Exploring the Role of H-migration on Aromaticity, Spectroscopic, Photovoltaic and Optical Properties of Planar Heterocyclic Compounds: A DFT Study

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Table S1: Cartesian coordinates of **IB1**

Atom	X-axis	Y-axis	Z-axis
C	-7.368679	0.696525	-0.005319
C	-7.368677	-0.696527	0.005411
C	-6.156789	-1.392087	-0.003119
C	-4.942988	-0.711142	-0.011071
C	-4.942989	0.711141	0.011139
C	-6.156789	1.392085	0.003198
N	-3.728601	-1.371316	-0.020844
C	-2.492795	-0.701573	-0.011169
C	-2.492796	0.701573	0.011199
N	-3.728602	1.371316	0.020902
C	-0.065030	-0.703334	-0.011706
C	-0.065029	0.703335	0.011685
C	2.392699	-0.723288	-0.012126
C	2.392699	0.723289	0.012070
C	3.579477	-1.409707	-0.023613
C	4.830604	-0.722900	-0.012347
C	4.830604	0.722898	0.012283
C	3.579478	1.409708	0.023552
C	7.118171	-0.721568	-0.014736
C	7.118170	0.721565	0.014657
N	5.969339	1.426027	0.025998
C	9.554753	-0.722878	0.009795
C	9.554752	0.722873	-0.009878
C	8.362046	1.408355	0.007431
N	10.807067	1.355547	0.012771
N	10.807057	-1.355551	-0.012842
H	-6.184245	-2.475769	0.013040
H	-6.184247	2.475768	-0.012960
H	-1.283221	-2.479256	-0.039420
H	-1.283222	2.479257	0.039422
H	3.598464	-2.495954	-0.042196
H	3.598465	2.495955	0.042136
H	8.340849	2.494815	-0.003694
H	10.753281	2.358083	-0.129728
H	11.471455	0.939530	-0.634714
H	11.471499	-0.939438	0.634523
H	10.753301	-2.358072	0.129760
N	-8.586675	1.495997	-0.165380
O	-8.607443	2.596807	0.388050
O	-9.472229	1.043967	-0.884718
N	-8.586670	-1.496002	0.165488
O	-8.607450	-2.596802	-0.387963
O	-9.472225	-1.043964	0.884819
H	1.158222	2.375986	0.039427
H	1.158222	-2.375985	-0.039451
H	-3.729929	-2.379480	-0.064136
C	-1.282665	1.391776	0.022524
C	-1.282665	-1.391775	-0.022520
N	1.158825	1.366595	0.022878

N	1.158825	-1.366593	-0.022928
C	8.362045	-1.408360	-0.007522
N	5.969338	-1.426030	-0.026066
H	-3.729929	2.379480	0.064185
H	8.340849	-2.494829	0.003575

Table S2: Cartesian coordinates of **IB2**

Atom	X-axis	Y-axis	Z-axis
C	7.373280	-0.697944	-0.004283
C	7.373278	0.697944	0.004901
C	6.164383	1.393313	-0.005077
C	4.950293	0.710190	-0.011719
C	4.950291	-0.710189	0.011721
C	6.164382	-1.393313	0.005395
N	3.736359	1.367290	-0.022000
C	2.496640	0.718548	-0.011928
C	2.496638	-0.718548	0.011282
N	3.736354	-1.367288	0.021702
C	1.310612	1.407964	-0.024016
C	0.063746	0.719300	-0.012854
C	0.063746	-0.719296	0.011923
C	1.310607	-1.407962	0.023196
N	-1.081710	1.426265	-0.025248
C	-2.223361	0.724527	-0.013152
C	-2.223360	-0.724524	0.012075
N	-1.081714	-1.426260	0.024169
C	-3.470661	1.410429	-0.025300
C	-4.662086	0.725049	-0.013311
C	-4.662091	-0.725059	0.011548
C	-3.470663	-1.410428	0.023960
N	-5.888319	1.364411	-0.024276
C	-7.120357	0.701806	-0.011663
C	-7.120363	-0.701814	0.010872
N	-5.888323	-1.364439	0.021716
C	-8.334147	1.390307	-0.005407
C	-9.552589	0.706046	0.007344
C	-9.552622	-0.706035	-0.005403
C	-8.334162	-1.390316	0.006091
N	-10.798634	-1.367557	0.027875
N	-10.798818	1.367482	-0.024611
H	6.191068	2.477095	0.009916
H	6.191072	-2.477095	-0.009586
H	1.291712	2.494134	-0.042081
H	1.291703	-2.494133	0.041220
H	-3.451987	2.496485	-0.044070
H	-3.451990	-2.496484	0.042796
H	-8.330081	2.478646	0.000773
H	-8.330124	-2.478656	-0.000061
H	-10.722457	-2.367234	-0.126539
H	-11.457919	-0.968635	-0.637233
H	-11.456808	0.969230	0.642243
H	-10.722348	2.367295	0.128936
H	-5.890227	-2.374017	0.041004
H	-5.890214	2.373997	-0.043140
N	8.592546	-1.495740	-0.167460
O	8.616883	-2.596853	0.384474
O	9.475220	-1.040410	-0.888114

