

Supporting information for the article entitled

CHANGE IN THE FLUORESCENCE OF 1,1'-DIARYL-2,2'-BIIMIDAZOLES UPON THE ADDITION OF ACID

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Table of Contents:

1. Orbitals and energies of 1c (Figure S1)S2
2. Cartesian coordinates of the result of DFT and TDDFT calculation of 1b , 1b•H⁺ , 1c , and 1c•H⁺S2
3. Copies of ¹ H and ¹³ C NMR spectra of described compoundsS6

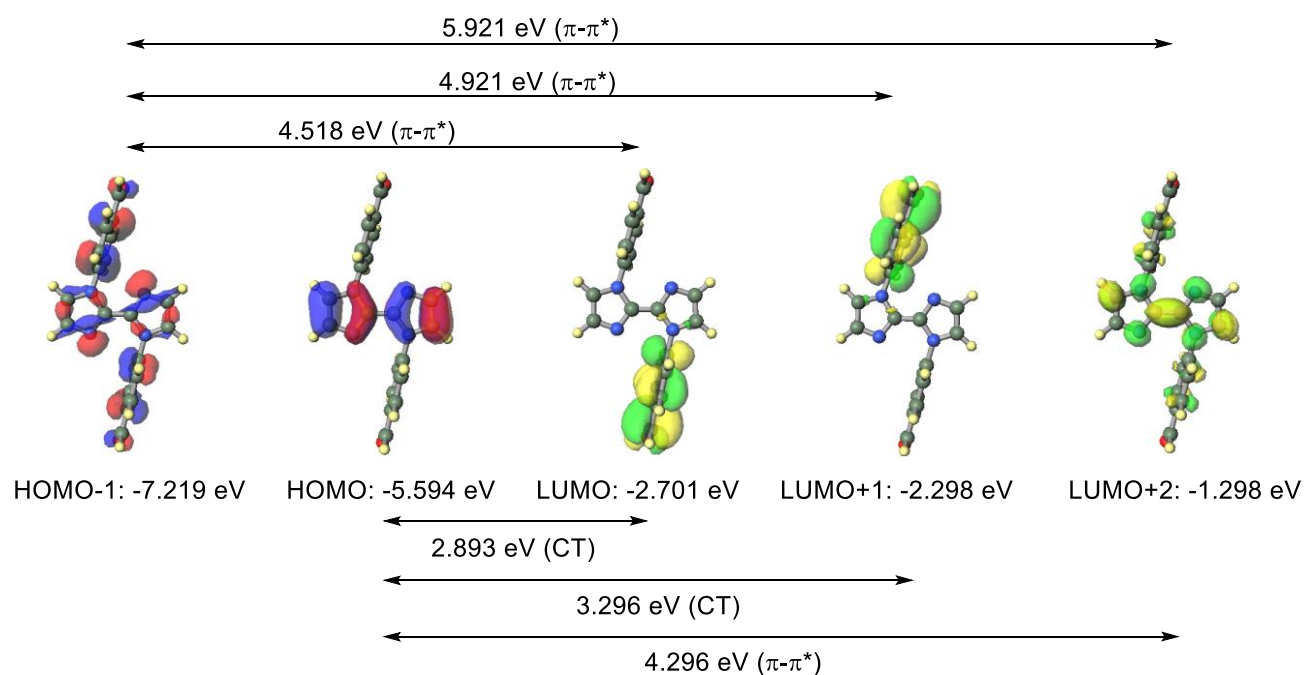
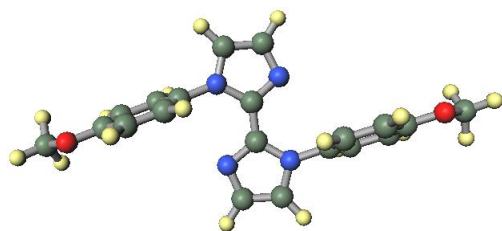


Figure S1. Orbitals and energies of **1c** calculated using the TDDFT/B3LYP/6-31+G** level of theory and the optimized structure obtained using the TDDFT method.

Energies and Cartesian coordinates of the results of TDDFT calculation.

Optimized structures were estimated by TDDFT/B3LYP/6-31+G** with nstate=1 using the Gaussian16 suite of programs.

1,1'-Bis(4-methoxyphenyl)-1*H*,1*H'*-2,2'-biimidazole (**1b**)



Total energy: -1142.43753313 A.U.

