Electronic Supplementary Material (ESI) for RSC Advances.

A theoretical exploration on the nonradiative deactivation of hydrogen-bond complexes: isoindole-pyridine and quinoline-pyrrole

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This supplementary file contains two Tables:

Table SM1: xyz coordinates revealed to the ground optimized geometry of monomer and dimers considered in the present study.

Table SM2: Vertical transition energies and configuration structures of the lowest-lying singlet electronic transitions of monomers and dimers, calculated at the CC2/aug-cc-pVDZ level of theory.

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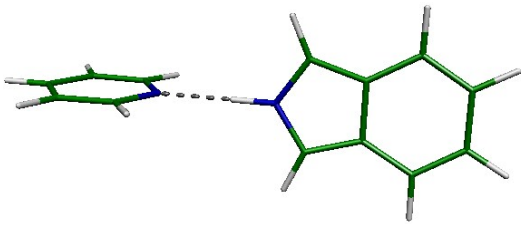
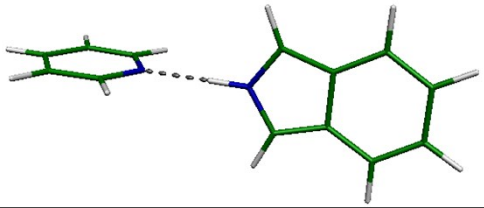
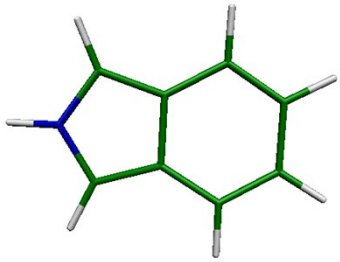
Table SM1:

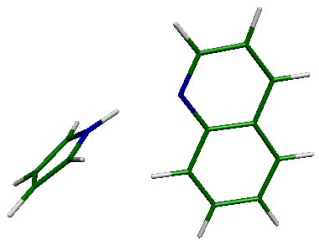
Isoindole - pyridine			
C	0.00000	1.13958	1.16727
N	0.00000	0.00000	0.40182
C	0.00000	-1.13958	1.16727
C	0.00000	-0.72841	2.52273
C	0.00000	0.72841	2.52273
C	0.00000	1.44039	3.75435
C	0.00000	0.71484	4.94603
C	0.00000	-0.71484	4.94603
C	0.00000	-1.44039	3.75435
H	0.00000	2.12719	0.71028
H	0.00000	0.00000	-0.63322
H	0.00000	-2.12719	0.71028
H	0.00000	-2.53542	3.76938
H	0.00000	-1.24855	5.90170
H	0.00000	1.24855	5.90170
H	0.00000	2.53542	3.76938
N	0.00000	0.00000	-2.50312
C	1.15814	0.00000	-3.20167
C	1.20741	0.00000	-4.60575
C	0.00000	0.00000	-5.32439
C	-1.20741	0.00000	-4.60575
C	-1.15814	0.00000	-3.20167
H	2.07718	0.00000	-2.60707
H	2.17255	0.00000	-5.11883
H	0.00000	0.00000	-6.41792
H	-2.17255	0.00000	-5.11883
H	-2.07718	0.00000	-2.60707
			

Isoindole - pyridine			
C	1.10507	1.14126	-0.00020
N	0.33825	0.00265	-0.00019
C	1.10226	-1.13786	-0.00023
C	2.45824	-0.72837	-0.00015
C	2.46004	0.72842	-0.00014
C	3.69251	1.43889	0.00002
C	4.88326	0.71183	0.00020
C	4.88148	-0.71783	0.00019
C	3.68894	-1.44193	0.00002
H	0.64959	2.12957	-0.00027
H	-0.69682	0.00387	-0.00013
H	0.64420	-2.12498	-0.00034
H	3.70228	-2.53699	0.00001
H	5.83661	-1.25254	0.00032
H	5.83968	1.24423	0.00034
H	3.70867	2.53391	0.00001
N	-2.56653	0.00264	-0.00004
C	-3.26512	0.00124	-1.15812
C	-4.66920	-0.00141	-1.20731
C	-5.38778	-0.00274	0.00011
C	-4.66907	-0.00139	1.20746
C	-3.26500	0.00126	1.15813
H	-2.67058	0.00239	-2.07721
H	-5.18229	-0.00239	-2.17246
H	-6.48131	-0.00477	0.00017
H	-5.18206	-0.00236	2.17266
H	-2.67036	0.00242	2.07715

