Electronic Supplementary Information

Highly emissive 4-carbazole-appended salen–indium complex: the effect of strong donor–acceptor interaction

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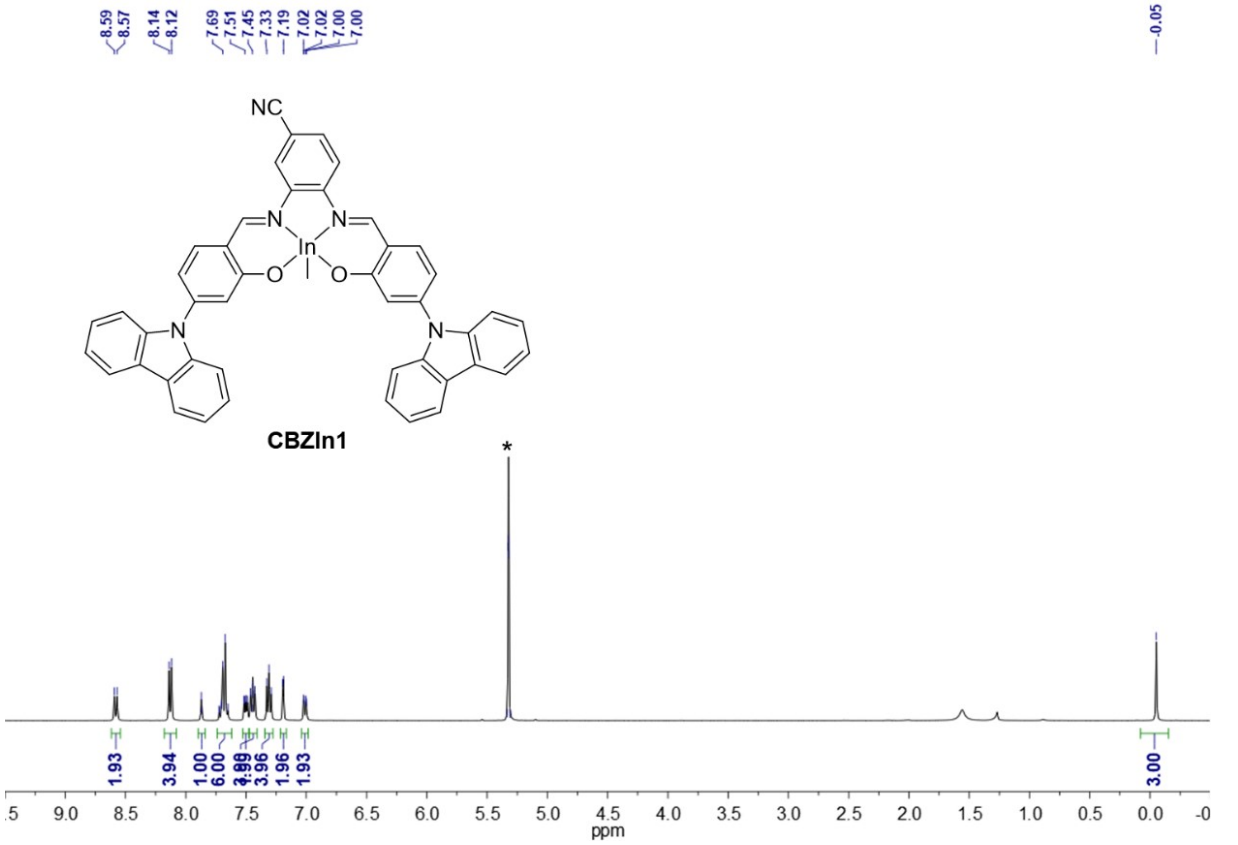
Contents

