Electronic supplementary information

High radiative efficiency based on intramolecular charge transfer in 9,9'–bianthracene–*ortho*–carboranyl luminophore

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Contents

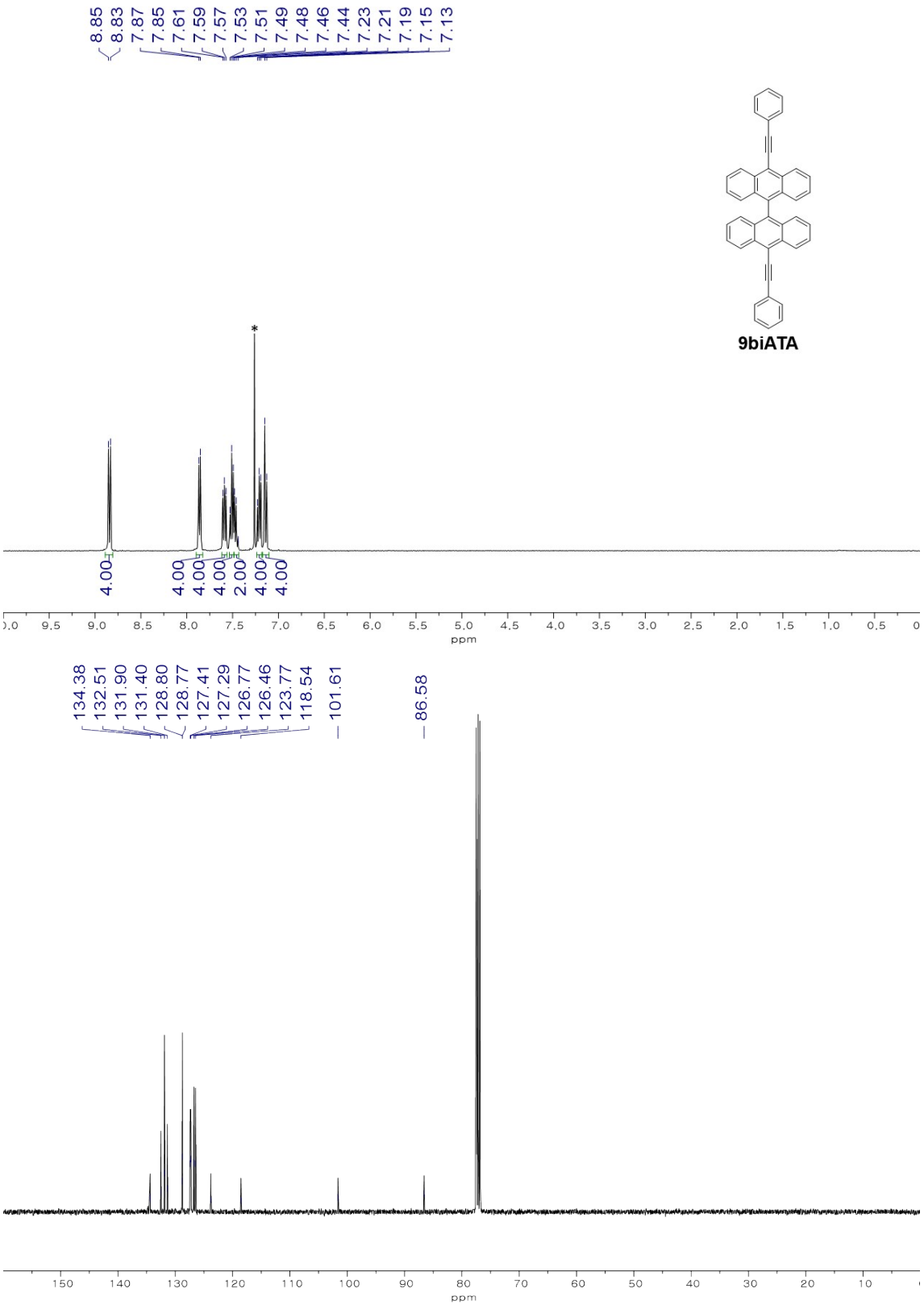


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **9biATA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

