700	2.23864900
C	-3.63384700	-2.74437400	0.27577600
H	-3.92215600	-2.53063300	-1.84582200
H	-3.19664800	-2.69835000	2.38242200
C	-2.07133800	2.17839100	-0.17821500
C	-1.36940900	3.38656900	-0.13974600
N	-3.38410900	2.11116700	-0.40568900
C	-2.06923200	4.56105000	-0.35160600
H	-0.30446900	3.38502900	0.05595100
C	-4.04317000	3.25023500	-0.60939200
C	-3.43765500	4.49817500	-0.59368300
H	-1.55558000	5.51634400	-0.32565700
H	-5.10998500	3.15306200	-0.79140300
H	-4.02268300	5.39476800	-0.76348200
F	1.77977900	-2.33758600	-0.89239200
F	4.46051400	-2.47067300	-1.20940000
F	6.03957500	-0.43742700	-0.31967400

F	4.90500000	1.69402900	0.91626200
F	2.26571000	1.80306000	1.31168300
C	-4.37860300	-3.96780500	0.35449000
N	-4.97488300	-4.95083600	0.41760900
Z12			
C	-1.35009000	0.60071600	-0.06020400
N	-0.19836400	0.02447900	-0.05912500
N	0.93505300	0.73089600	-0.18262000
H	0.89771100	1.72253800	0.04318300
C	2.14313200	0.05613800	-0.09264800
C	3.22792900	0.68463700	0.51844900
C	2.36293700	-1.21533500	-0.62666900
C	4.47091600	0.08651300	0.61493800
C	3.59907700	-1.83373400	-0.51391300
C	4.65828100	-1.18796900	0.10370200
C	-2.49736300	-0.33625000	0.08397400
C	-2.46066800	-1.57818200	-0.55466500
C	-3.59587000	-0.02147000	0.88798500
C	-3.49781800	-2.48218400	-0.40349900
H	-1.60240800	-1.83090700	-1.16588000
C	-4.63782200	-0.92055300	1.04795500
H	-3.63188600	0.92914200	1.40951600
C	-4.59455300	-2.15487900	0.39760900
H	-3.46458700	-3.44230600	-0.90548600
H	-5.48186000	-0.67349100	1.68174500
C	-1.60235600	2.05673400	-0.22638800
C	-2.80314000	2.52123300	-0.77345000
N	-0.62053900	2.90096100	0.12533300
C	-2.98776600	3.88447400	-0.93276500

H	-3.57125300	1.82120400	-1.07742500
C	-0.81159900	4.20938200	-0.02554600
C	-1.97797700	4.75412200	-0.54150900
H	-3.90894200	4.26410700	-1.36171100
H	0.01378300	4.84666800	0.27810400
H	-2.08347000	5.82746700	-0.64549500
F	1.40564700	-1.85586400	-1.29111500
F	3.77798100	-3.04497500	-1.02745800
F	5.84257400	-1.78067600	0.19712100
F	5.47424800	0.72051300	1.20957700
F	3.05489400	1.90802300	1.03058900
C	-5.67426200	-3.08498400	0.55354600
N	-6.54345200	-3.83034600	0.67835800

E13

C	1.38503300	1.17341800	-0.01618300
N	0.10268100	1.10925500	-0.01514900
N	-0.50704100	-0.07858300	0.02091400
H	0.04063800	-0.92680200	0.09706200
C	-1.89129800	-0.17467400	0.01493600
C	-2.47516600	-1.43981900	0.12737100
C	-2.70723300	0.95284100	-0.11036300
C	-3.85212800	-1.57554600	0.11583700
C	-4.08313200	0.80560200	-0.11995300
H	-2.25525400	1.93096400	-0.20574900
C	-4.66539100	-0.45408400	-0.01007600
H	-4.29290300	-2.56167600	0.20212100
H	-4.70950500	1.68478600	-0.22183800
C	2.26297300	-0.03306300	-0.01176800
C	2.98509600	-0.38026400	1.12976800