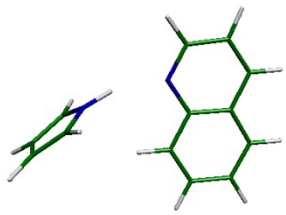


Isoindole			
C	-1.44148	0.00000	0.91975
C	-0.71514	0.00000	2.10942
C	0.71514	0.00000	2.10942
C	1.44148	0.00000	0.91975
C	-0.72767	0.00000	-0.31170
C	0.72767	0.00000	-0.31170
C	-1.14508	0.00000	-1.66353
N	0.00000	0.00000	-2.42470
C	1.14508	0.00000	-1.66353
H	-2.53614	0.00000	0.93406
H	-1.24808	0.00000	3.06525
H	1.24808	0.00000	3.06525
H	2.53614	0.00000	0.93406
H	-2.13166	0.00000	-2.12115
H	2.13166	0.00000	-2.12115
H	0.00000	0.00000	-3.43953
			

Quinoline - pyrrole			
N	0.31045	1.34459	0.00000
C	0.89450	2.54557	0.00000
C	1.12196	0.23033	0.00000
C	2.30294	2.74450	0.00000
C	3.13804	1.63488	0.00000
C	2.55990	0.33300	0.00000
H	2.70706	3.76034	0.00000
H	0.21983	3.40880	0.00000
H	4.22771	1.74425	0.00000
C	0.51132	-1.05960	0.00000
C	1.30585	-2.20262	0.00000
C	2.72662	-2.10247	0.00000
C	3.34725	-0.85734	0.00000
H	4.43906	-0.77418	0.00000
H	3.33329	-3.01298	0.00000
H	0.83159	-3.18818	0.00000
H	-0.57994	-1.12917	0.00000
C	-3.06763	-0.10458	1.12827
C	-4.09988	-0.95640	0.71455
C	-4.09988	-0.95640	-0.71455
C	-3.06763	-0.10458	-1.12827
N	-2.46931	0.41156	0.00000
H	-2.72564	0.17439	2.12318
H	-4.77469	-1.50379	1.37167
H	-4.77469	-1.50379	-1.37167
H	-2.72564	0.17439	-2.12318
H	-1.59245	0.94948	0.00000



Quinoline - pyrrole			
N	0.24420	1.31868	0.00110
C	0.82893	2.51932	0.00104
C	1.05514	0.20398	0.00026
C	2.23748	2.71748	0.00011
C	3.07198	1.60741	-0.00079
C	2.49312	0.30585	-0.00080
H	2.64213	3.73311	0.00013
H	0.15475	3.38294	0.00182
H	4.16170	1.71618	-0.00142
C	0.44377	-1.08560	0.00036
C	1.23766	-2.22907	-0.00059
C	2.65849	-2.12974	-0.00166
C	3.27980	-0.88494	-0.00172
H	4.37166	-0.80237	-0.00244
H	3.26464	-3.04059	-0.00248
H	0.76281	-3.21434	-0.00050
H	-0.64752	-1.15465	0.00119
C	-3.13448	-0.13009	1.12907
C	-4.16623	-0.98225	0.71475
C	-4.16551	-0.98214	-0.71433
C	-3.13346	-0.12977	-1.12747
N	-2.53594	0.38654	0.00114
H	-2.79304	0.14879	2.12419
H	-4.84118	-1.52984	1.37157
H	-4.83965	-1.52982	-1.37191
H	-2.79119	0.14952	-2.12219
H	-1.65906	0.92440	0.00156