^{1}H and ^{13}C NMR Spectra



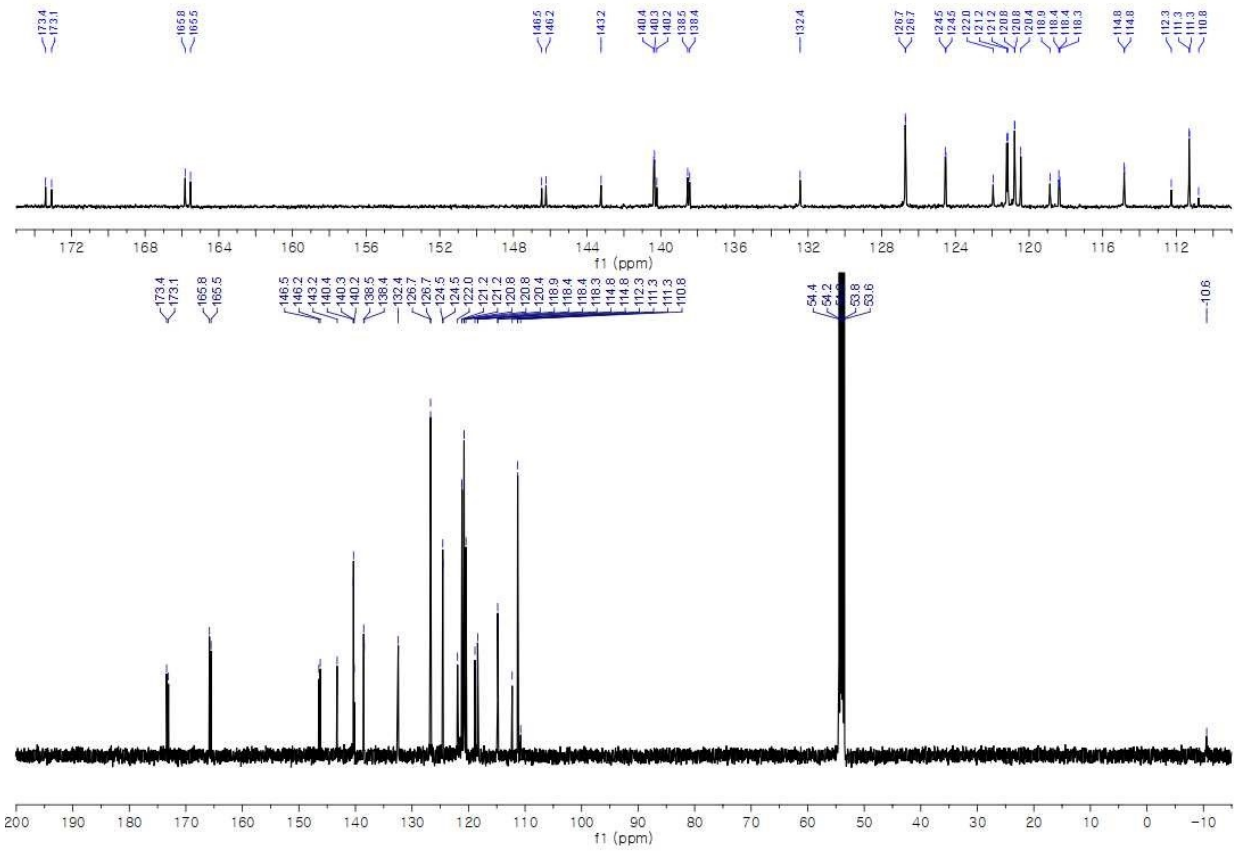


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **CBZIn1** (∗ from residual CH_2Cl_2 in CD_2Cl_2).

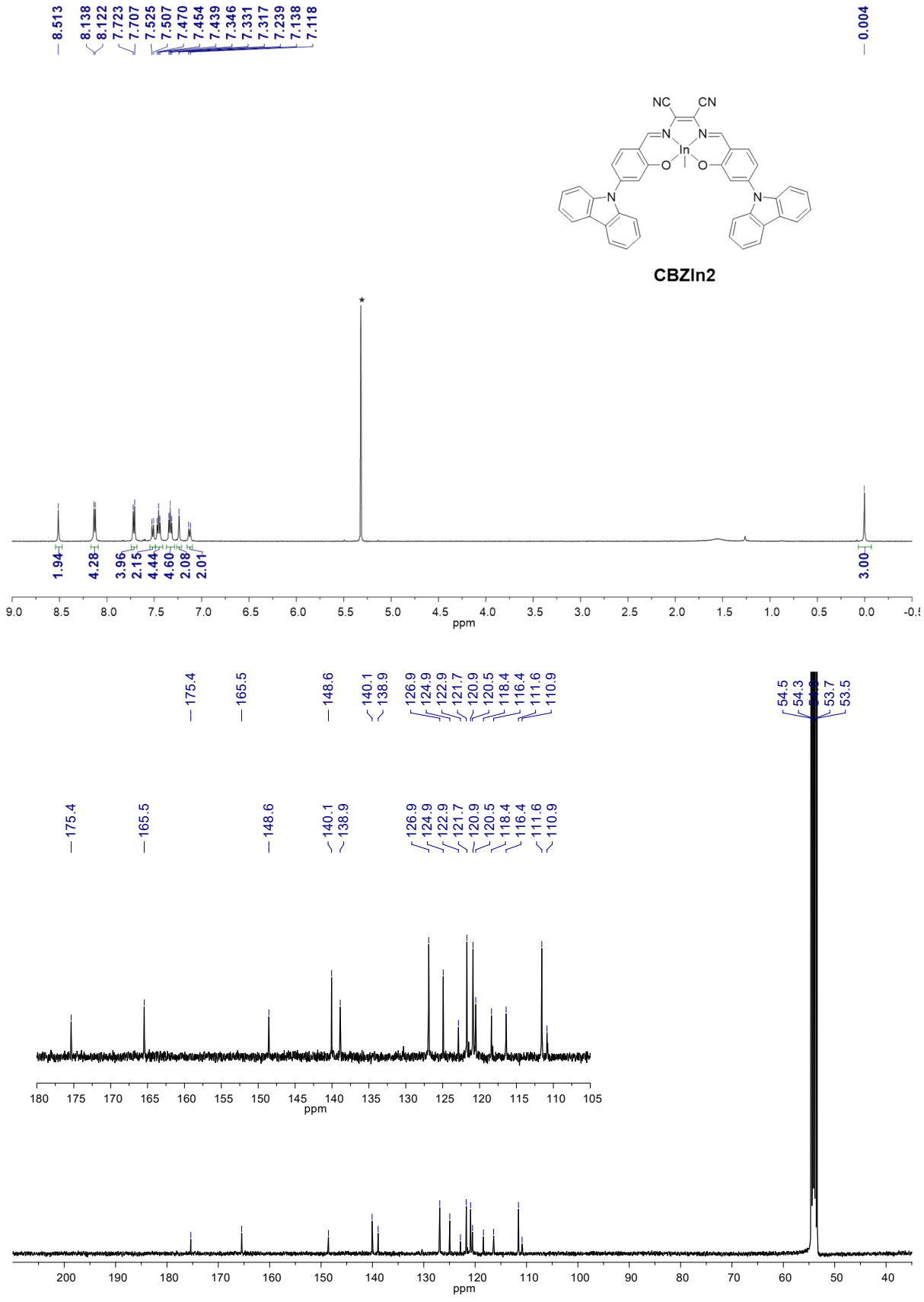


Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **CBZIn2** (∗ from residual CH_2Cl_2 in CD_2Cl_2).

Table S1 Crystallographic data and parameters for **CBZIn1**

Compound	$C_{45}H_{30}InN_4O_2\cdot(C_7H_8)\cdot0.5(C_2N_2)$
Formula	$C_{53}H_{38}InN_5O_2$
Formula weight	891.70
Crystal system	Triclinic
Space group	$P\bar{1}$
a (Å)	11.7454(4)
b (Å)	12.2305(4)
c (Å)	15.3406(5)
α (°)	78.228(2)
β (°)	78.289(2)
γ (°)	69.581(2)
V (Å^3)	2000.83(12)
Z	2
ρ_{calc}(g cm^{-3})	1.480
μ (mm^{-1})	0.642
F(000)	912
T (K)	100
Scan mode	*multi-scan*
hkl range	$-14 < h < 14$, $-14 < k < 14$, $-18 < l < 18$
Measurement reflns	27090
Unique reflns [R_{int}]	7557[0.0898]
Reflns used for refinement	7557
Refined parameters	570
R_1[a] (I > 2σ(I))	0.0559
wR_2[b] all data	0.0984
GOF on F^2	0.981
ρ_{fin} (max/min) (e Å^{-3})	0.519, −0.936