C	2.33783300	-0.84209200	-1.14628800
C	3.77256300	-1.52056700	1.14513200
H	2.93885700	0.25385700	2.00785900
C	3.12447100	-1.98481800	-1.14776600
H	1.78553500	-0.56866500	-2.03926700
C	3.82674400	-2.30491800	0.00279800
H	4.34113800	-1.80297700	2.02148400
H	3.20001600	-2.61872000	-2.02155200
C	2.01231700	2.51640300	-0.02529400
C	1.24761200	3.68074000	0.09718900
N	3.34048100	2.53774100	-0.15897300
C	1.89507900	4.90252200	0.06789400
H	0.17380700	3.60993800	0.21474300
C	3.94934300	3.72165200	-0.18390100
C	3.27846200	4.93116800	-0.07730800
H	1.33054200	5.82445600	0.16071100
H	5.02982700	3.69519400	-0.29664900
H	3.82460500	5.86703000	-0.10441700
H	-1.84896500	-2.32202500	0.22303400
C	-6.15681200	-0.58660900	0.03134900
F	-6.76711500	0.29846600	-0.77774200
F	-6.57102200	-1.81133000	-0.33638500
F	-6.65027400	-0.37074600	1.26948400
C	4.69849149	-3.57439176	0.01242539
N	5.35513245	-4.53061875	0.01967719
Z13			
C	1.33500600	0.87866900	0.01506600
N	0.14941800	0.36433200	0.00374600
N	-0.94594200	1.10737600	-0.02890100

H	-0.84535800	2.10878400	-0.17523100
C	-2.19866300	0.50625900	-0.03749800
C	-3.32679100	1.32595500	-0.11635400
C	-2.35596000	-0.88104800	0.03579700
C	-4.59521200	0.76950900	-0.12145800
C	-3.62631400	-1.42660600	0.02929500
H	-1.48042900	-1.51463600	0.08895400
C	-4.75256100	-0.60904000	-0.04882800
H	-5.46266300	1.41552400	-0.18349200
H	-3.74283700	-2.50373000	0.08442200
C	2.43053300	-0.12951700	0.00988300
C	2.37542100	-1.23282200	0.86436600
C	3.50291600	-0.01548700	-0.87960900
C	3.36694900	-2.20056100	0.83993300
H	1.54453900	-1.32669200	1.55373700
C	4.49996100	-0.97617000	-0.91972300
H	3.54984400	0.82493200	-1.56396500
C	4.41766900	-2.05553400	-0.05313500
H	3.33676200	-3.05448400	1.50399800
H	5.32550500	-0.90348300	-1.61546500
C	1.67372800	2.32239800	0.06225900
C	2.93052600	2.75154300	0.50978600
N	0.72326000	3.20472200	-0.28867100
C	3.20250100	4.10716300	0.56538700
H	3.67562900	2.03072500	0.82103200
C	0.99954200	4.50615000	-0.23594200
C	2.22290400	5.01171400	0.17444700
H	4.16835400	4.45512400	0.91603400
H	0.19614500	5.17334600	-0.53483400

H	2.39530500	6.08117300	0.19857700
H	-3.20948800	2.40371000	-0.17458100
C	-6.11214400	-1.23731400	-0.03129000
F	-7.09488700	-0.34638000	-0.24089400
F	-6.37526200	-1.83781800	1.14827600
F	-6.23868700	-2.19239600	-0.97379500
C	5.52645820	-3.12379900	-0.08470075
N	6.36165006	-3.92846615	-0.10847756

E14

C	-0.95220300	0.83791000	0.00579000
N	0.33087800	0.87237000	0.00138500
N	1.02088300	-0.27386700	-0.02696000
H	0.52796200	-1.15678500	-0.08182700
C	2.40493100	-0.28027000	-0.02450000
C	3.06657400	-1.51149000	-0.10692200
C	3.14965800	0.90012100	0.06317800
C	4.44662100	-1.56310800	-0.10171500
C	4.53105500	0.84129100	0.06681600
H	2.63849600	1.85093700	0.13141700
C	5.19493600	-0.38563300	-0.01545100
H	4.95201000	-2.51980200	-0.16702000
H	5.10607800	1.75785700	0.13569400
C	-1.73372900	-0.43375000	0.00515700
C	-2.34448100	-0.88718900	-1.16317000
C	-1.82568400	-1.19666000	1.16912600
C	-3.04034500	-2.08516200	-1.17286600
H	-2.28289200	-0.29160500	-2.06740000
C	-2.52380400	-2.39476500	1.17173000
H	-1.35780000	-0.84207600	2.08163200