	Quinoline	aug-cc-pVDZ	
C	-0.77722	-1.75064	0.00000
C	0.42214	-2.45673	0.00000
C	1.66747	-1.76442	0.00000
C	1.70269	-0.37343	0.00000
C	-0.77364	-0.32517	0.00000
C	0.48650	0.37405	0.00000
N	-1.98688	0.32435	0.00000
C	-1.96359	1.65908	0.00000
C	-0.77313	2.44244	0.00000
C	0.45707	1.79851	0.00000
H	-1.74573	-2.25884	0.00000
H	0.41092	-3.55069	0.00000
H	2.60242	-2.33283	0.00000
H	2.65803	0.16215	0.00000
H	-2.94051	2.15554	0.00000
H	-0.84241	3.53393	0.00000
H	1.39588	2.36270	0.00000

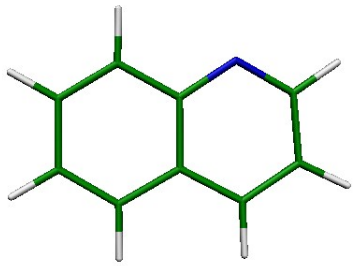


Table SM2

state	Energy (eV)	oscillator strengths	configuration
Isoindole - pyridine			
S_1 (^{1}B2)1	4.04	0.0668	(π_1/ π_1*)72.9% (π_1/ π_2*)16.6%
S_2 (^{1}A2)1	4.17	0.0000	(π_1/ σ_1*)47.0% (π_1/ σ_2*)18.4%
S_3(^{1}B1)1	4.29	0.0000	(π_1/π*)72.1% (π_1/ π_3*)12.4%
S_4(^{1}B1)2	4.56	0.0030	(π_1/σ_4*)85.5%
S_5(^{1}A2)2	4.59	0.0000	(π_1/σ_5*)63.4% (π_1/σ_2*)14.8%
S_6(^{1}A1)1	4.69	0.0005	(π_1/σ_6*)38.2% (π_2/ π_2*)25.7%
S_7(^{1}B2)2	4.71	0.0233	(π_1/π_4*)43.0% (π_1/σ_7*)29.1% (π_1/π_2*)14.8%
S_8(^{1}A1)2	4.80	0.0168	(π_1/σ_6*)54.3% (π_2/ π_2*)18.4%

state	Energy (eV)	oscillator strengths	configuration
Isoindole			
S1 (^{1}B1) 1	4.15	0.0841	(π_1/ π_1*)61.0% (π_1/ π_2*)29.7%
S2 (^{1}A2) 1	4.21	0.0000	(π_1/ σ_1*)83.9%
S3 (^{1}A2) 2	4.74	0.0000	(π_1/ σ_2*)74.0%
S4 (^{1}A1) 1	4.76	0.0020	(π_2/ π_1*)31.1% (π_1/ π_3*)22.8% (π_2/ π_2*)20.1%
S5 (^{1}B2)1	4.85	0.0038	(π_1/ σ_3*)88.0%
S6 (^{1}B1) 2	5.16	0.0413	(π_1/ π_2*)60.5% (π_1/ π_1*)25.6%
S7 (^{1}B2) 2	5.41	0.0190	(π_1/ σ_4*)84.8%
S8 (^{1}A1)2	6.01	0.7500	(π_1/ π_4*)47.7% (π_2/ π_1*)23.5%

state	Energy (eV)	oscillator strengths	configuration
pyridine			
S_1 (^{1}B2)1	4.98	0.0046	(n/ π_1*)77.5%
S_2 (^{1}B1)1	5.21	0.0310	(n/σ_1*)86.0%
S_3(^{1}A2)1	5.24	0.0000	(nσ_1/ π_2*)85.2%
S_4(^{1}A1)2	6.60	0.0144	(π_1/π_2*)53.2% (π_2/ π_1*)26.3%
S_5(^{1}A1)1	6.15	0.0058	(nσ_1/σ_2*)74.6%
S_6(^{1}A2)2	6.61	0.0000	(π_1/σ_2*)80.3%
S_7(^{1}B1)2	6.70	0.0256	(nσ_1/σ_1*)86.0%
S_8(^{1}B2)2	7.16	0.0454	(π_1/σ_1*)65.9% (π_2/σ_2*)19.8%