N	8.592504	1.495734	0.168383
O	8.616954	2.596880	-0.383481
O	9.474983	1.040399	0.889270
H	3.737981	2.377005	-0.052023
H	3.737969	-2.377003	0.051728

Table S3: Cartesian coordinates of **IB3**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-7.350627	-0.706779	-0.008118
C	-7.394023	0.698790	-0.009855
C	-6.185039	1.411256	0.005293
C	-4.978763	0.736999	0.012779

C	-4.910988	-0.695790	-0.017929
C	-6.150649	-1.386673	-0.024353
N	-3.758649	1.412211	0.027618
C	-2.550764	0.757871	0.013392
C	-2.593860	-0.685780	-0.016405
N	-3.755384	-1.388067	-0.030176
C	-0.132110	0.743118	0.013604
C	-0.152158	-0.671185	-0.016576
C	2.320537	0.733310	0.013884
C	2.295819	-0.699729	-0.016876
C	3.526620	1.408909	0.028620
C	4.768257	0.720979	0.013906
C	4.714423	-0.727889	-0.017234
C	3.500003	-1.411100	-0.032035
C	7.090054	0.700535	0.016231
C	7.134840	-0.722422	-0.015180
N	5.914203	-1.382156	-0.031662
C	9.536054	0.713971	-0.005394
C	9.553364	-0.713529	0.007926
C	8.347783	-1.413399	-0.013270
N	10.797191	-1.351582	-0.009657
N	10.781667	1.371756	0.029267
H	-6.230870	2.494688	-0.008193
H	-6.137389	-2.469800	-0.017342
H	-1.332916	2.535927	0.051337
H	-1.382771	-2.446968	-0.054683
H	3.557282	2.493676	0.052237
H	3.482773	-2.498547	-0.055659
H	8.354827	-2.502045	-0.010066
H	10.761794	-2.344334	0.190786
H	11.489187	-0.886355	0.571806
H	11.425098	1.028307	-0.680401
H	10.697498	2.379919	-0.045638
N	5.914610	-2.394423	-0.055066
O	-8.559444	-1.538761	0.155116
O	-8.730137	-2.440415	-0.660465
N	-9.253655	-1.317725	1.140385
O	-8.621742	1.442389	-0.151731
O	-8.595762	2.651933	0.121560
H	-9.619624	0.844927	-0.569222
H	1.062835	-2.333820	-0.052133
C	1.103868	2.389681	0.049119
C	-3.769851	2.423155	0.052444
N	-1.361166	-1.361597	-0.031332
N	-1.341864	1.448289	0.028201
C	1.078645	-1.321968	-0.030356
N	1.094726	1.378436	0.027477
H	8.324844	1.386436	0.010805
H	5.920405	1.400814	0.029414
H	8.292596	2.472141	0.005706

Table S4: Cartesian coordinates of **IB4**

Atom	X-axis	Y-axis	Z-axis
C	-7.394005	0.698780	-0.009736
C	-7.350645	-0.706746	-0.008186
C	-6.150637	-1.386644	-0.024560
C	-4.911036	-0.695755	-0.018042
C	-4.978760	0.737031	0.012642
C	-6.185036	1.411292	0.005372
N	-3.755384	-1.388026	-0.030280
C	-2.593887	-0.685774	-0.016499
C	-2.550746	0.757882	0.013155
N	-3.758647	1.412233	0.027281
C	-0.152168	-0.671187	-0.016581