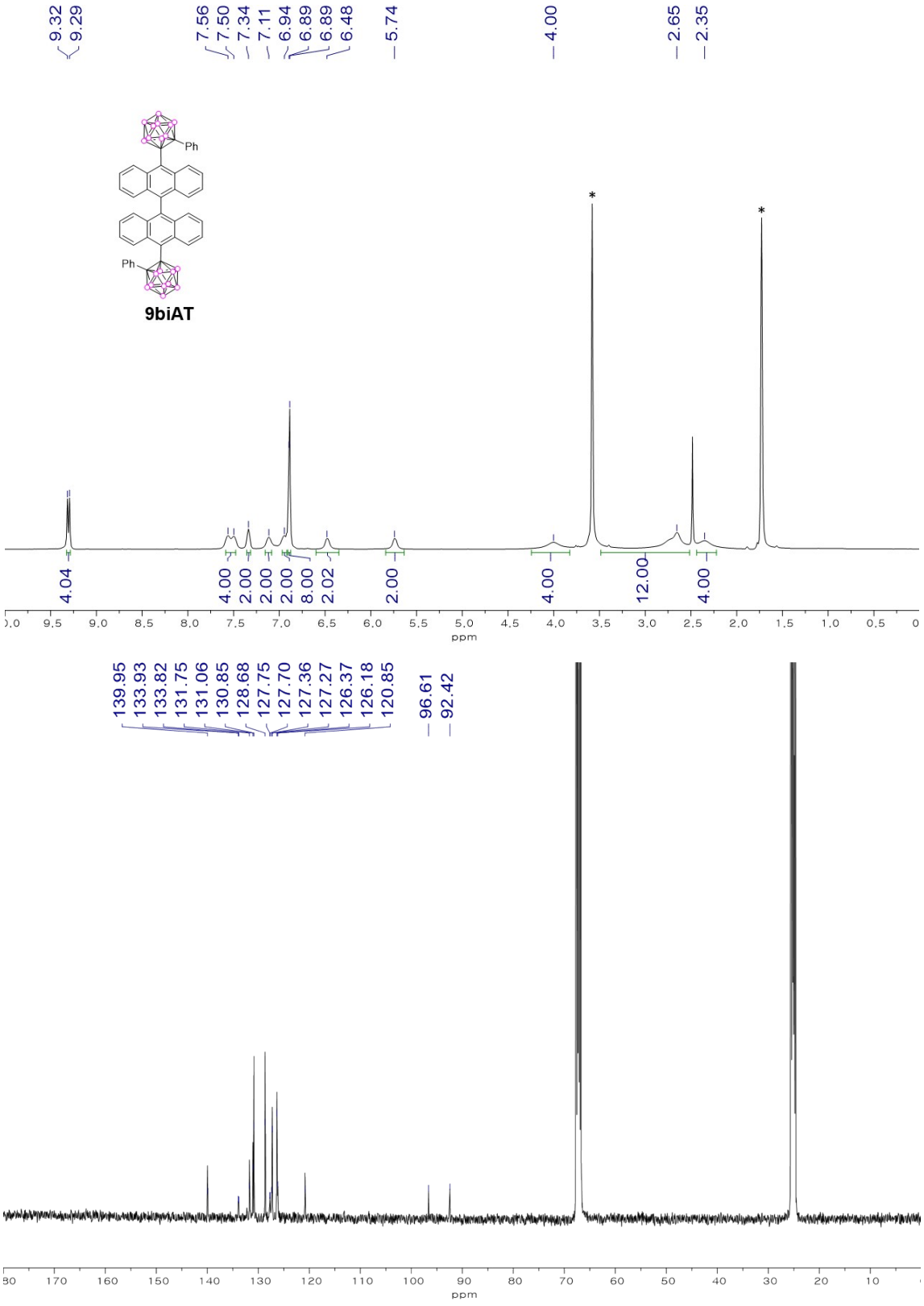


Fig. S2 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **9biAT** in THF-d_8 (* from residual THF in THF-d_8).

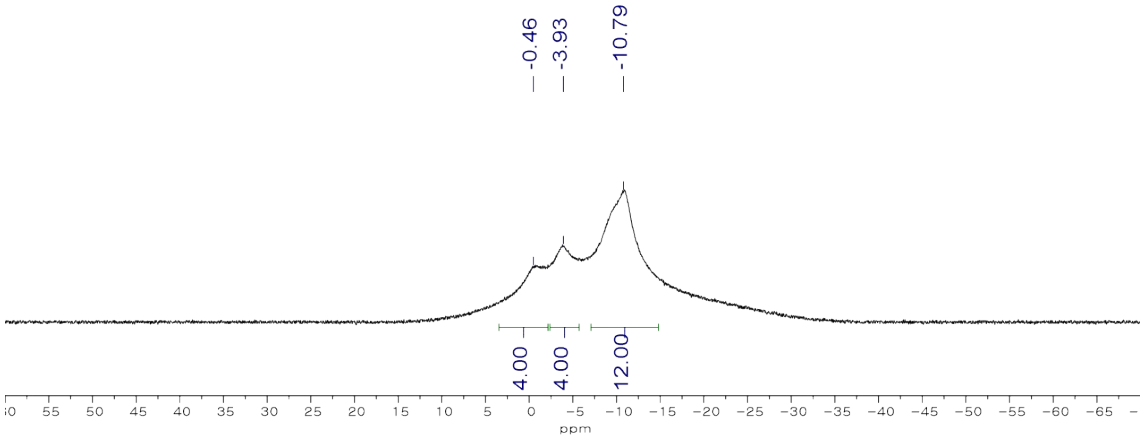


Fig. S3 $^{11}B\{^{1}H\}$ (top) NMR spectrum of **9biAT** in THF-d_8.

Table S1 Crystallographic data and parameters for **9biAT**.

Compound	**9biAT**
Formula	$C_{44}H_{46}B_{20}$
Formula weight	791.01
Crystal system	Triclinic
Space group	P_{-1}
a (Å)	11.9622(7)
b (Å)	13.4561(8)
c (Å)	14.6657(9)
α (°)	75.096(2)
β (°)	73.810(2)
γ (°)	79.007(2)
V (Å^3)	2172.7(2)
Z	2
ρ_{calc}(g cm^{-3})	1.209
μ (mm^{-1})	0.061
F(000)	820
T (K)	296(2)
Scan mode	*φ and ω scan*
hkl range	$-14 < h < 14$, $-16 < k < 16$, $-17 < l < 17$
Measd reflns	32778
Unique reflns [R_{int}]	7915 [0.0929]
Reflns used for refinement	7915
Refined parameters	577
R_1[a] (I > 2σ(I))	0.0804
wR_2[b] all data	0.2004
GOF on F^2	0.981
ρ_{fin} (max/min) (e Å^{-3})	0.198, −0.196

[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 **9biAT**

Compound	**9biAT**
length (Å)	
C9–C13	1.427(4)
C9–C15	1.522(4)
C15–C16	1.829(4)
angles (°)	
C13–C9–C15	120.3(3)
C9–C15–C16	116.6(2)