state	Energy (eV)	oscillator strengths	configuration
Quinoline - pyrrole			
S1 (^{1}A'1)	4.35	0.0260	(π_1/π_1^*)54.3% (π_2/π_2^*)22.3%
S2 (^{1}A'2)	4.49	0.0268	(π_3/π_1^*)71.3% (π_2/π_1^*)16.6%
S3(^{1}A"1)	4.60	0.0010	(n_1/π_1^*)76.8%
S4(^{1}A'3)	4.63	0.0431	(π_2/π_1^*)66.8% (π_3/π_1^*)17.2%
S5(^{1}A"2)	5.08	0.0000	(π_3/σ_1^*)41.7% (π_3/σ_2^*)16.1%
S6(^{1}A"3)	5.29	0.0000	(π_4/π_1^*)81.0%
S7(^{1}A'4)	5.46	0.0158	(π_3/σ_3^*)59.4% (π_3/π_2^*)12.8%
S8(^{1}A"4)	5.56	0.0113	(π_3/σ_4^*)40.9% (π_3/σ_5^*)18.5%
S9(^{1}A'5)	5.59	0.0674	(π_3/π_2^*)52.2% (π_3/π_3^*)15.9% (π_3/σ_3^*)14.9%
S10(^{1}A"5)	5.76	0.0399	(π_3/σ_6^*)24.1% (π_3/σ_7^*)15.2% (π_3/σ_8^*)12.7%

state	Energy (eV)	oscillator strengths	configuration
Quinoline			
S1 (^{1}A'1)	4.37	0.0247	(π_1/π_1^*)57.4% (π_2/π_2^*)28.5%
S2 (^{1}A"1)	4.44	0.0018	(σ_1/π_1^*)89.7%
S3 (^{1}A'2)	4.72	0.0588	(π_2/π_1^*)87.8%
S4 (^{1}A"2)	5.37	0.0000	(σ_1/π_2^*)77.3%
S5 (^{1}A"3)	5.81	0.0000	(π_2/σ_1^*)73.5%
S6 (^{1}A'3)	5.82	0.6325	(π_2/π_2^*)28.3% (π_1/π_1^*)20.3%
S7 (^{1}A'4)	6.07	0.0010	(π_2/π_3^*)19.4% (π_2/π_4^*)18.8%
S8 (^{1}A'5)	6.10	0.0142	(σ_1/σ_1^*)59.1% (σ_2/σ_1^*)5.7%
S9 (^{1}A"4)	6.21	0.0021	(π_2/σ_1^*)63.7%
S10 (^{1}A"5)	6.31	0.0196	(π_1/σ_1^*)60.5% (π_2/σ_2^*)14.0%

state	Energy (eV)	oscillator strengths	configuration
Pyrrole			
S_1 (^{1}A2)1	5.02	0.0000	(π_1/σ_1*)84.2%
S_2 (^{1}B2)1	5.74	0.0145	(π_2/σ_1*)51.6% (π_1/σ_2*)33.1%
S_3(^{1}A2)2	5.78	0.0000	(π_1/σ_3*)81.6%
S_4(^{1}B2)2	5.82	0.0244	(π_1/σ_2*)56.3% (π_2/σ_1*)28.9%
S_5(^{1}B1)1	6.22	0.1934	(π_1/π_1*)81.7%
S_6(^{1}A1)1	6.33	0.0002	(π_2/π_2*)26.6% (π_1/π_3*)19.1% (π_2/π_1*)16.6%
S_7(^{1}B1)2	6.97	-0.0002	(π_1/π_4*)62.2% (π_1/π_2*)17.6%
S_8(^{1}A1)2	7.40	0.0000	(π_2/π_1*)72.4%