C	-3.13113600	-2.84221200	-0.00254400
H	-3.51731200	-2.43673000	-2.08039400
H	-2.60406500	-2.98175000	2.07937700
C	-1.68609800	2.12562400	0.01318400
C	-1.02209900	3.34904500	-0.11497500
N	-3.01113600	2.03507900	0.14961500
C	-1.77076500	4.51228400	-0.09121000
H	0.05396700	3.36919100	-0.23308600
C	-3.71795400	3.16307800	0.17069100
C	-3.15115600	4.42423700	0.05612600
H	-1.28570800	5.47771300	-0.19016600
H	-4.79197700	3.04594700	0.28622500
H	-3.77477100	5.31057200	0.07874400
H	2.49542800	-2.43250500	-0.17657000
C	6.62459600	-0.43679500	-0.00984300
N	7.77631200	-0.47804300	-0.00517900
C	-3.85115800	-4.08282000	-0.00786800
N	-4.42636300	-5.08030700	-0.01329400

Z14

C	-0.88846000	0.53518600	-0.00438300
N	0.28333600	-0.00754200	0.00081200
N	1.39662000	0.71458800	0.02938200
H	1.31631900	1.71675500	0.18449700
C	2.63320100	0.08864200	0.03096800
C	2.76288300	-1.30085500	-0.05847300
C	5.03393300	0.30862400	0.11649900
C	4.02074100	-1.87422800	-0.06006800
H	1.87438900	-1.91534300	-0.11881100
C	5.16807400	-1.07978200	0.02562800

H	5.91844100	0.93168900	0.18479900
H	4.12088300	-2.95158300	-0.12904300
C	-2.01170100	-0.44289700	0.00259800
C	-2.00098700	-1.53604400	-0.86520300
C	-3.06765400	-0.30978200	0.90779800
C	-3.02084700	-2.47324100	-0.83685300
H	-1.18252300	-1.64566600	-1.56741400
C	-4.09008400	-1.24275300	0.94840000
H	-3.08149900	0.52363200	1.60250000
C	-4.07217700	-2.32882700	0.07075700
H	-3.01009000	-3.31536600	-1.51940800
H	-4.89825000	-1.14048600	1.66356300
C	-1.19273300	1.98774500	-0.04528900
C	-2.43931600	2.44678600	-0.49075800
N	-0.22280700	2.84633200	0.31083700
C	-2.68071100	3.80865300	-0.53920300
H	-3.20004400	1.74386700	-0.80519800
C	-0.46983000	4.15384500	0.26572400
C	-1.68153100	4.68866700	-0.14252900
H	-3.63822400	4.18030300	-0.88832700
H	0.34807800	4.80120200	0.56883300
H	-1.83040300	5.76177800	-0.16034500
C	3.77977600	0.88721100	0.11838600
H	3.68227900	1.96613000	0.18874500
C	6.46647800	-1.68026600	0.02195000
N	7.51320600	-2.16264200	0.01893300
C	-5.13297600	-3.29266400	0.10137500
N	-5.98690100	-4.06516900	0.12455900

E15

C	1.34150100	0.83632700	-0.00704300
N	0.05954200	0.89174800	-0.00314000
N	-0.64952000	-0.24448400	0.02476000
H	-0.17118200	-1.13528500	0.08232300
C	-2.03090900	-0.22610900	0.02288200
C	-2.71506200	-1.44680100	0.10565300
C	-2.75281000	0.97003300	-0.06529000
C	-4.09525000	-1.47441300	0.10095600
C	-4.13464100	0.93970200	-0.06907900
H	-2.22307800	1.91039300	-0.13323700
C	-4.79621900	-0.27832200	0.01408300
H	-4.63379600	-2.41085100	0.16537600
H	-4.70671700	1.85590100	-0.13766500
C	2.10403600	-0.44664000	-0.00728300
C	2.72000500	-0.90198600	1.15754200
C	2.17455900	-1.21630100	-1.16826500
C	3.39979800	-2.10903600	1.16672400
H	2.67561300	-0.30073400	2.05901400
C	2.85686100	-2.42350400	-1.17126800
H	1.70325100	-0.85990700	-2.07831800
C	3.46945100	-2.87298500	-0.00057400
H	3.88083500	-2.46234600	2.07140600
H	2.92075100	-3.01610200	-2.07656400
C	2.09475600	2.11344300	-0.01136600
C	1.44883100	3.34538900	0.12422800
N	3.41774000	2.00389400	-0.15255300
C	2.21418900	4.49793700	0.10281900
H	0.37364300	3.38110900	0.24617700
C	4.14077900	3.12155500	-0.17131400