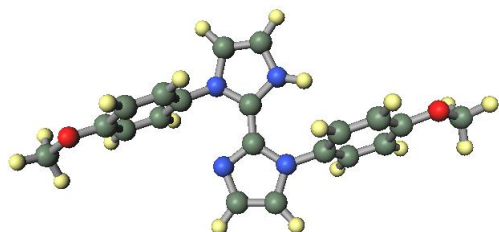
Number of imaginary frequency: 0

Cartesian coordinates:

C1	0.995260	-2.587810	-0.367202	N4	-1.347339	1.427664	-0.201798
C2	-0.412899	-2.689714	-0.519778	H1	1.770468	-3.337189	-0.327252
N1	-0.962198	-1.478949	-0.477044	C7	2.666202	-0.808856	-0.005646
C3	0.076705	-0.613350	-0.320348	C8	-2.661944	0.874150	0.018679
N2	1.292340	-1.290247	-0.243634	H2	-1.893716	3.482298	-0.209516
C4	-0.092834	0.791835	-0.302416	H3	-0.998764	-3.589411	-0.649000
N3	0.888054	1.703640	-0.439468	H4	0.851737	3.818332	-0.542842
C5	0.293928	2.898053	-0.440324	C9	3.024000	-0.487331	1.288524
C6	-1.099069	2.755424	-0.286265	C10	3.540847	-0.807651	-1.102143

C11	4.906783	-0.371152	-0.847198	H9	-3.263904	1.126977	-2.029066
C12	4.379083	-0.060933	1.538623	H10	-5.543348	0.258982	-1.657971
C13	5.275341	-0.019987	0.445499	H11	-2.319719	0.509128	2.117345
H5	3.185960	-0.970582	-2.112110	H12	-4.617656	-0.384528	2.499354
H6	5.610061	-0.342260	-1.668327	O2	-6.448756	-0.630264	0.771697
H7	2.310990	-0.566354	2.102228	C19	-7.431401	-0.750287	-0.254109
H8	4.713671	0.239379	2.522267	C20	7.523873	0.472488	-0.242597
O1	6.549673	0.400064	0.779078	H13	-7.686725	0.229104	-0.676352
C14	-3.031228	0.451615	1.299840	H14	-7.091623	-1.420508	-1.052743
C15	-3.565275	0.807838	-1.036372	H15	-8.310508	-1.177200	0.228634
C16	-4.853541	0.308839	-0.824809	H16	7.706825	-0.510399	-0.698494
C17	-4.307311	-0.048546	1.515966	H17	7.231886	1.179321	-1.031675
C18	-5.226442	-0.125058	0.454859	H18	8.440563	0.824342	0.236236

Protonated 1,1'-Bis(4-methoxyphenyl)-1*H*,1*H*'-2,2'-bimidazole (1*b*•H⁺)



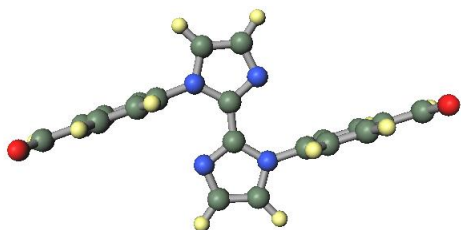
Total energy: -1142.83558044 A.U.

Number of imaginary frequency: 0

Cartesian coordinates:

C1	-1.030297	2.805235	-0.659732	H7	-2.364597	1.526844	1.793619
C2	0.296305	2.980220	-0.507791	H8	-4.649114	0.705851	2.430724
N1	0.900642	1.732342	-0.385907	O1	-6.277427	-0.405103	0.888043
C3	-0.076745	0.740467	-0.371712	C14	2.920810	-0.235818	1.282517
N2	-1.297321	1.408506	-0.672968	C15	3.495080	-1.122373	-0.894147
C4	0.038726	-0.647962	-0.254890	C16	4.809455	-0.674032	-0.737861
N3	-1.028664	-1.474060	-0.357043	C17	4.221151	0.231653	1.437791
C5	-0.532755	-2.741827	-0.237466	C18	5.177482	0.012860	0.429465
C6	0.828868	-2.725979	-0.056173	H9	3.205570	-1.641665	-1.802449
N4	1.208237	-1.384810	-0.055082	H10	5.527553	-0.858558	-1.527272
H1	-1.807588	3.526349	-0.853920	H11	2.194869	-0.101771	2.079332
C7	-2.565046	0.900666	-0.262770	H12	4.528447	0.745427	2.342532
C8	2.544538	-0.904989	0.105799	O2	6.418145	0.498778	0.681428
H2	1.551989	-3.510979	0.097769	C19	7.456309	0.284444	-0.276564
H3	0.875481	3.889880	-0.531700	C20	-7.250146	-1.057388	0.032808
H4	-1.176825	-3.608705	-0.281907	H13	7.634221	-0.785691	-0.432553
C9	-3.013722	1.058634	1.063701	H14	7.218750	0.766473	-1.232010
C10	-3.404863	0.291574	-1.238027	H15	8.347710	0.743159	0.150178
C11	-4.660164	-0.157815	-0.908071	H16	-7.543702	-0.382048	-0.773737
C12	-4.264512	0.610539	1.421500	H17	-6.830965	-1.985713	-0.360674
C13	-5.104043	-0.009287	0.436167	H18	-8.096562	-1.265766	0.682509
H5	-3.020600	0.181356	-2.243900	H19	1.832160	1.579754	-0.024785
H6	-5.290165	-0.625519	-1.653687				

4,4'-(1*H*,1'*H*-(2,2'-Biimidazol)-1,1'-diyl)dibenzaldehyde (1c)



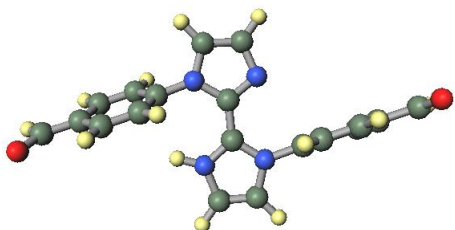
Total energy: -1140.04009868 A.U.