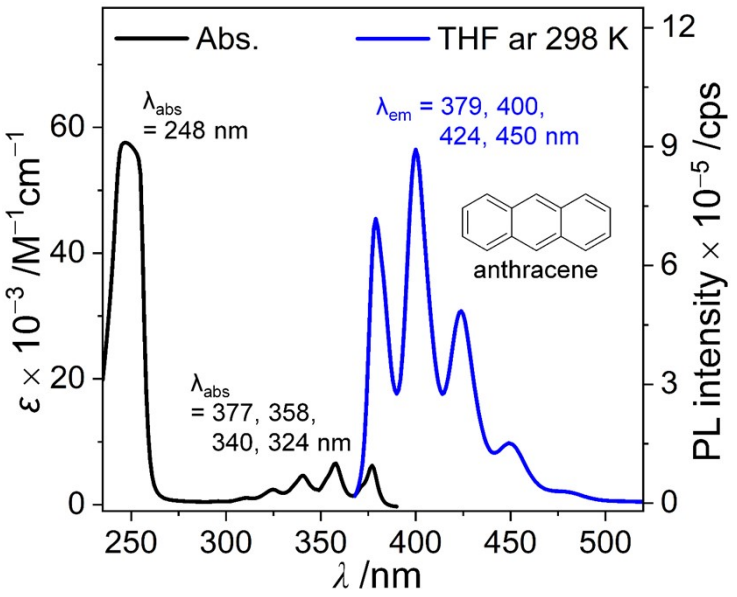


Fig. S4 UV-vis absorption (left side) and PL spectra (right side) for anthracene in THF (4.0×10^{-5} M, $\lambda_{ex} = 358$ nm).

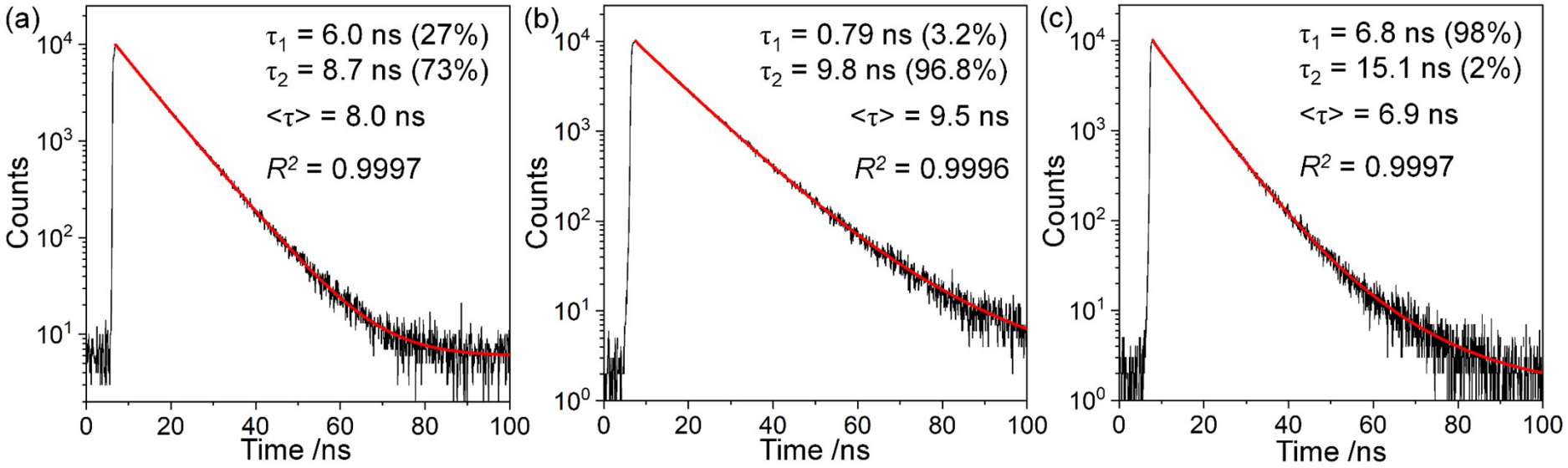


Fig. S5 Emission decay curves for **9biAT** in (a) film (5 wt% doped with PMMA), (b) in f_w (water fraction in a THF–water mixture) = 90% (2.0×10^{-5} M), and (c) crystalline states detected at each emissive maxima at 298 K. Each red-line is its double exponential fitting curve for the decay curves.