C	3.59237300	4.39035100	-0.04955200
H	1.74319900	5.46968000	0.20745900
H	5.21259900	2.98965900	-0.29088800
H	4.22890600	5.26749000	-0.07049800
H	-2.16079000	-2.37778200	0.17534900
N	-6.25882700	-0.30403000	0.00870900
O	-6.84492100	0.75910800	-0.07887600
O	-6.80722800	-1.38756700	0.09229700
C	4.17369900	-4.12260700	0.00400400
N	4.73653300	-5.12709100	0.00873100

Z15

C	-1.29184500	0.56414600	0.00707400
N	-0.09072300	0.09126100	0.01198000
N	0.98032000	0.87705400	0.03229400
H	0.84233700	1.87572300	0.16970500
C	2.24756300	0.32224000	0.03127100
C	3.34931000	1.18624600	0.09339900
C	2.45169200	-1.06096600	-0.03558000
C	4.63357800	0.67949000	0.08937300
C	3.73789500	-1.56664800	-0.03990900
H	1.59766000	-1.72366500	-0.07583900
C	4.81832500	-0.69553900	0.02104400
H	5.49232600	1.33624700	0.13700000
H	3.91369600	-2.63344900	-0.09010300
C	-2.35327300	-0.48114500	0.01268900
C	-2.27858100	-1.56057600	-0.86873100
C	-3.41041600	-0.42510400	0.92424300
C	-3.23773500	-2.55987600	-0.84834000
H	-1.45838000	-1.61034900	-1.57562500

C	-4.37238000	-1.42085200	0.95725200
H	-3.47217700	0.39746700	1.62924300
C	-4.29137400	-2.49239300	0.06538100
H	-3.17812900	-3.39112200	-1.54156300
H	-5.18162800	-1.37819900	1.67713000
C	-1.68283000	1.99594500	-0.03935900
C	-2.96381700	2.37689000	-0.45902000
N	-0.75667500	2.91305500	0.28652300
C	-3.28459400	3.72235500	-0.51540700
H	-3.69006100	1.62824500	-0.74826200
C	-1.07936000	4.20341900	0.23349700
C	-2.32894200	4.66286500	-0.15262000
H	-4.27043200	4.03349100	-0.84425800
H	-0.29393200	4.90025900	0.51137000
H	-2.53887100	5.72552400	-0.17904200
H	3.19304300	2.25904000	0.14507800
N	6.17790500	-1.23536000	0.01577200
O	6.30949500	-2.44352900	-0.05089900
O	7.10243100	-0.44540600	0.07828300
C	-5.29023600	-3.52052100	0.08881000
N	-6.09493400	-4.34423700	0.10710100
E16			
C	-0.28597900	0.83687600	-0.00118300
N	0.99296800	0.71742900	-0.00577200
N	1.54888500	-0.49375600	-0.03943000
H	0.99248500	-1.33866500	-0.10743200
C	2.92462000	-0.66081000	-0.03713400
N	3.31189000	-1.93037800	-0.11975500
C	3.81188600	0.41743900	0.05238400