[a] $R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for **CBZIn1**

Compound	**CBZIn1**
	lengths
In–O1	2.092(3)
In–O2	2.071(3)
In–N1	2.251(3)
In–N2	2.288(4)
In–C45	2.126(5)
	Angles
O1–In–O2	91.98(11)
O1–In–N1	82.75(12)
O1–In–N2	140.68(12)
O2–In–N1	125.89(13)
O2–In–N2	82.21(12)
O1–In–C45	111.95(16)
O2–In–C45	111.49(15)
N1–In–N2	70.10(12)
C45–In–N1	120.39(15)
C45–In–N2	106.28(2)

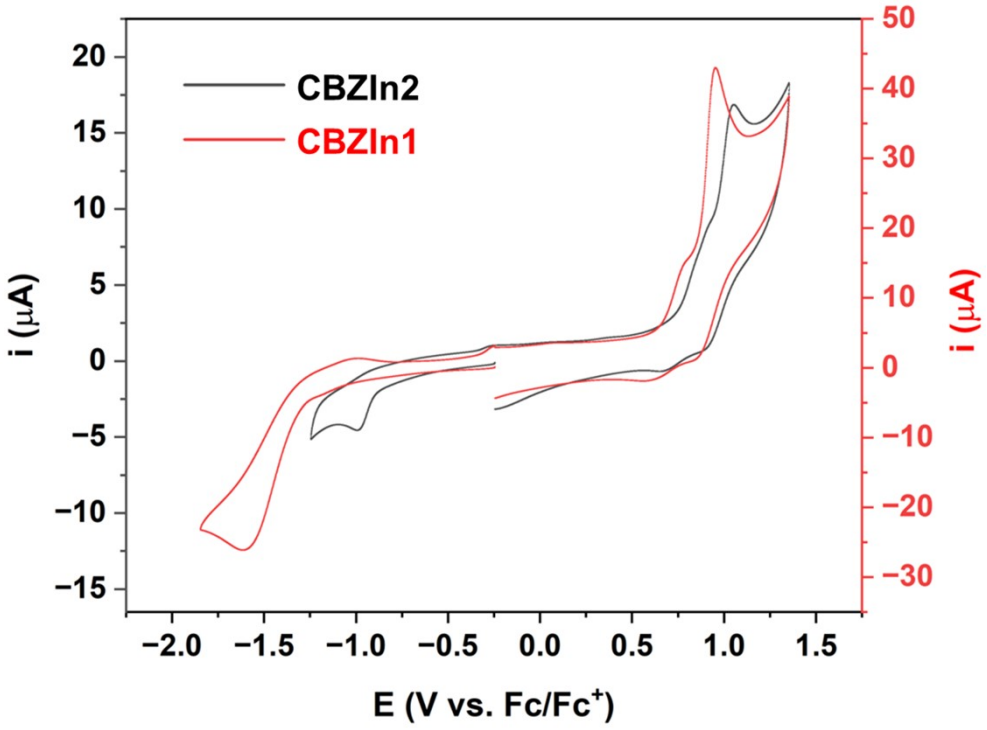


Fig. S3 Cyclic voltammograms (CV) for **CBZIn1** and **CBZIn2** (1 mM in MeCN, scan rate = 100 mV/s).

Table S3 Electrochemical data of **CBZIn1** and **CBZIn2**

Compound	E_{ox} (V)[a]	E_{red} (V)[a]	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)[b]
CBZIn1	0.79	−1.33	−5.59	−3.47	2.12
CBZIn2	0.80	−0.87	−5.60	−3.93	1.67

[a]The oxidation and reduction onset potentials in MeCN (1 mM, scan rate 100 mVs^{-1}) with reference to a ferrocene/ferrocenium (Fc/Fc^+) redox couple. [b]Electrochemical band gap.

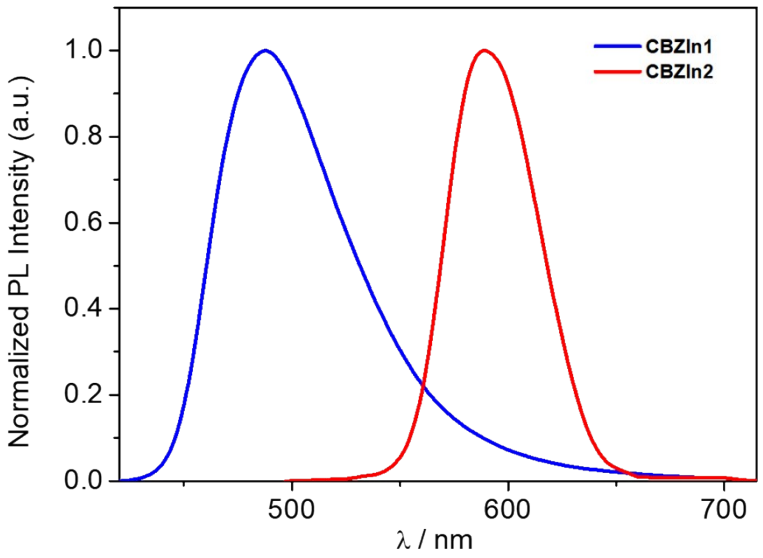


Fig. S4 PL spectra of **CBZIn1** and **CBZIn2** in THF (20 μM) at 298 K.