C	-0.132097	0.743127	0.013396
C	2.295823	-0.699737	-0.016813
C	2.320543	0.733313	0.013725
C	3.500000	-1.411110	-0.031832
C	4.714432	-0.727878	-0.017111
C	4.768258	0.720979	0.013799
C	3.526624	1.408928	0.028377
C	7.134856	-0.722409	-0.015000
C	7.090079	0.700551	0.016173
N	5.920419	1.400812	0.029222
C	9.553372	-0.713512	0.008134
C	9.536080	0.713974	-0.005443
C	8.324863	1.386453	0.010667
N	10.781649	1.371767	0.029143
N	10.797274	-1.351561	-0.009441
H	-6.137366	-2.469772	-0.017761
H	-6.230893	2.494720	-0.007948
H	-1.382799	-2.446975	-0.054496
H	-1.332926	2.535944	0.050868
H	3.482805	-2.498557	-0.055288
H	3.557323	2.493693	0.051822
H	8.292609	2.472156	0.005409
H	10.697582	2.379862	-0.046732
H	11.425454	1.027550	-0.679806
H	11.489048	-0.886611	0.572531
H	10.761733	-2.344355	0.190826
H	-8.621833	1.442389	-0.151143
N	-8.595819	2.651874	0.122247
O	-9.619825	0.844897	-0.568293
O	-8.559419	-1.538783	0.154831
N	-8.730360	-2.439814	-0.661392
O	-9.253326	-1.318395	1.140439
O	1.103877	2.389673	0.048689
H	1.062835	-2.333819	-0.051846
H	-1.341855	1.448304	0.027874
H	-1.361157	-1.361604	-0.031276
C	1.094735	1.378425	0.027198
C	1.078646	-1.321966	-0.030224
N	8.347801	-1.413386	-0.012935
N	5.914208	-1.382145	-0.031402
C	-3.769853	2.423180	0.051820
N	5.914618	-2.394414	-0.054654
H	8.354847	-2.502030	-0.009541

Table S5: Cartesian coordinates of **IB5**

Atom	X-axis	Y-axis	Z-axis
C	7.371332	-0.710827	0.000690
C	7.371327	0.710840	0.000364
C	6.188810	1.407931	-0.016098
C	4.948550	0.718022	-0.016437
C	4.948549	-0.718020	0.016603
C	6.188812	-1.407923	0.016718
N	3.798849	1.430035	-0.027799
C	2.662953	0.729578	-0.014477
C	2.662952	-0.729590	0.013818
N	3.798848	-1.430040	0.027548
C	1.416765	1.414415	-0.028395
C	0.225681	0.726920	-0.015193
C	0.225680	-0.726945	0.013658
C	1.416764	-1.414434	0.027289
N	-0.997742	1.360182	-0.028262
C	-2.228170	0.699102	-0.015247

C	-2.228171	-0.699140	0.012888
N	-0.997743	-1.360214	0.026282
C	-3.445326	1.393390	-0.029201
C	-4.658362	0.709694	-0.015333
C	-4.658362	-0.709744	0.012127
C	-3.445329	-1.393431	0.026513
N	-5.880608	1.371967	-0.027384
C	-7.114718	0.702345	-0.013139
C	-7.114719	-0.702371	0.011808
N	-5.880609	-1.372038	0.023347
C	-8.327355	1.387704	-0.008351
C	-9.549717	0.703868	0.006133
C	-9.549752	-0.703832	-0.002778
C	-8.327379	-1.387702	0.009447
N	-10.794730	-1.369825	0.033032
N	-10.794784	1.369880	-0.027336
H	6.192978	2.491205	0.001795
H	6.192991	-2.491197	-0.001174
H	1.435706	2.500048	-0.050129
H	1.435703	-2.500067	0.049029
H	-3.442293	2.480820	-0.050564
H	-3.442298	-2.480860	0.047937
H	-8.324263	2.476280	-0.005567
H	-8.324317	-2.476277	0.006719
H	-10.714332	-2.368941	-0.123327
H	-11.454079	-0.973948	-0.634043
H	-11.452642	0.974500	0.641510
H	-10.713980	2.369090	0.128220
H	-5.882711	-2.380059	0.046889
H	-5.882716	2.380019	-0.049536
N	8.608908	-1.481316	-0.183744
O	8.686848	-2.569854	0.382055
O	9.451249	-1.006892	-0.941475
N	8.608828	1.481336	0.185250
O	8.686938	2.569902	-0.380465
O	9.450885	1.006913	0.943295
H	-1.000270	-2.370554	0.046766
H	-1.000266	2.370521	-0.048770

Table S6: GRD of studied compounds **IB1-IB5**.

