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Supporting Information

for

On the aromaticity and photophysics of 1-arylbenzo[*a*]imidazo[5,1,2-*cd*]indolizines as bicolor fluorescent molecules for barium tagging in the study of double-beta decay of ^{136}Xe

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Energies, calculated absorption and emission wavelengths

Table S1. Total energies (E), zero-point vibrational energies (ZPVE) and thermal corrections for Gibbs energies (TCGE) calculated for compounds **1-15**.[a]

Compound	E (a.u)	ZPVE (a. u.)	TCGE (a.u.)
1 (S_0)	-609.9060587	0.176762	0.141739
1 (S_1)	-609.8996567		
2	-611.0968762	0.199189	0.163241
3	-611.0866456	0.199260	0.163686
4	-612.3055856	0.222345	0.186106
5	-611.090726	0.199031	0.163115
6	-611.0904228	0.199084	0.163161
7	-612.3213374	0.222925	0.186554
8	-379.9757466	0.117380	0.087238
9	-381.1757085	0.140157	0.109153
10	-381.169404	0.139909	0.109333
11	-382.3796935	0.163231	0.131183
12	-233.5049978	0.121901	0.094336
13	-234.7365585	0.145754	0.117773
14	-232.330161	0.100194	0.075076

[a] Values computed at the B3LYP-D3BJ/6.311++G(d,p)%DefTZVPP(Ba) level.

Table S2. Total energies (E), zero-point vibrational energies (ZPVE) and thermal corrections for Gibbs energies (TCGE) calculated for compounds **15a-d, 16a-d, 17a-d**, **19** and **·Ba(ClO$_4$)$_2$**.[a]

Compound	E (a.u)	ZPVE (a. u.)	TCGE (a.u.)
15a	-640.6658645	0.248434	0.208982
15b	-794.6007494	0.309634	0.264037
15c	-948.533772	0.371660	0.320205
15d	-1102.443735	0.433721	0.378415
16a	-615.5355929	0.245247	0.207758
16b	-769.4247609	0.306950	0.262335
16c	-923.3163967	0.368607	0.320017
16d	-1077.208118	0.429505	0.373651
17a	-873.050199	0.349293	0.295361
17b	-1026.9762566	0.410893	0.353034

17c	-1180.8999491	0.472725	0.411279
17d	-1334.7818278	0.534993	0.470533
19 (S_0)	-1971.2608099	0.661267	0.584192
19 (S_1)	-1971.1557349		
19·Ba(ClO$_4$)$_2$ (S_0)	-3518.7683558	0.686340	0.591384
19·Ba(ClO$_4$)$_2$ (S_1)	-3518.6550761		

[a] Values computed at the B3LYP-D3BJ/6.311++G(d,p)%DefTZVPP(Ba) level.

Table S3. Total energies calculated for compounds **19** and **19·Ba(ClO$_4$)$_2$** at S_0 and S_1 states with different functionals.[a]

Functional	S_0		S_1	
	19	**Ba(ClO$_4$)$_2$**	**19**	**Ba(ClO$_4$)$_2$**
BHandH	-1957.14463621	-3498.81290051	-1956.9999427	-3498.6296551
BHandHLYP	-1969.94831606	-3516.90526237	-1969.8128635	-3516.7529069
B3LYP	-1971.2608099	-3518.76835587	-1971.1557349	-3518.6550761
CAM-B3LYP	-1970.15492224	-3517.34937615	-1970.0276974	-3517.2112303
M06	-1969.78065911	-3516.87448682	-1969.6462543	-3516.7563090
M06-L	-1970.84848954	-3518.23281981	-1969.6714904	-3518.1215546
M06-2X	-1970.33142837	-3517.42930374	-1970.2099690	-3517.2858321
PBE	-1968.84831481	-3515.32524575	-1968.7408013	-3515.1955066
wB97XD	-1970.47373002	-3517.74326079	-1970.3499872	-3517.6037878

[a] Values computed with the 6.311++G(d,p)&DefTZVPP(Ba) basis set.