Table S4 UV–vis absorption and PL data of **CBZIn2** in various organic solvents (20 μM) at 298 K

Solvent	λ_{abs} /nm (ε, × 10^{-3} M^{-1} cm^{-1})	λ_{ex} /nm	λ_{em} /nm	Φ_{PL} /%
THF	382 (54.46), 431 (34.29), 561 (29.14), 590 (28.01)	384	589	53.9
DMF	381 (143.36), 431 (92.59), 551 (58.73), 577 (54.70)	398	550	18.5
DMSO	383 (44.62), 433 (32.08), 559 (31.44), 578 (29.99)	394	531	6.8

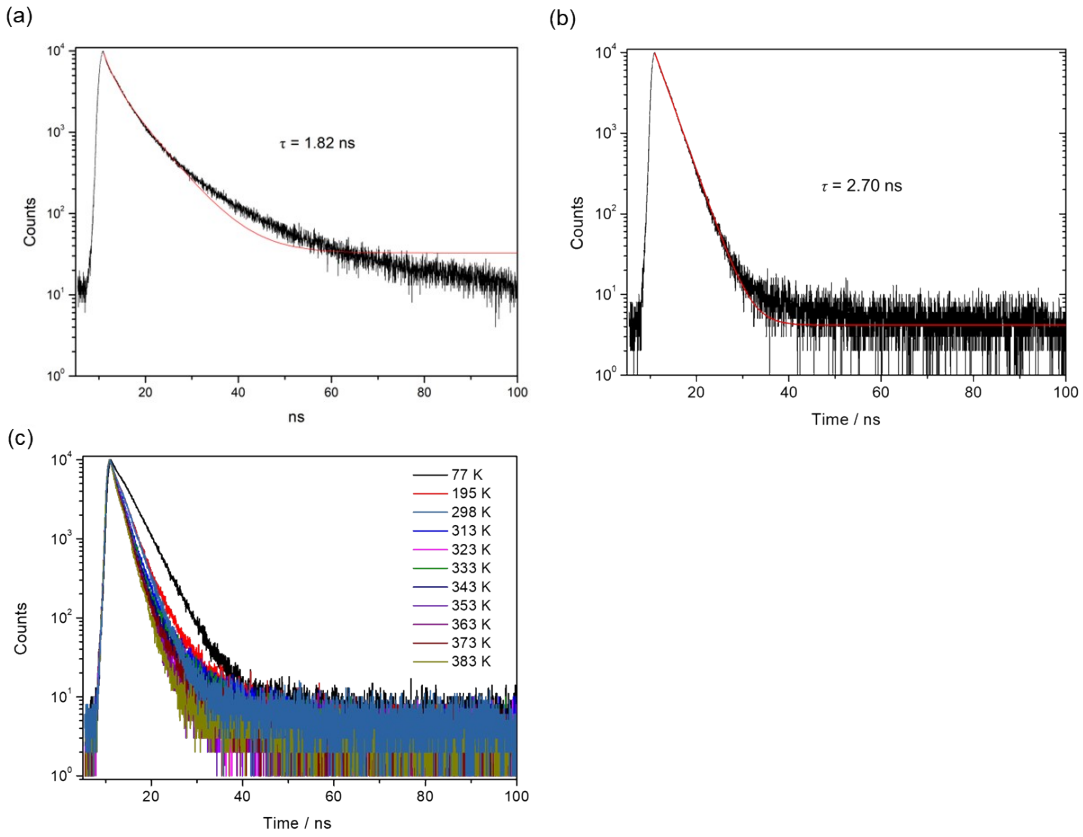


Fig. S5 Emission decay curves of (a) **CBZIn1** and (b) **CBZIn2** in toluene (20 μM) solutions at 298 K (The red-line corresponds to the single-exponential fitting curves). (c) Emission decay curves of **CBZIn2** in toluene at variable temperature.

Table S5 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **CBZIn1** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0)- and first singlet excited state (S_1)-optimized geometries in toluene

state	λ_{calc} (nm)	f_{calc}	major contribution
		S_0	
1	490.51	0.5086	HOMO → LUMO (75.7%)
2	464.99	0.2153	HOMO−1 → LUMO (82.8%)
3	445.41	0.3551	HOMO → LUMO+1 (82.8%)
4	428.81	0.0132	HOMO−4 → LUMO (62.5%)
5	423.66	0.0482	HOMO−1 → LUMO+1 (61.3%)
		S_1	
1	623.27	0.1495	HOMO → LUMO (90.3%)
2	575.08	0.2750	HOMO−1 → LUMO (92.5%)
3	542.65	0.0046	HOMO−2 → LUMO (96.6%)
4	498.57	0.0010	HOMO−3 → LUMO (99.5%)
5	480.10	0.0001	HOMO−4 → LUMO (99.8%)

Table S6 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **CBZIn1** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in toluene

	E (eV)	benzonitrile	In–Me	4-CBZ	Phenoxy
			S_0		
LUMO+3	−0.84	0.1	0.0	99.1	0.8
LUMO+2	−1.14	71.6	0.2	3.4	24.8
LUMO+1	−2.28	35.6	0.3	3.9	60.3
LUMO	−2.51	40.2	0.2	3.5	56.1
HOMO	−5.48	7.9	0.6	75.6	15.9
HOMO−1	−5.54	3.0	0.0	85.1	11.8
HOMO−2	−5.88	0.0	0.0	99.8	0.2
HOMO−3	−5.90	0.2	0.1	98.6	1.0
			S_1		
LUMO+3	−0.86	0.0	0.0	99.5	0.5
LUMO+2	−1.24	76.5	0.2	1.9	21.4
LUMO+1	−2.10	37.5	0.4	3.4	58.8
LUMO	−3.02	35.3	0.4	3.0	61.4
HOMO	−5.34	5.9	0.4	77.0	16.7
HOMO−1	−5.59	4.9	0.6	81.3	13.1
HOMO−2	−5.73	8.0	3.2	19.9	69.0
HOMO−3	−5.86	0.0	0.0	99.9	0.2