	HOMO	**LUMO**	**IP**	**EA**	**X**	**η**	**μ**	**ω**	**σ**
IB1	-0.16252	-0.09419	0.163	0.094	0.128	0.034	-0.128	0.241	14.635
IB2	-0.14277	-0.10739	0.143	0.107	0.125	0.018	-0.125	0.442	28.265
IB3	-0.14277	-0.10739	0.143	0.107	0.125	0.018	-0.125	0.442	28.265
IB4	-0.16468	-0.09589	0.165	0.096	0.130	0.034	-0.130	0.247	14.537
IB5	-0.15431	-0.09461	0.154	0.095	0.124	0.030	-0.124	0.259	16.750

Table S7: NBO analysis of **IB1-IB5** at B3LYP level of theory.

Compounds	Donor(i)	Type	Acceptor(j)	Type	E(2)[a]Kcal/mol]	E(j)-E(i)[b] (a.u)	F (i, j) [c] (a.u)
IB1	C 1 - C 2	π	N 41 O43	π*	14.59	0.18	0.05
	N41- O43	π	C 1 - C 2	π*	3.54	0.46	0.041
	C15 -H31	σ	C13 - C14	σ*	5.39	1.01	0.066
	N38 -O39	σ	C 1 - C 2	σ*	0.88	1.62	0.034
	O 42	LP (3)	N41-O43	π*	144.88	0.16	0.137
IB2	C28 - C29	π	C25 - C30	π*	20.19	0.27	0.067
	N47 - O49	π	C1 - C 2	π*	3.52	0.46	0.041
	C 1 - C 6	σ	C2 - N50	σ*	4.44	1.01	0.061
	N50 -O52	σ	C 2 - C3	σ*	0.87	1.61	0.034
	O51	LP (3)	N50 - O52	π*	144.8	0.16	0.137
IB3	C 2 - C 3	π	N 42 -O44	π*	27.18	0.16	0.065
	N39 -O41	π	C 1 - C 6	π*	1.79	0.49	0.029
	C52 -H54	σ	C 22 -C23	σ*	4.79	1.04	0.063
	N39 -O40	σ	C 1 - C 2	σ*	0.66	1.62	0.029
	O43	LP (3)	N42 - O44	π*	143.15	0.15	0.134
IB4	C 1 - C 6	π	N38 - O40	π*	27.18	0.16	0.065
	N41 -O43	π	C 2 - C 3	π*	1.78	0.49	0.029
	C 6 H28	σ	C 4 - C 5	σ*	5.04	1.04	0.065
	N 41 O42	σ	C 1 - C 2	σ*	0.66	1.61	0.029
	O39	LP (3)	N38 - O40	π*	143.18	0.15	0.134
IB5	C 1 - C 6	π	N47 -O49	π*	17.68	0.18	0.056
	N 50 -O52	π	C 2 - C 3	π*	3.26	0.48	0.038
	C14-H36	σ	C 8 - C 9	σ*	4.15	1.01	0.058
	N 47-O49	σ	C 1 - C 6	σ*	0.88	1.64	0.034
	O 48	LP (3)	N47 -O49	π*	142.17	0.16	0.137

[a]$E^{(2)}$ means energy of hyper conjugative interaction (stabilization energy in *kcal/mol*).
[b]Energy difference between donor and acceptor i and j NBO orbitals
[c]F(i;j) is the Fock matrix element between i and j NBO orbitals.