C	4.62072000	-2.17864700	-0.11805400
C	5.16389100	0.13093400	0.05138100
H	3.43614800	1.42927100	0.12267600
C	5.59090100	-1.19252100	-0.03547400
H	4.89819400	-3.22689600	-0.18809100
H	5.88635000	0.93788700	0.11930500
H	6.64306000	-1.45039900	-0.03846700
C	-1.21496700	-0.33031600	0.00088600
C	-1.94102800	-0.66453500	-1.14144500
C	-1.33540000	-1.11963700	1.14431500
C	-2.77456900	-1.77068700	-1.14599900
H	-1.85813700	-0.04776500	-2.02941100
C	-2.17019100	-2.22647000	1.15253800
H	-0.77578900	-0.86054700	2.03713700
C	-2.89105500	-2.55510100	0.00386400
H	-3.33842500	-2.02981600	-2.03472800
H	-2.26713500	-2.83489000	2.04425800
C	-0.85119800	2.20725500	0.01261000
C	-0.03030100	3.33639500	-0.07971100
N	-2.17897500	2.29183400	0.12309400
C	-0.61878000	4.58718100	-0.04451700
H	1.04089800	3.21494500	-0.17759300
C	-2.73083300	3.50337100	0.15323800
C	-2.00181100	4.68093900	0.07621000
H	-0.00833300	5.48182100	-0.11230800
H	-3.81335100	3.52785200	0.24649600
H	-2.50345600	5.64126900	0.10797000
C	-3.75395300	-3.70083500	0.00361300
N	-4.44680000	-4.62070800	0.00258700

Z16

C	0.23667200	0.45296800	-0.01459900
N	-0.77355100	-0.35284000	-0.01859200
N	-2.02570500	0.07220200	-0.04319200
H	-2.22923600	1.05721000	-0.19432700
C	-3.07604900	-0.83577000	-0.03793000
N	-4.27638000	-0.27172300	-0.14071000
C	-2.87395700	-2.21595300	0.07235700
C	-5.33837000	-1.07582700	-0.13711200
C	-3.99328200	-3.02659200	0.07374700
H	-1.87201400	-2.61664200	0.14708600
C	-5.25956100	-2.45562200	-0.03217200
H	-6.30191100	-0.58098100	-0.22472300
H	-3.87905600	-4.10255100	0.15759300
H	-6.15793600	-3.06133300	-0.03426500
C	1.55832900	-0.23224800	-0.01859500
C	2.57641100	0.17170100	-0.88667200
C	1.78529300	-1.32522800	0.82038200
C	3.79076700	-0.49356700	-0.91718300
H	2.41098900	1.00685800	-1.55931900
C	2.99646400	-1.99628100	0.80119900
H	0.99844500	-1.64541600	1.49346100
C	4.00758500	-1.58075000	-0.06804000
H	4.56990300	-0.18065300	-1.60287700
H	3.16714400	-2.83880400	1.46175400
C	0.18356900	1.93535400	0.03537400
C	1.27718300	2.68038100	0.49736700
N	-0.96260100	2.53349400	-0.32450700
C	1.17593200	4.05930900	0.56176400

H	2.18520000	2.18274200	0.81344300
C	-1.04672000	3.86004800	-0.26079000
C	-0.00709100	4.67153400	0.16667700
H	2.01117500	4.65013400	0.92280900
H	-1.99790600	4.28799200	-0.56404700
H	-0.12849000	5.74782600	0.20042500
C	5.26546100	-2.26770100	-0.08865900
N	6.27707600	-2.81840600	-0.10438400

E17

C	1.43505200	-0.79526300	0.02160400
N	0.27444600	-1.34854400	0.02861300
N	-0.82019500	-0.58800100	0.01509800
H	-0.77466300	0.42296000	-0.06131600
C	1.63827000	0.68198300	0.03290300
C	2.15731700	1.33573200	-1.08393300
C	1.27638200	1.42762000	1.15462200
C	2.30994700	2.71191000	-1.08594300
H	2.45090600	0.75934000	-1.95406100
C	1.42909600	2.80528800	1.16595300
H	0.87391400	0.92400600	2.02731000
C	1.94504700	3.45106500	0.04181100
H	2.71384400	3.21829000	-1.95502100
H	1.15150600	3.38147300	2.04104000
C	2.61932000	-1.68653000	0.00124600
C	2.48593800	-3.07060600	-0.15529400
N	3.80673000	-1.09163500	0.14034400
C	3.62789000	-3.85050100	-0.15570500
H	1.50162600	-3.50489500	-0.27515200
C	4.89698200	-1.85620200	0.13660800