Number of imaginary frequency: 0

Cartesian coordinates:

C1	0.949466	-2.634988	-0.290400	C13	5.350906	-0.006956	0.031114
C2	-0.465716	-2.709962	-0.340422	H5	2.931480	-0.765225	-2.296878
N1	-0.984656	-1.484828	-0.307524	H6	5.279828	-0.027437	-2.141963
C3	0.077788	-0.638664	-0.243033	H7	2.680182	-0.867555	2.023507
N2	1.285257	-1.339006	-0.231296	H8	5.046978	-0.116833	2.171582
C4	-0.072871	0.768298	-0.202395	C14	6.717462	0.427611	0.131419
N3	0.920401	1.675510	-0.226120	C15	-3.207236	0.546973	1.163391
C5	0.341139	2.875609	-0.191468	C16	-3.405214	0.753100	-1.258484
C6	-1.061768	2.743088	-0.141008	C17	-4.712208	0.272807	-1.182816
N4	-1.326462	1.416198	-0.149005	C18	-4.510797	0.068192	1.229222
H1	1.706509	-3.404222	-0.287793	C19	-5.268202	-0.072923	0.055487
C7	2.665912	-0.862700	-0.143511	H9	-2.958848	1.013899	-2.212385
C8	-2.666267	0.876366	-0.082994	H10	-5.301980	0.165270	-2.089415
H2	-1.852156	3.477266	-0.092564	H11	-2.606949	0.656816	2.060715
H3	-1.078110	-3.599434	-0.396183	H12	-4.961126	-0.200051	2.179365
H4	0.913076	3.792777	-0.200480	C20	-6.662590	-0.584756	0.117194
C9	3.256199	-0.679330	1.120360	O1	-7.227731	-0.906091	1.144702
C10	3.397115	-0.624398	-1.324945	H13	-7.179381	-0.661009	-0.862409
C11	4.711858	-0.207168	-1.232081	O2	7.334805	0.627608	1.210733
C12	4.569875	-0.260277	1.208229	H14	7.233035	0.588959	-0.838116

Protonated 4,4'-(1*H*,1'*H*-(2,2'-Biimidazol)-1,1'-diyl)dibenzaldehyde (1c•H⁺)



Total energy: -1140.42289075 A.U.

Number of imaginary frequency: 0

Cartesian coordinates:

C1	-0.944089	2.770986	-0.192205	C7	-2.595447	0.910899	-0.071959
C2	0.434876	2.847469	-0.260345	C8	2.620356	-0.862026	-0.168835
N1	0.975853	1.601382	-0.272281	H2	1.776384	-3.456596	-0.479673
C3	-0.049970	0.758370	-0.215180	H3	1.050537	3.734713	-0.295637
N2	-1.262893	1.434343	-0.158835	H4	-0.986093	-3.734786	-0.625825
C4	0.100600	-0.673139	-0.293855	C9	-3.042420	0.303563	1.122502
N3	-0.889839	-1.586112	-0.420124	C10	-3.487882	1.088986	-1.155888
C5	-0.364145	-2.860549	-0.521237	C11	-4.790369	0.645836	-1.061308
C6	0.985557	-2.724524	-0.451861	C12	-4.340379	-0.156928	1.230023
N4	1.268035	-1.369373	-0.307688	C13	-5.257479	0.004792	0.134177
H1	-1.711336	3.528490	-0.139492	H5	-3.141069	1.574963	-2.062540

H6	-5.466458	0.786861	-1.898789	H10	5.338486	-0.123303	-2.046088
H7	-2.366064	0.217933	1.968289	H11	2.487701	-0.749492	1.982796
H8	-4.676717	-0.610170	2.155661	H12	4.853472	0.047359	2.220604
C14	-6.584817	-0.435135	0.222073	C20	6.636712	0.490314	0.248880
C15	3.118915	-0.608113	1.111419	O1	7.152467	0.749116	1.317066
C16	3.399441	-0.703254	-1.312743	H13	7.200232	0.599339	-0.700281
C17	4.714235	-0.259473	-1.167056	O2	-7.166483	-1.019529	1.195525
C18	4.429840	-0.164270	1.244164	H14	-7.281852	-0.290007	-0.625097
C19	5.230782	0.013355	0.105319	H15	-1.873204	-1.339177	-0.424505
H9	2.984115	-0.907447	-2.294172				