Table S8: Wavelength λ_{max} (nm), E (Transition Energy), f_o (oscillator strength) and MO contributions of all the studied compounds IB1-IB5 at CAM-B3LYP level of theory

Compounds	λ_{max} (nm)	E (eV)	f_o	MO contributions	Percentage
IB1	246	5.05	1.40	H-1 -> L+3	18%
IB2	441	2.81	1.34	H->L+1	87%
IB3	962	1.29	1.11	H->L	102%
IB4	962	1.29	1.11	H->L	102%
IB5	542	2.29	0.89	H->L	90%

Table S9*:* Calculated values for the dipole moment (μ), linear polarizability (a.u.), and total first hyper polarizability (a.u.) of complexes **IB1-IB5** at the CAM-B3LYP/6-31G(d) level determined.

Complex	**IB1**	**IB2**	**IB3**	**IB4**	**IB5**
μ	10.8747	15.0665	28.092	28.0872	19.1587
α_o	478.5047	555.4646	986.4844	986.4844	515.2016
β_x	2815209.882	698452209	3166227254	3161630020	3799755295
β_y	0.008555325	0.086411	33850023.89	33854297.28	0.069573505
β_z	6416.084605	13882.19	497386.2257	166285.886	4225.90871
β_{tot}	1679.76962	25065.63	56573.62163	56530.08583	61642.18946

Calculated values for the dipole moment (μ), linear polarizability (a.u.), and total first hyper polarizability (a.u.) of complexes **IB1-IB5** at the ωB97XD/6-31G(d) level determined.

Complex	**IB1**	**IB2**	**IB3**	**IB4**	**IB5**
μ	10.9625	14.5844	29.3244	29.3192	18.9061
α_0	474.8977	500.2591	1016.333002	1016.30905	504.6750
β_x	2279698	368230479	954859186.3	954859186.3	2462967457
β_y	0.007277	0.07274753	20116987.15	20116987.15	0.054111553
β_z	5051.246	4851.016563	420746.5816	420746.5816	2949.275882
β_{tot}	1511.539	19189.45885	31231.34515	31231.34515	49628.32263

Calculated values for the dipole moment (μ), linear polarizability (a.u.), and total first hyper polarizability (a.u.) of complexes **IB1-IB5** at the B3LYP/6-31G(d) level determined.

Complex	**IB1**	**IB2**	**IB3**	**IB4**	**IB5**
μ(Debye)	11.397	16.1146	26.1404	26.1366	21.837
α_0	541.9337	576.8560	921.1584	921.1584	627.3361
β_x	31562823	2142724365	7313799820	7313799820	21733903118
β_y	0.029132	0.31369308	3359568.851	3359568.851	0.136500692
β_z	34109.44	26027.3135	1745383.256	1745383.256	26688.25297
β_{tot}	5621.115	46289.8519	85550.59773	85550.59773	147424.3189

Table S10. β_{tot} of complexes **IB1-IB5** along x, y and z axis at CAM-B3LYP.

Complex	IB1	IB2	IB3	IB4	IB5
β_{xxx}	2549.357577	-24110.5	57288.2271	-57246.91595	61363.83273
β_{xxy}	0.0907213	-0.2246	-5817.875281	-5818.133196	0.2026424
β_{xyy}	-896.4162124	-1061.87	-1064.70034	1064.418472	324.135386
β_{yyy}	0.0030559	-0.029	4.9687241	4.8350506	0.0056962
β_{xxz}	-0.0112304	0.329213	552.0778717	-549.0038024	5.666549
β_{xyz}	80.1149185	117.1835	147.5679607	146.7896862	59.2833199
β_{yyz}	0.0075755	0.117018	16.1342735	-16.1108452	0.02642
β_{xzz}	24.9173551	107.0077	45.7122006	-45.876323	-45.8129416
β_{yzz}	-0.0012822	-0.04036	-5.1707796	-5.1464307	0.0554293
β_{zzz}	-0.0032224	0.30996	5.6103095	-5.5675484	0.0571208
β_{x}	2815210	628272068	3166227254	3161630020	3799755295
β_{y}	0.008555	0.086410894	33850023.89	33854297.28	0.069573505
β_{z}	6416.085	13882.19349	497386.2257	166285.886	4225.90871
β_{tot}	1679.770	25065.633	56573.622	56530.086	61642.189

β_{tot} of complexes **IB1-IB5** along x, y and z axis at M06-2X.