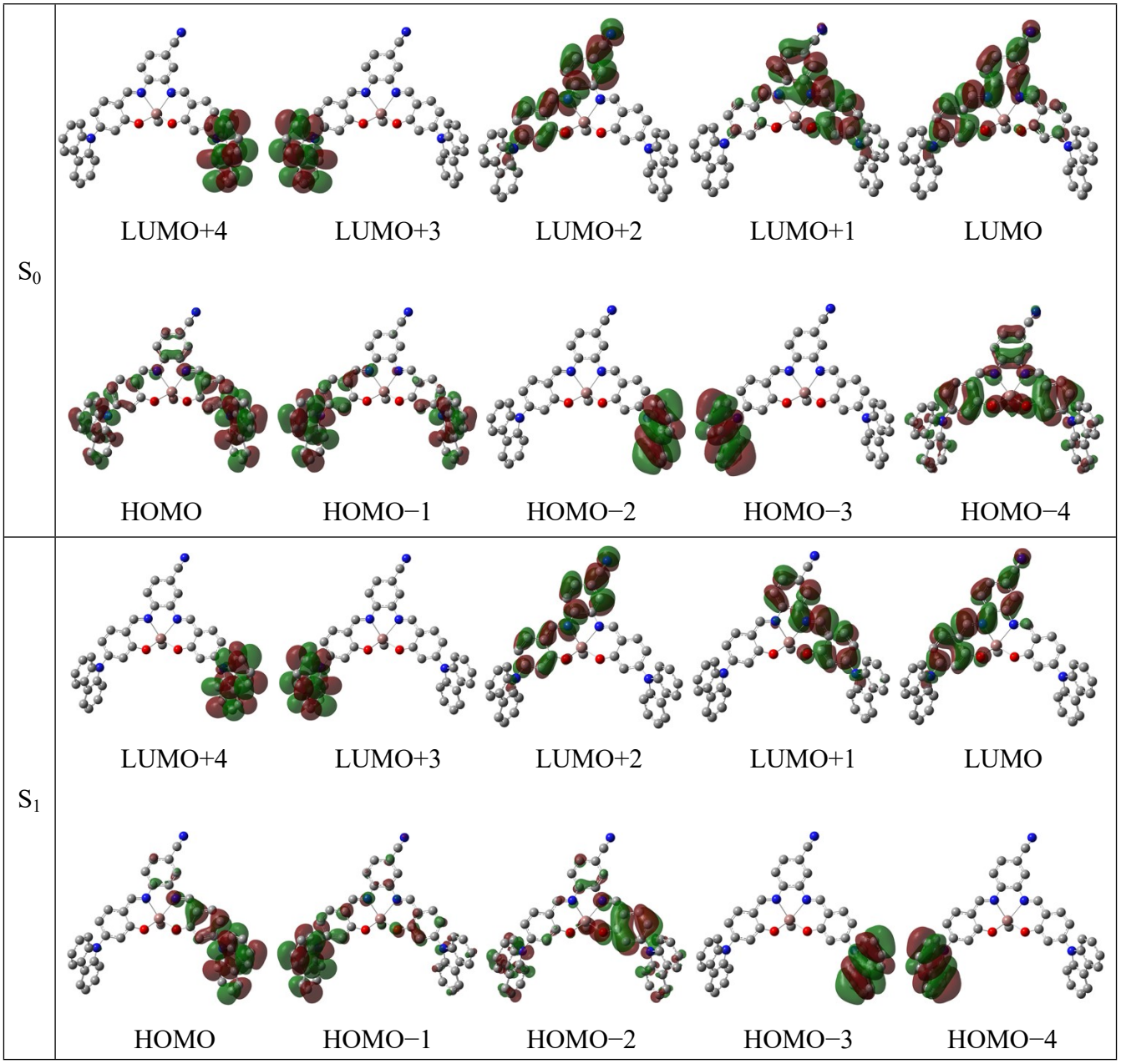


Fig. S6 The selected frontier orbitals of **CBZIn1** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0)- and first singlet excited state (S_1)-optimized geometries in toluene.

Table S7 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **CBZIn2** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0)- and first singlet excited state (S_1)-optimized geometries in toluene

state	λ_{calc} (nm)	f_{calc}	major contribution
		S_0	
1	649.34	0.6496	HOMO → LUMO (98.6%)
2	591.56	0.1697	HOMO−1 → LUMO (99.1%)
3	533.83	0.0724	HOMO−2 → LUMO (97.8%)
4	522.73	0.0001	HOMO−3 → LUMO (53.8%)
5	471.71	0.0735	HOMO−5 → LUMO (95.2%)
		S_1	
1	871.51	0.0008	HOMO → LUMO (99.1%)
2	729.03	0.3077	HOMO−1 → LUMO (99.3%)
3	638.20	0.0104	HOMO−2 → LUMO (98.2%)
4	618.08	0.0039	HOMO−3 → LUMO (98.5%)
5	604.91	0.2047	HOMO−4 → LUMO (95.8%)

Table S8 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **CBZIn2** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in toluene

	E (eV)	1,2-dicyanoethylene	In–Me	4-CBZ	Phenoxy
			S_0		
LUMO+3	−0.92	0.1	0.0	99.1	0.8
LUMO+2	−1.44	61.9	0.1	4.1	34.0
LUMO+1	−2.21	28.1	1.2	5.0	65.6
LUMO	−3.27	42.1	0.2	4.1	53.6
HOMO	−5.55	10.5	0.9	69.4	19.2
HOMO−1	−5.68	1.8	0.0	86.6	11.6
HOMO−2	−5.98	0.0	0.0	100.0	0.0
HOMO−3	−5.98	0.0	0.0	100.0	0.0
			S_1		
LUMO+3	−0.90	0.2	0.0	99.2	0.6
LUMO+2	−1.62	61.0	0.1	1.9	37.0
LUMO+1	−2.35	30.5	1.2	2.7	65.6
LUMO	−3.61	44.6	0.2	2.1	53.0
HOMO	−5.40	0.0	0.0	97.7	2.3
HOMO−1	−5.64	3.8	0.2	85.3	10.6
HOMO−2	−5.89	0.2	0.1	98.5	1.3
HOMO−3	−5.95	0.0	0.0	99.8	0.2