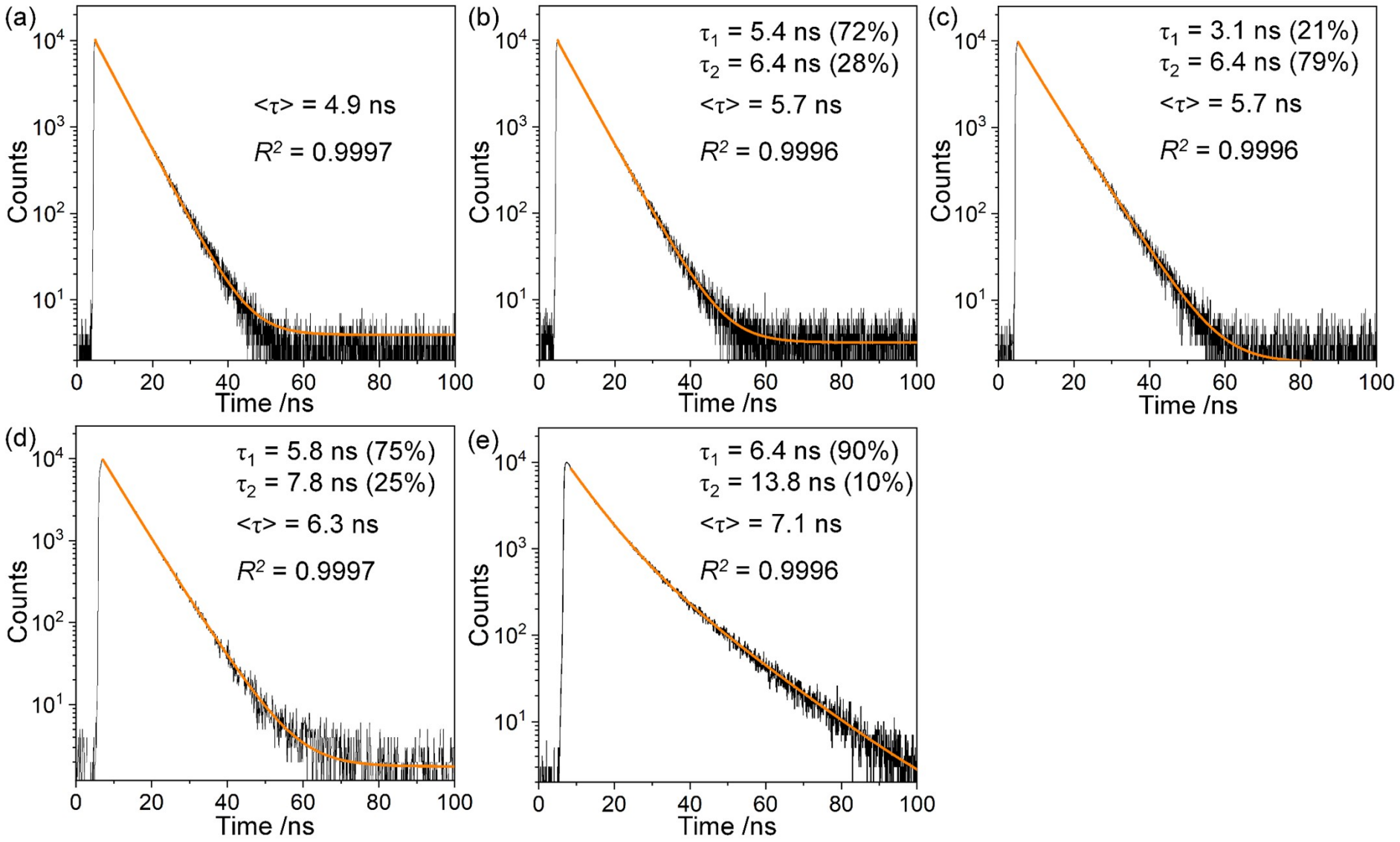


Fig. S6 Emission decay curves for **9biAT** in (a) cyclohexane (2.0×10^{-5} M), (b) toluene, (c) diethyl ether, (d) tetrahydrofuran, and (e) dichloromethane detected at each emissive maxima at 298 K. Each orange-line is its single or double exponential fitting curve for the decay curves.

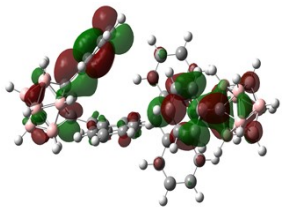
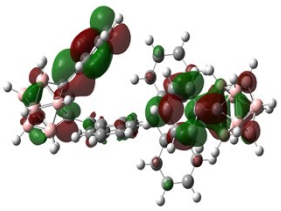
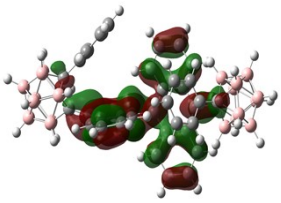
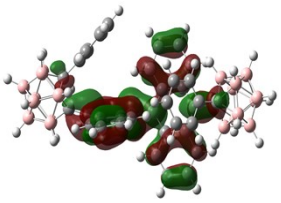
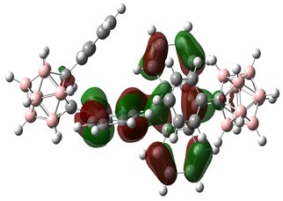
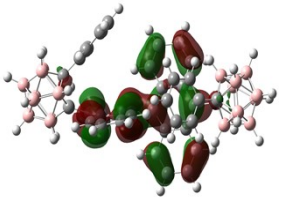
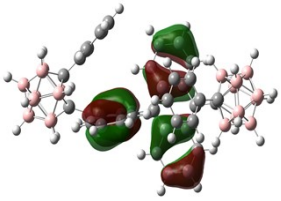
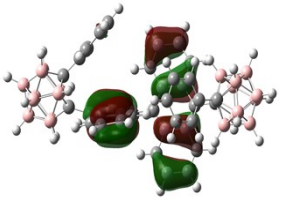
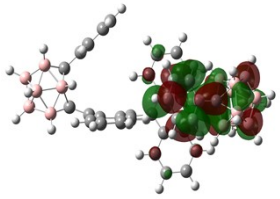
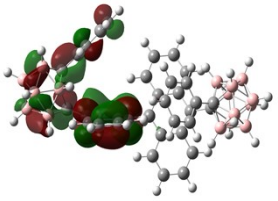
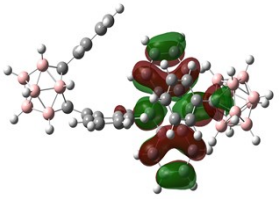
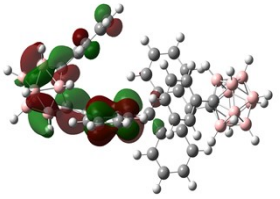
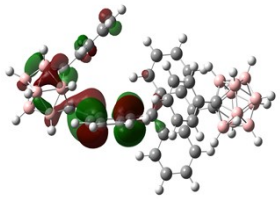
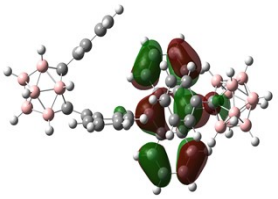
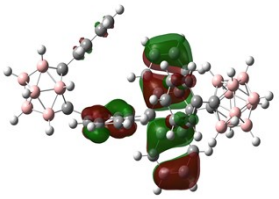
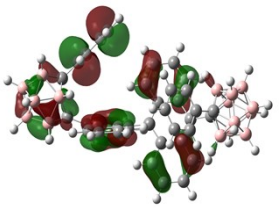
S_0	 LUMO+3	 LUMO+2	 LUMO+1	 LUMO
	 HOMO	 HOMO–1	 HOMO–2	 HOMO–3
S_1	 LUMO+3	 LUMO+2	 LUMO+1	 LUMO
	 HOMO	 HOMO–1	 HOMO–2	 HOMO–3

Fig. S7 The selected frontier orbitals of **9biAT** from PBE0 calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimised geometries in THF.