C	4.86699500	-3.23572600	-0.00530100
H	3.55471700	-4.92640100	-0.27691000
H	5.84232500	-1.33312500	0.25457700
H	5.78742900	-3.80839000	-0.00165500
C	-2.08112600	-1.14821600	0.03309800
C	-3.17784400	-0.23147700	-0.04248400
C	-2.32697700	-2.49842300	0.12658500
C	-4.50199000	-0.73124500	-0.02189200
C	-3.65320600	-2.97639600	0.14504300
H	-1.49491900	-3.18826700	0.18813000
C	-3.87940100	1.94125600	-0.20114800
C	-5.54258900	0.22433300	-0.09967100
C	-4.72482900	-2.12680000	0.07367000
H	-3.81750800	-4.04628000	0.22151900
C	-5.23749800	1.55476000	-0.18902400
H	-3.61359900	2.99304800	-0.27322200
H	-6.57541600	-0.11177300	-0.08710500
H	-5.74131200	-2.50645800	0.09063100
H	-6.01290000	2.30979700	-0.24986900
N	-2.88532800	1.09111900	-0.13082200
C	2.09970400	4.87689200	0.04406400
N	2.22137100	6.02219600	0.04537000
Z17			
C	1.10290000	0.40025500	0.03568400
N	0.13677600	-0.45956500	0.03861400
N	-1.13529800	-0.09752400	0.02777300
H	-1.39416200	0.87483300	-0.12803500
C	2.45952200	-0.20883600	-0.00419700
C	2.75516100	-1.32950200	0.77582900

C	3.44578000	0.29303300	-0.85854000
C	3.99962700	-1.93291600	0.70967200
H	1.99391600	-1.72530900	1.43798700
C	4.69300300	-0.30366900	-0.93505200
H	3.22871800	1.15048200	-1.48685900
C	4.97714200	-1.42071600	-0.14685900
H	4.22228200	-2.79894800	1.32276800
H	5.44614000	0.08455100	-1.61133300
C	0.96639500	1.87626000	0.09710900
C	2.00432000	2.67760400	0.59262900
N	-0.20264900	2.41020400	-0.28564900
C	1.82240700	4.04754300	0.66522300
H	2.93098800	2.22831000	0.92716100
C	-0.36529300	3.72854100	-0.21284400
C	0.61549000	4.59455200	0.24559800
H	2.61293800	4.68281900	1.05085400
H	-1.33308200	4.10189900	-0.53552000
H	0.43310900	5.66212400	0.28440900
C	-2.12916500	-1.05924500	0.06362500
C	-3.47581100	-0.58817700	-0.04766900
C	-1.88805200	-2.40695400	0.20067900
C	-4.54022800	-1.52253000	-0.01310000
C	-2.96034800	-3.32038100	0.23324100
H	-0.86654500	-2.75728000	0.27759900
C	-4.89896700	1.18549300	-0.29844400
C	-5.85044300	-1.00184100	-0.13442000
C	-4.26081400	-2.90315300	0.13147100
H	-2.74008100	-4.37728100	0.34259500
C	-6.03412000	0.34554600	-0.27763000

H	-5.02235400	2.26001400	-0.41257900
H	-6.69658800	-1.68266900	-0.11460100
H	-5.07977600	-3.61480100	0.15679900
H	-7.02468500	0.77513200	-0.37566600
N	-3.66983200	0.74807000	-0.18846400
C	6.26821000	-2.03898800	-0.21725100
N	7.30655900	-2.53481200	-0.27286000

E18

C	-1.38793800	0.85022900	-0.02194000
N	-0.10927200	0.73983500	-0.04212100
N	0.44880000	-0.47355600	-0.07208900
H	-0.13800600	-1.29815200	-0.09153200
C	1.82855800	-0.62499000	-0.05892900
C	2.31110100	-1.98121200	-0.13214100
C	2.68802400	0.43529600	0.01904300
C	3.63485800	-2.27351900	-0.12791600
C	4.08054900	0.15855600	0.02400200
H	2.32855400	1.45299600	0.07850900
C	4.56448800	-1.19592200	-0.04890500
H	3.99427600	-3.29395400	-0.18449800
C	-2.30273700	-0.32949200	-0.00555900
C	-2.88662200	-0.78959500	-1.18482000
C	-2.54142400	-1.00763600	1.18936600
C	-3.70103500	-1.91082100	-1.17454200
H	-2.70850300	-0.26025400	-2.11450900
C	-3.35716100	-2.12847800	1.21154400
H	-2.09248000	-0.64718500	2.10892700
C	-3.93755500	-2.58327200	0.02626500
H	-4.15769500	-2.26731400	-2.09060700