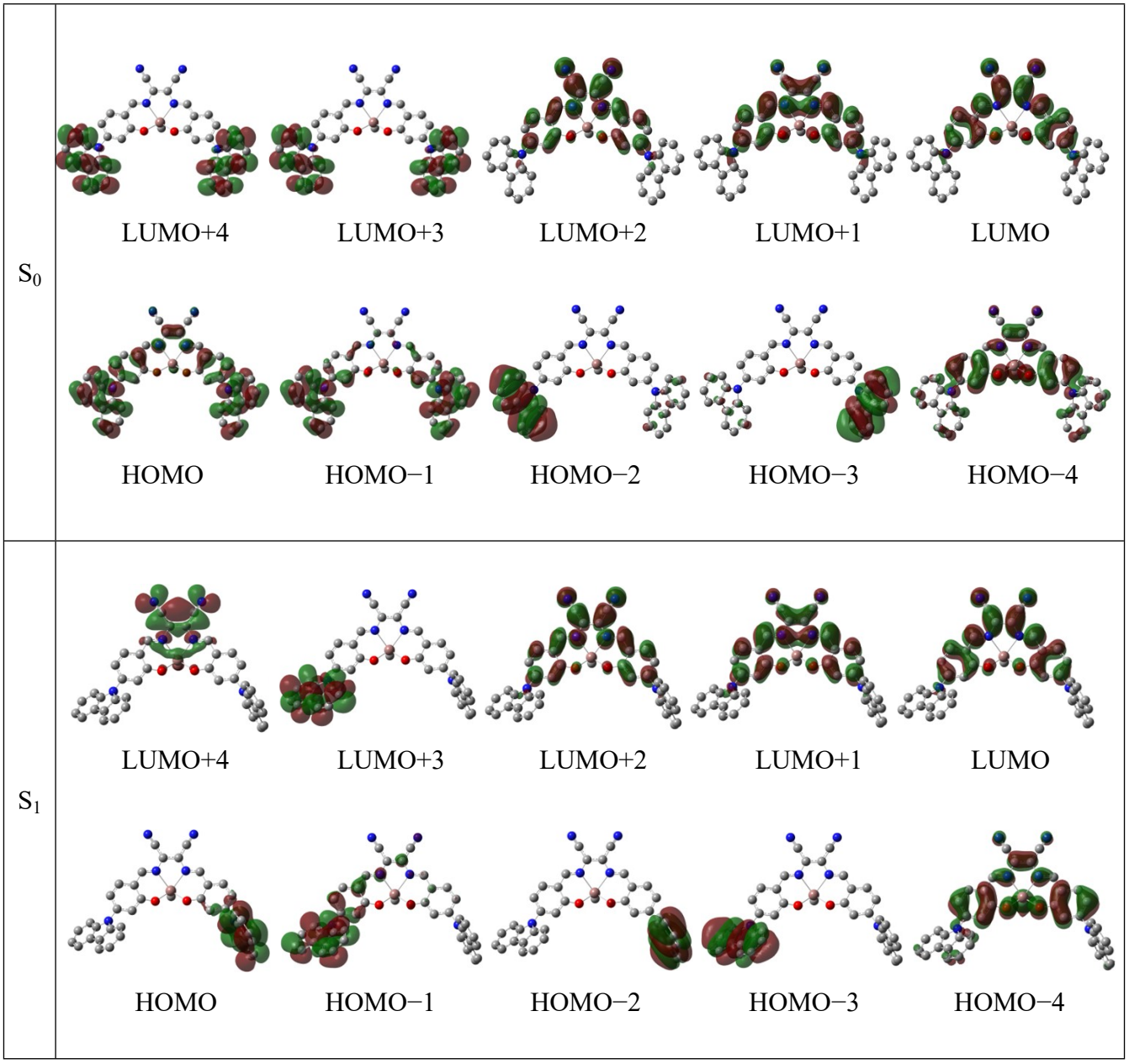


Fig. S7 The selected frontier orbitals of **CBZIn2** from TD-B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0)- and first singlet excited state (S_1)-optimized geometries in toluene.

Table S9 Cartesian coordinates of the ground state (S_0) fully optimized geometry in toluene of **CBZIn1** from B3LYP calculations (in Å)

Atom	X	Y	Z
N	-1.227474	3.242579	0.011058
N	1.408243	3.123476	0.000917
O	-1.499897	0.488184	-0.752563
O	1.425971	0.351399	-0.753277
C	-2.684457	0.612263	-0.228332
C	-3.536487	-0.522128	-0.220441
C	-4.808282	-0.478967	0.332737
C	-5.292925	0.712488	0.931631
C	-4.478715	1.819684	0.955957
H	-4.842767	2.738867	1.408280
C	-3.177688	1.822416	0.383526
C	-2.423040	3.025780	0.498442
H	-2.897671	3.820540	1.082094
C	2.575621	2.799153	0.492403
H	3.119658	3.547524	1.077114
C	3.219826	1.531141	0.377868
C	4.515778	1.413351	0.947780
H	4.960719	2.296385	1.399892
C	5.229439	0.238090	0.921044
C	4.640189	-0.904474	0.322754
C	3.367410	-0.834930	-0.226227
C	2.619595	0.370323	-0.231886
H	6.234192	0.184401	1.321593
H	-6.297689	0.747851	1.334119
In	0.027609	1.770375	-1.211565
C	0.045269	2.392637	-3.256685
H	0.005255	1.526010	-3.923443
H	-0.814138	3.030803	-3.484193
H	0.954410	2.954737	-3.491290
H	2.896900	-1.714540	-0.649145
H	-3.146322	-1.439644	-0.644308
C	6.040293	-2.708106	1.360622
C	5.553999	-2.927896	-0.852605
C	6.100918	-2.309853	2.699874
C	6.665115	-3.900557	0.916035
C	5.120018	-2.738770	-2.168220
C	6.360238	-4.037311	-0.493322
C	6.826600	-3.107984	3.582978
H	5.595578	-1.416323	3.047690
C	7.387301	-4.685262	1.822823
C	5.485231	-3.693480	-3.116003
H	4.522850	-1.879190	-2.448906
C	6.712305	-4.983070	-1.463676
C	7.469712	-4.281165	3.152703
H	6.889337	-2.815866	4.627186
H	7.870553	-5.600580	1.493000
C	6.268319	-4.808560	-2.771503
H	5.155539	-3.568195	-4.143214
H	7.328504	-5.837640	-1.198827
H	8.027530	-4.879889	3.866290
H	6.531768	-5.535490	-3.533751
N	5.365341	-2.117629	0.280093
C	-5.894894	-2.420893	-0.833156
C	-6.360379	-2.147630	1.379079
C	-5.446603	-2.277448	-2.149714
C	-6.793195	-3.454870	-0.467660
C	-6.385098	-1.739473	2.716469
C	-7.084988	-3.284559	0.940868
C	-5.892277	-3.203143	-3.091925
H	-4.778140	-1.473905	-2.435549
C	-7.225122	-4.372818	-1.432371
C	-7.175423	-2.468456	3.603940
H	-5.804183	-0.891475	3.060181
C	-7.870706	-4.000309	1.851810
C	-6.767807	-4.244976	-2.741012
H	-5.553019	-3.112814	-4.119668
H	-7.912133	-5.169922	-1.162676
C	-7.917015	-3.584243	3.179755
H	-7.211483	-2.167302	4.646831
H	-8.430393	-4.872787	1.526816
H	-7.092418	-4.951404	-3.498907
H	-8.523121	-4.129770	3.896587
N	-5.637701	-1.622784	0.295048
C	-0.566136	4.466103	0.197210
C	0.855219	4.403551	0.189896
C	-1.202226	5.707304	0.343479
C	1.598282	5.577181	0.325981
C	-0.459057	6.870070	0.501990
H	-2.284351	5.768523	0.304548
C	0.945465	6.808330	0.493919
H	2.680861	5.550098	0.277473
H	-0.956265	7.827713	0.607413
C	1.716194	8.008243	0.629593