Table S3 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **9biAT** from TD-PBE0 calculations using the PBE0 geometries at the ground state (S_0) and first singlet excited state (S_1) optimised geometries in THF

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	450.03	0.0819	HOMO–1 → LUMO+1 (12.94%)
			HOMO → LUMO (86.46%)
2	447.27	0.0000	HOMO–1 → LUMO (55.23%)
			HOMO → LUMO+1 (44.23%)
3	434.38	0.3207	HOMO–1 → LUMO+1 (86.38%)
			HOMO → LUMO (12.84%)
4	416.81	0.0117	HOMO–1 → LUMO (43.65%)
			HOMO → LUMO+1(54.57%)
5	332.24	0.0151	HOMO–3 → LUMO+1(18.50%)
			HOMO–2 → LUMO (44.26%)
			HOMO–1 → LUMO+5 (8.89%)
			HOMO → LUMO+4 (21.31%)
			S_1
1	626.50	0.5279	HOMO → LUMO (98.96%)
2	465.50	0.2310	HOMO–1 → LUMO (98.56%)
3	439.72	0.0020	HOMO → LUMO+1 (97.89%)
4	403.54	0.0918	HOMO–1 → LUMO+1 (99.52%)
5	373.15	0.0185	HOMO–4 → LUMO (10.80%)
			HOMO–2 → LUMO (76.61%)

Table S4 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **9biAT** at the ground state (S_0) and first singlet excited state (S_1) optimised geometries in THF

	E (eV)	anthracene1	carborane1	carborane phenyl1	anthracene2	carborane2	carborane phenyl2
				S_0			
LUMO+3	−1.32	5.33	17.91	26.77	5.33	17.90	26.76
LUMO+2	−1.32	5.12	18.32	26.55	5.13	18.33	26.56
LUMO+1	−2.50	41.43	8.25	0.33	41.42	8.25	0.33
LUMO	−2.56	40.08	9.57	0.35	40.09	9.57	0.35
HOMO	−6.01	47.47	2.47	0.07	47.46	2.47	0.07
HOMO−1	−6.04	47.59	2.31	0.10	47.60	2.31	0.10
HOMO−2	−7.22	49.13	0.13	0.74	49.13	0.13	0.74
HOMO−3	−7.31	48.34	0.73	0.93	48.34	0.73	0.93
				S_1			
LUMO+3	−1.30	1.40	0.01	0.00	6.06	33.01	59.51
LUMO+2	−2.02	62.03	28.43	9.00	0.52	0.00	0.01
LUMO+1	−2.69	1.90	0.18	0.04	87.77	7.88	0.23
LUMO	−3.50	32.51	59.73	5.63	2.07	0.05	0.00
HOMO	−5.97	81.14	12.64	3.00	3.10	0.07	0.06
HOMO−1	−6.16	2.99	0.38	0.06	92.05	4.44	0.07
HOMO−2	−7.36	9.44	9.90	35.70	43.58	0.11	1.28
HOMO−3	−7.38	17.71	10.56	37.27	33.63	0.20	0.63

Table S5 Cartesian coordinates of the ground state (S_0) fully optimised geometry of **9biAT** in THF from TD-PBE0 calculations (in Å).