Complex	IB1	IB2	IB3	IB4	IB5
β_{xxx}	3028.787283	-25553.6274	43335.92359	-43303.993	70355.99928
β_{xxy}	0.0961126	-0.2386389	-5742.802337	-5742.6018	0.2168595
β_{xyy}	-862.1265208	-975.422050	-999.3738076	999.10276	362.769131
β_{yyy}	0.0032756	-0.0278918	5.1232618	5.0069311	0.0078708

β_{xxz}	-0.0134186	0.1674753	537.0840388	-534.21322	5.8665294
β_{xyz}	79.0898089	107.808706	146.4639902	145.71079	62.7246971
β_{yyz}	0.0076428	0.1004035	16.0700228	-16.048765	0.0276855
β_{xzz}	28.402976	100.8030305	50.2925038	-50.450178	-47.4927083
β_{yzz}	-0.0013308	-0.0381903	-5.2267256	-5.202104	0.0546799
β_{zzz}	-0.0034261	0.2757584	5.7830895	-5.7378434	0.0629359
β_{x}	4818304.813	698452209	1796644399	1.794E+09	4994429209
β_{y}	0.009615254	0.092854888	32980967.03	32979717	0.07807006
β_{z}	6252.533667	11718.48245	475177.3909	155425.39	4713.394015
β_{tot}	2196.487504	26428.46813	42779.67442	42744.708	70671.30905

β_{tot} of complexes **IB1-IB5** along x, y and z axis at ωB97XD.

Complex	**IB1**	**IB2**	**IB3**	**IB4**	**IB5**
β_{xxx}	2305.999755	-18481.7987	31943.77031	31943.77	49461.65528
β_{xxy}	0.0806251	-0.2079411	-4479.270776	-4480.14	0.1711023
β_{xyy}	-823.9340212	-743.594735	-1090.967318	1090.629	214.1617323
β_{yyy}	0.0057466	-0.0245699	-0.6220752	-0.72379	0.0104218
β_{xxz}	-0.0103853	0.4591381	494.1921387	-490.419	5.1672245
β_{xyz}	71.0859737	69.1263008	148.6803084	147.8653	49.0820108
β_{yyz}	0.00654	0.0555729	16.0287521	-15.9985	0.0111016
β_{xzz}	27.8009872	36.0610303	47.9928889	-48.1595	-47.5240942
β_{yzz}	-0.0010681	-0.0372065	-5.3035938	-5.27822	0.0510948
β_{zzz}	-0.0034701	0.0638006	5.7773672	-5.73343	0.0580007

β_x	2279697.515	368230479.7	954859186.3	1.09E+09	2462967458
β_y	0.007276704	0.07274753	20116987.15	20125487	0.054111553
β_z	5051.246	4851.016563	420746.5816	121303.7	2949.275882
β_{tot}	1511.538543	19189.45885	31231.34515	33291.72	49628.32263

β_{tot} of complexes **IB1-IB5** along x, y and z axis at B3LYP.

Complex	**IB1**	**IB2**	**IB3**	**IB4**	**IB5**
β_{xxx}	-4010.6497	-44815.16	84778.93	84778.93476	146249.47
β_{xxy}	0.1724297	-0.4999878	1000.359	1000.358995	0.2751346
β_{xyy}	-1621.5686	-1503.0728	639.6102	639.6101861	1218.742775
β_{yyy}	0.0006617	-0.0032502	844.7499	844.7499403	0.0102983
β_{xxz}	0.0176657	0.0029945	934.4359	934.4359401	5.3757752
β_{xyz}	184.673001	161.25535	396.1509	396.1508528	157.9222024
β_{yyz}	0.0117043	0.1006925	78.90926	78.9092625	0.1088709
β_{xzz}	14.1383489	28.662139	102.2117	102.2117183	-43.9843542
β_{yzz}	-0.0024091	-0.0568451	-12.19627	-12.1962665	0.0840271
β_{zzz}	-0.0032534	0.0714842	-9.457255	-9.4572551	0.0674195
β_x	31562823.4	2.143E+09	7.31E+09	7313799820	21733903118
β_y	0.02913245	0.3136931	3359569	3359568.851	0.136500692
β_z	34109.4406	26027.314	1745383	1745383.256	26688.25297
β_{tot}	5621.1149	46289.852	85550.6	85550.59773	147424.3189