N	2.342180	8.982577	0.744256

Table S10 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in toluene of **CBZIn1** from B3LYP calculations (in Å)

Atom	X	Y	Z
N	-1.164935	3.199371	0.072205
N	1.492396	3.091863	-0.054768
O	-1.463020	0.344820	-0.414262
O	1.433476	0.274113	-0.531407
C	-2.725490	0.560249	-0.075459
C	-3.598758	-0.541870	-0.055978
C	-4.942663	-0.417041	0.301981
C	-5.459023	0.839357	0.667180
C	-4.616298	1.934896	0.671650
H	-5.013361	2.906561	0.955566
C	-3.239772	1.859144	0.307065
C	-2.480522	3.056752	0.379740
H	-3.007308	3.922483	0.775071
C	2.685179	2.821226	0.364296
H	3.274891	3.605570	0.849057
C	3.332969	1.528685	0.284587
C	4.674409	1.461493	0.709112
H	5.164917	2.375991	1.030885
C	5.387932	0.276860	0.715724
C	4.733468	-0.907142	0.286680
C	3.415940	-0.888512	-0.133966
C	2.663139	0.319638	-0.156200
H	6.435318	0.255452	0.990040
H	-6.507084	0.942109	0.927206
In	-0.065539	1.650411	-1.033080
C	0.060535	2.023937	-3.142370
H	0.204016	1.090197	-3.694717
H	-0.857211	2.494324	-3.508554
H	0.896815	2.689913	-3.377207
H	2.905198	-1.798064	-0.426593
H	-3.188438	-1.510718	-0.319624
C	6.264344	-2.599228	1.302549
C	5.580793	-2.992192	-0.831730
C	6.410173	-2.095405	2.601090
C	6.896977	-3.798939	0.884992
C	5.004350	-2.898922	-2.103405
C	6.460464	-4.048912	-0.481204
C	7.253415	-2.790301	3.468199
H	5.877509	-1.210730	2.928107
C	7.725444	-4.479999	1.769488
C	5.306217	-3.905490	-3.020808
H	4.349581	-2.078617	-2.369745
C	6.748052	-5.040980	-1.412448
C	7.906619	-3.961883	3.060294
H	7.392014	-2.423451	4.479546
H	8.218641	-5.400166	1.473216
C	6.159814	-4.964958	-2.682603
H	4.869805	-3.863967	-4.012984
H	7.419602	-5.857109	-1.165759
H	8.550294	-4.485483	3.759313
H	6.372969	-5.735117	-3.416447
N	5.480538	-2.111699	0.253662
C	-6.059822	-2.375510	-0.811599
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C	-8.034639	-3.879534	1.916014
C	-6.917123	-4.239937	-2.684525
H	-5.687570	-3.142489	-4.079079
H	-8.070631	-5.136514	-1.096078
C	-8.076105	-3.416288	3.229657
H	-7.371957	-1.946823	4.645860
H	-8.605610	-4.756410	1.623043
H	-7.238639	-4.961000	-3.430196
H	-8.686637	-3.931996	3.964906
N	-5.792881	-1.563576	0.291499
C	-0.515062	4.397998	0.166798
C	0.923097	4.377858	0.085760
C	-1.129210	5.669526	0.347165
C	1.665578	5.548319	0.128793
C	-0.380952	6.827631	0.409921
H	-2.208493	5.742433	0.400865
C	1.029532	6.795616	0.294380
H	2.743313	5.517109	0.009890
H	-0.879624	7.784471	0.528167
C	1.793024	7.995286	0.325537

N	2.423789	8.977244	0.354850

Table S11 Cartesian coordinates of the ground state (S_0) fully optimized geometry in toluene of **CBZIn2** from B3LYP calculations (in Å)