Atom	X	Y	Z
C	-5.488528	-0.892841	0.452071
C	-5.012815	0.453254	-0.659410
B	-5.915627	0.711466	0.804141
H	-5.401616	1.237075	1.722238
B	-7.048877	-0.619573	1.063362
H	-7.244181	-0.959649	2.183180
B	-6.764880	-1.784566	-0.225072
H	-6.758298	-2.953454	-0.021609
B	-5.467619	-1.126738	-1.228707
H	-4.651912	-1.842643	-1.681296
B	-6.050827	0.361347	-2.008399
H	-5.621298	0.710716	-3.056084
B	-7.144391	-1.011349	-1.767923
H	-7.518531	-1.652190	-2.697571
B	-8.141622	-0.673095	-0.332050
H	-9.254892	-1.076466	-0.213106
B	-7.608382	0.889691	0.333622
H	-8.319984	1.631529	0.932078
B	-6.335919	1.525739	-0.721392
H	-6.104511	2.675902	-0.886225
B	-7.699537	0.641722	-1.424426
H	-8.483788	1.212875	-2.113701
C	-4.443635	-1.568720	1.287300
C	-3.802160	-2.722706	0.822055
H	-4.020768	-3.104512	-0.168315
C	-2.897680	-3.402744	1.629223
H	-2.414371	-4.298934	1.252941
C	-2.624104	-2.945142	2.915256
H	-1.929466	-3.487078	3.550146
C	-3.256788	-1.797800	3.386802
H	-3.056793	-1.435309	4.390457
C	-4.160906	-1.114464	2.580419
H	-4.660308	-0.235048	2.969920
C	5.488544	-0.892731	-0.452274
C	5.012826	0.453126	0.659486
B	5.467637	-1.126976	1.228454
H	4.651927	-1.842982	1.680880
B	6.764906	-1.784584	0.224675
H	6.758343	-2.953429	0.020970
B	7.048894	-0.619329	-1.063525
H	7.244178	-0.959171	-2.183417
B	5.915631	0.711639	-0.804018
H	5.401624	1.237451	-1.721996
B	6.335920	1.525609	0.721681
H	6.104505	2.675737	0.886748
B	7.608384	0.889789	-0.333478
H	8.319973	1.631759	-0.931784
B	8.141639	-0.673128	0.331877
H	9.254911	-1.076469	0.212848
B	7.144412	-1.011686	1.767683
H	7.518567	-1.652718	2.697193
B	6.050845	0.360953	2.008455
H	5.621321	0.710104	3.056215
B	7.699551	0.641464	1.424523
H	8.483804	1.212480	2.113910
C	4.443633	-1.568468	-1.287597
C	3.802590	-2.722852	-0.822737
H	4.021561	-3.105076	0.167392
C	2.898083	-3.402748	-1.629992
H	2.415120	-4.299251	-1.254011
C	2.624034	-2.944597	-2.915728
H	1.929363	-3.486403	-3.550692
C	3.256282	-1.796857	-3.386889
H	3.055918	-1.433931	-4.390313
C	4.160433	-1.113664	-2.580419
H	4.659481	-0.233921	-2.969632
C	-3.544675	0.833175	-0.674243
C	-3.021712	1.804411	0.234083
C	-3.800638	2.830613	0.854519
H	-4.836892	2.950296	0.583457
C	-3.262796	3.735231	1.728144
H	-3.896431	4.513859	2.142098
C	-1.893263	3.682060	2.077432
H	-1.481259	4.389484	2.790043
C	-1.090582	2.761205	1.471513
H	-0.028279	2.737753	1.687770
C	-1.604989	1.835480	0.512342
C	-0.727540	0.975454	-0.168993
C	-1.208283	0.196134	-1.232278
C	-0.294710	-0.551494	-2.037213
H	0.753430	-0.558825	-1.757555
C	-0.708635	-1.209549	-3.157421
H	0.003267	-1.753607	-3.769301
C	-2.068250	-1.132472	-3.540166
H	-2.392933	-1.579136	-4.475167
C	-2.982001	-0.484190	-2.755874
H	-3.995245	-0.412345	-3.117226
C	-2.619804	0.167764	-1.536015
C	3.544684	0.833034	0.674389
C	3.021718	1.804446	-0.233748
C	3.800639	2.830783	-0.853967
H	4.836888	2.950427	-0.582871
C	3.262796	3.735571	-1.727416
H	3.896426	4.514294	-2.141203
C	1.893270	3.682448	-2.076738
H	1.481267	4.390006	-2.789217
C	1.090593	2.761461	-1.471014
H	0.028295	2.738036	-1.687295
C	1.604998	1.835561	-0.512010
C	0.727547	0.975421	0.169178
C	1.208290	0.195914	1.232326
C	0.294708	-0.551829	2.037144
H	-0.753436	-0.559080	1.757500
C	0.708633	-1.210092	3.157230
H	-0.003276	-1.754227	3.769033
C	2.068260	-1.133134	3.539957
H	2.392948	-1.579985	4.474866
C	2.982016	-0.484736	2.755766
H	3.995270	-0.412996	3.117108
C	2.619815	0.167462	1.536039

Table S6 Cartesian coordinates of the first excited state (S_1) fully optimised geometry of **9biAT** in THF from TD-PBE0 calculations (in Å)