H	-3.54904700	-2.64999500	2.14216100
C	-1.97234800	2.21116000	-0.00723300
C	-1.16880700	3.35338300	-0.08080900
N	-3.30308100	2.26978900	0.08424500
C	-1.78048300	4.59339000	-0.05097500
H	-0.09394200	3.25192800	-0.16064700
C	-3.87669400	3.47116300	0.11097400
C	-3.16656400	4.66131700	0.04834300
H	-1.18522500	5.49895000	-0.10534900
H	-4.96064600	3.47640300	0.18826000
H	-3.68531400	5.61265000	0.07546500
H	1.58412100	-2.78643900	-0.19393900
N	5.88887100	-1.29337300	-0.03256200
N	5.06082700	1.05682200	0.09498200
S	6.46190200	0.22553300	0.06864200
C	-4.77709100	-3.74627800	0.04094000
N	-5.44803700	-4.68206500	0.05172100

Z18

C	-1.43443900	0.60953900	0.02885900
N	-0.18771000	0.27071600	0.04759600
N	0.79345600	1.15948100	0.07115700
H	0.55464700	2.13815800	0.20953600
C	2.11563000	0.72953000	0.06684900
C	3.11019600	1.76978800	0.13133100
C	2.46528400	-0.59041900	-0.00134200
C	4.43818500	1.49558000	0.12713300
C	3.84889800	-0.90731000	-0.00879000
H	1.71902400	-1.37153100	-0.04268000
C	4.84473600	0.13129600	0.05494400

H	5.18433600	2.27941100	0.17569700
C	-2.37326600	-0.54644300	0.02880800
C	-2.12691400	-1.64434300	-0.79816400
C	-3.48104700	-0.57920700	0.88009000
C	-2.96647400	-2.74552800	-0.78491700
H	-1.26496000	-1.62794400	-1.45496000
C	-4.32647700	-1.67618900	0.90342600
H	-3.67608200	0.25508800	1.54590500
C	-4.07420800	-2.76422800	0.06533100
H	-2.77090100	-3.59122300	-1.43428000
H	-5.17659400	-1.69856700	1.57572900
C	-1.97219100	1.99086600	-0.03860000
C	-3.27309900	2.23581800	-0.49845400
N	-1.15531700	3.00136200	0.30369400
C	-3.73021900	3.53988700	-0.57376200
H	-3.90910500	1.41495800	-0.80394700
C	-1.60856200	4.25122600	0.23014600
C	-2.88772200	4.57680500	-0.19190800
H	-4.73307300	3.74486900	-0.93301800
H	-0.90602800	5.02658900	0.52199100
H	-3.20618600	5.61173800	-0.23218300
H	2.77326400	2.80118700	0.18395400
N	4.37636700	-2.12866800	-0.07300000
N	6.09339300	-0.32189700	0.03757500
S	5.99396500	-1.94317800	-0.05217300
C	-4.95235800	-3.89727300	0.07847000
N	-5.66126400	-4.80503100	0.08816900

References

- (1) Mravec, B.; Budzák, Š.; Medved', M.; Pašteka, L. F.; Slavov, C.; Saßmannshausen, T.; Wachtveitl, J.; Kožíšek, J.; Hegedüsová, L.; Filo, J.; Cigáň, M. Design of High-Performance Pyridine/Quinoline Hydrazone Photoswitches. *J. Org. Chem.* **2021**, *86* (17), 11633–11646. <https://doi.org/10.1021/acs.joc.1c01174>.
- (2) Le Bahers, T.; Adamo, C.; Ciofini, I. A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. *J. Chem. Theory Comput.* **2011**, *7* (8), 2498–2506. <https://doi.org/10.1021/ct200308m>.