Atom	X	Y	Z
N	-1.340638	3.382270	-0.129573
N	1.340796	3.382310	-0.129631
O	-1.474745	0.538656	-0.287407
O	1.474752	0.538724	-0.287092
C	-2.748842	0.730265	-0.097218
C	-3.588378	-0.405547	0.014624
C	-4.956167	-0.288155	0.220409
C	-5.557963	0.993925	0.344751
C	-4.764927	2.110850	0.268298
H	-5.217089	3.094791	0.361455
C	-3.358928	2.034405	0.049225
C	-2.639106	3.255125	0.066077
H	-3.220820	4.153390	0.290967
C	2.639266	3.255164	0.065978
H	3.221010	4.153429	0.290788
C	3.359047	2.034416	0.049168
C	4.765072	2.110820	0.268076
H	5.217292	3.094751	0.361062
C	5.558065	0.993865	0.344567
C	4.956188	-0.288202	0.220485
C	3.588373	-0.405549	0.014828
C	2.748887	0.730289	-0.097080
H	6.630424	1.078715	0.467884
H	-6.630302	1.078811	0.468228
In	0.000058	1.746282	-1.016993
C	0.000164	1.977232	-3.142934
H	0.001029	1.001476	-3.637808
H	-0.885276	2.524839	-3.479812
H	0.884808	2.526283	-3.479552
H	3.116796	-1.378788	-0.045373
H	-3.116854	-1.378802	-0.045719
C	6.760511	-1.686003	1.255580
C	5.726890	-2.536608	-0.590145
C	7.129669	-0.928642	2.371571
C	7.361637	-2.939982	0.983888
C	4.947260	-2.737815	-1.732949
C	6.708760	-3.477707	-0.192375
C	8.140099	-1.429489	3.191596
H	6.644734	0.011939	2.605054
C	8.372829	-3.422065	1.822735
C	5.145846	-3.913143	-2.456215
H	4.215124	-2.007508	-2.056192
C	6.888468	-4.650754	-0.934378
C	8.762755	-2.659350	2.920533
H	8.445038	-0.855500	4.061623
H	8.840477	-4.381897	1.622958
C	6.100315	-4.865652	-2.061767
H	4.547507	-4.091236	-3.344816
H	7.637420	-5.379049	-0.636773
H	9.546754	-3.020603	3.578958
H	6.226846	-5.772328	-2.645398
N	5.764687	-1.440614	0.292634
C	-5.727150	-2.536467	-0.590254
C	-6.760387	-1.685904	1.255704
C	-4.947742	-2.737662	-1.733210
C	-6.709038	-3.477510	-0.192386
C	-7.129306	-0.928566	2.371785
C	-7.361673	-2.939812	0.984024
C	-5.146558	-3.912921	-2.456527
H	-4.215602	-2.007397	-2.056539
C	-6.888980	-4.650486	-0.934441
C	-8.139651	-1.429368	3.191943
H	-6.644253	0.011965	2.605234
C	-8.372774	-3.421849	1.823005
C	-6.101039	-4.865375	-2.061981
H	-4.548392	-4.090998	-3.345248
H	-7.637952	-5.378731	-0.636766
C	-8.762455	-2.659161	2.920911
H	-8.444409	-0.855395	4.062045
H	-8.840540	-4.381629	1.623256
H	-6.227756	-5.771997	-2.645658
H	-9.546383	-3.020384	3.579437
N	-5.764721	-1.440526	0.292600
C	-0.691828	4.596528	0.019712
C	0.691971	4.596550	0.019670
C	1.425653	5.810579	0.207964
C	-1.425531	5.810536	0.208049
N	2.075535	6.764746	0.358182
N	-2.075421	6.764693	0.358300

Table S12 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in toluene of **CBZIn2** from B3LYP calculations (in Å)

Atom	X	Y	Z
N	1.374708	3.390657	-0.374645
N	-1.343635	3.431686	-0.344152
O	1.446157	0.547229	0.057768
O	-1.461869	0.595349	0.065872
C	2.739643	0.703221	-0.106106
C	3.563903	-0.445349	-0.042146
C	4.941856	-0.370842	-0.210508
C	5.566010	0.870802	-0.446382
C	4.781121	2.005864	-0.510620
H	5.251230	2.966017	-0.708528
C	3.373381	1.972214	-0.351879
C	2.671724	3.212425	-0.518412
H	3.279453	4.068657	-0.821926
C	-2.649982	3.294731	-0.434276
H	-3.248722	4.166625	-0.707435
C	-3.376776	2.061706	-0.244574
C	-4.784296	2.129254	-0.335629
H	-5.242507	3.101573	-0.496340
C	-5.601015	1.010782	-0.235959
C	-4.975058	-0.225062	-0.046414
C	-3.596808	-0.354226	0.051485
C	-2.752596	0.781548	-0.034032
H	-6.679905	1.087813	-0.308113
H	6.637554	0.921942	-0.600360
In	0.024893	1.877676	0.647209
C	0.000238	2.302049	2.750784
H	0.066407	1.381645	3.339537
H	0.844554	2.939757	3.031155
H	-0.919928	2.821193	3.037825
H	-3.130410	-1.322476	0.196482
H	3.083314	-1.395184	0.163084
C	-6.203880	-2.189387	-1.019370
C	-6.262971	-1.969871	1.224001
C	-5.940172	-1.990115	-2.382292
C	-6.980187	-3.280419	-0.535317
C	-6.070447	-1.509499	2.535227
C	-7.018041	-3.138882	0.919890
C	-6.478326	-2.917009	-3.274294
H	-5.341917	-1.151887	-2.717682
C	-7.504071	-4.187150	-1.438346
C	-6.656960	-2.250537	3.559875
H	-5.486933	-0.618743	2.732812
C	-7.590796	-3.857941	1.952649
C	-7.245833	-3.994788	-2.814125
H	-6.298466	-2.801964	-4.336885
H	-8.100085	-5.031521	-1.109234
C	-7.403060	-3.402388	3.276897
H	-6.532599	-1.931841	4.588303
H	-8.172365	-4.753659	1.762932
H	-7.652336	-4.701755	-3.528979
H	-7.847993	-3.961349	4.092765
N	-5.788839	-1.420399	0.050216
C	6.842364	-1.755645	0.671813
C	5.533468	-2.709816	-0.916336
C	7.403329	-0.906583	1.631695
C	7.367494	-3.052482	0.432317
C	4.574265	-2.973511	-1.899684
C	6.534309	-3.659995	-0.583833
C	8.513707	-1.367546	2.336255
H	6.987518	0.076121	1.823834
C	8.484720	-3.490839	1.154446
C	4.620587	-4.212732	-2.535150
H	3.820983	-2.238713	-2.160255
C	6.556932	-4.898793	-1.237129
C	9.055043	-2.644237	2.101047
H	8.967439	-0.724623	3.085143
H	8.897337	-4.480779	0.979961
C	5.597322	-5.170606	-2.208294
H	3.884787	-4.439962	-3.301379
H	7.317398	-5.635032	-0.991474
H	9.922390	-2.971480	2.666591
H	5.603479	-6.127499	-2.721759
N	5.728448	-1.555171	-0.150207
C	0.740060	4.589084	-0.630451
C	-0.681062	4.605469	-0.614464
C	-1.404509	5.785581	-0.926107
C	1.482715	5.751339	-0.951342
N	-2.063014	6.719344	-1.171561
N	2.148357	6.678378	-1.207068