Atom	X	Y	Z
C	-5.408965	-0.689303	0.798420
C	-5.001852	-0.039798	-0.791542
B	-5.962783	0.857909	0.338347
H	-5.496484	1.792721	0.879783
B	-7.010127	-0.262742	1.206889
H	-7.212597	-0.036825	2.352799
B	-6.615775	-1.886426	0.646673
H	-6.539875	-2.798840	1.399593
B	-5.335539	-1.726203	-0.553718
H	-4.456826	-2.506278	-0.604360
B	-5.973695	-0.834170	-1.953020
H	-5.518285	-0.995458	-3.034553
B	-6.995744	-1.988010	-1.077090
H	-7.299681	-3.021189	-1.579156
B	-8.051985	-1.061002	0.014710
H	-9.141482	-1.429644	0.315288
B	-7.639961	0.661030	-0.162832
H	-8.411996	1.549803	-0.001664
B	-6.370554	0.790298	-1.392467
H	-6.185855	1.721948	-2.099829
B	-7.652633	-0.413410	-1.581932
H	-8.441492	-0.300430	-2.464064
C	-4.353475	-0.800383	1.858534
C	-3.605234	-1.975656	1.994429
H	-3.749676	-2.798966	1.304828
C	-2.687297	-2.110820	3.029280
H	-2.118432	-3.030397	3.122048
C	-2.509387	-1.080117	3.947655
H	-1.801482	-1.194009	4.762799
C	-3.252700	0.090665	3.822656
H	-3.129527	0.896705	4.539162
C	-4.169792	0.231130	2.786630
H	-4.757480	1.139269	2.718498
C	5.516395	-1.256235	-0.008869
C	4.887160	0.993964	0.388999
B	5.341165	-0.414917	1.438752
H	4.512946	-0.786315	2.202915
B	6.734880	-1.532678	1.051226
H	6.816078	-2.621157	1.528979
B	7.014981	-1.151092	-0.662698
H	7.310780	-1.947543	-1.498055
B	5.732817	0.118215	-0.956610
H	5.202477	0.150458	-2.017542
B	6.266450	1.677038	-0.162003
H	6.185839	2.765782	-0.635639
B	7.476403	0.545360	-0.766973
H	8.177901	0.912587	-1.660036
B	8.072965	-0.462047	0.585526
H	9.205718	-0.823923	0.690121
B	7.027077	-0.066407	1.981872
H	7.397572	-0.149224	3.113459
B	5.984816	1.293461	1.562770
H	5.691732	2.092375	2.394602
B	7.624011	1.203290	0.882649
H	8.430123	2.026178	1.197604
C	4.532401	-2.290677	-0.403807
C	3.863594	-3.057694	0.561989
H	4.054766	-2.872407	1.613915
C	2.972131	-4.057471	0.189685
H	2.472566	-4.642405	0.956808
C	2.727342	-4.316640	-1.157740
H	2.041693	-5.107852	-1.448135
C	3.382666	-3.560481	-2.128335
H	3.208636	-3.756933	-3.182719
C	4.272552	-2.558423	-1.755965
H	4.784078	-1.982676	-2.520402
C	-3.553498	0.387317	-0.994478
C	-3.113323	1.714173	-0.672628
C	-3.961106	2.848584	-0.669861
H	-4.988335	2.756190	-0.982820
C	-3.496692	4.114810	-0.354478
H	-4.185267	4.951991	-0.393155
C	-2.161342	4.318599	-0.000661
H	-1.805589	5.306984	0.268001
C	-1.285817	3.249011	-0.038072
H	-0.235771	3.390012	0.190128
C	-1.719680	1.956556	-0.405779
C	-0.756495	0.929300	-0.553179
C	-1.170685	-0.303513	-1.109845
C	-0.199787	-1.284498	-1.409845
H	0.826012	-1.104537	-1.110026
C	-0.531476	-2.436164	-2.101073
H	0.235154	-3.167185	-2.332139
C	-1.848578	-2.617983	-2.527519
H	-2.113068	-3.476350	-3.135616
C	-2.835649	-1.710192	-2.180222
H	-3.828793	-1.873771	-2.567315
C	-2.556362	-0.551295	-1.414646
C	3.498783	1.335281	0.238626
C	2.948264	1.719447	-1.046579
C	3.737739	2.244407	-2.099121
H	4.788586	2.421497	-1.925912
C	3.212032	2.572459	-3.329063
H	3.859562	2.984561	-4.096924
C	1.842670	2.382860	-3.585057
H	1.425656	2.629902	-4.556904
C	1.029419	1.908417	-2.587120
H	-0.033422	1.796170	-2.776818
C	1.539130	1.590684	-1.296005
C	0.675137	1.175752	-0.255797
C	1.153404	1.060160	1.068537
C	0.259421	0.822202	2.150738
H	-0.797010	0.680946	1.943734
C	0.698548	0.795905	3.450047
H	-0.007583	0.635508	4.259036
C	2.061892	1.001883	3.725814
H	2.415230	1.020749	4.752251
C	2.956107	1.181916	2.694188
H	3.994960	1.348061	2.936871
C	2.559756	1.191271	1.334425

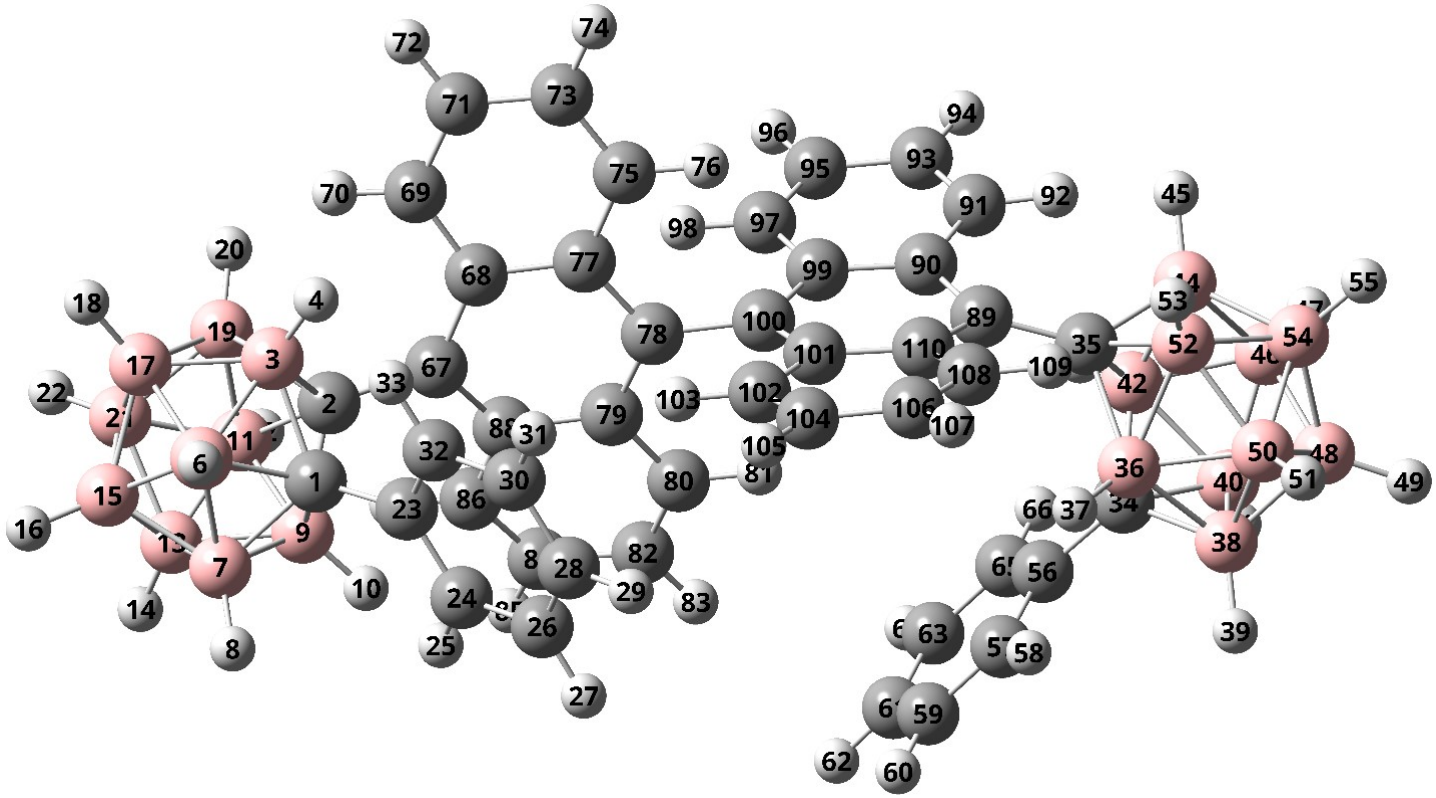


Fig. S8 Atomic tag for **9biAT** in S_1–optimized geometry.

Table S7 Calculated atomic charge for **9biAT** in S_1–optimized geometry in cyclohexane.

Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge
1	C	-0.31643	22	H	0.00471	45	H	0.02491	68	C	0.05680	91	C	-0.14812
2	C	-0.30391	23	C	0.13372	46	B	0.05194	69	C	-0.16340	92	H	0.16039
3	B	0.01109	24	C	-0.11663	47	H	-0.00542	70	H	0.16103	93	C	-0.13192
4	H	0.06631	25	H	0.15892	48	B	-0.10138	71	C	-0.14029	94	H	0.15439
5	B	0.02216	26	C	-0.14694	49	H	-0.00302	72	H	0.14770	95	C	-0.14102
6	H	0.03085	27	H	0.14922	50	B	0.05166	73	C	-0.14081	96	H	0.15071
7	B	0.02367	28	C	-0.11788	51	H	-0.00581	74	H	0.14706	97	C	-0.12884
8	H	0.03068	29	H	0.14428	52	B	0.00696	75	C	-0.14699	98	H	0.15666
9	B	0.01144	30	C	-0.15467	53	H	0.02439	76	H	0.14989	99	C	0.08510
10	H	0.06627	31	H	0.14821	54	B	-0.07578	77	C	0.07350	100	C	-0.14458
11	B	0.00740	32	C	-0.11929	55	H	-0.00371	78	C	-0.11675	101	C	0.08328
12	H	0.03408	33	H	0.15963	56	C	0.12724	79	C	0.07747	102	C	-0.13005
13	B	-0.00347	34	C	-0.28530	57	C	-0.12778	80	C	-0.14846	103	H	0.15951
14	H	0.00307	35	C	-0.26748	58	H	0.15425	81	H	0.15582	104	C	-0.13922
15	B	-0.09407	36	B	-0.05796	59	C	-0.14676	82	C	-0.13668	105	H	0.13796
16	H	0.00557	37	H	0.03502	60	H	0.14435	83	H	0.13848	106	C	-0.13252
17	B	-0.00315	38	B	0.03053	61	C	-0.12242	84	C	-0.13919	107	H	0.15315
18	H	0.00318	39	H	0.02233	62	H	0.14317	85	H	0.14634	108	C	-0.14847
19	B	0.00592	40	B	0.02946	63	C	-0.14985	86	C	-0.16757	109	H	0.16028
20	H	0.03523	41	H	0.02265	64	H	0.14503	87	H	0.16261	110	C	0.04060
21	B	-0.08043	42	B	-0.05903	65	C	-0.12846	88	C	0.05296			
			43	H	0.03657	66	H	0.15545	89	C	0.06393			
			44	B	0.00665	67	C	0.05506	90	C	0.04302			

Table S8 Calculated atomic charge for **9biAT** in S_1–optimized geometry in tetrahydrofuran.

Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge
1	C	-0.31477	22	H	-0.00047	45	H	0.02907	68	C	0.05696	91	C	-0.15316
2	C	-0.30367	23	C	0.13156	46	B	0.04650	69	C	-0.16810	92	H	0.16210
3	B	0.01011	24	C	-0.12317	47	H	-0.01011	70	H	0.16385	93	C	-0.13403
4	H	0.07235	25	H	0.16369	48	B	-0.10619	71	C	-0.14359	94	H	0.16272
5	B	0.01991	26	C	-0.15248	49	H	-0.00999	72	H	0.15532	95	C	-0.14489
6	H	0.03246	27	H	0.15738	50	B	0.04611	73	C	-0.14522	96	H	0.15963
7	B	0.02138	28	C	-0.12256	51	H	-0.01026	74	H	0.15500	97	C	-0.13303
8	H	0.03213	29	H	0.15446	52	B	0.00379	75	C	-0.15186	98	H	0.16135
9	B	0.01008	30	C	-0.15777	53	H	0.02881	76	H	0.15412	99	C	0.08633
10	H	0.07265	31	H	0.15710	54	B	-0.08017	77	C	0.07483	100	C	-0.14159
11	B	0.00443	32	C	-0.12494	55	H	-0.01052	78	C	-0.11537	101	C	0.08474
12	H	0.03881	33	H	0.16426	56	C	0.12473	79	C	0.07766	102	C	-0.13301
13	B	-0.00766	34	C	-0.28342	57	C	-0.13402	80	C	-0.15311	103	H	0.16068
14	H	0.00042	35	C	-0.26726	58	H	0.15817	81	H	0.15642	104	C	-0.14292
15	B	-0.09776	36	B	-0.05834	59	C	-0.15221	82	C	-0.14101	105	H	0.15013
16	H	0.00014	37	H	0.03906	60	H	0.15338	83	H	0.14690	106	C	-0.13440
17	B	-0.00727	38	B	0.02817	61	C	-0.12610	84	C	-0.14239	107	H	0.16232
18	H	0.00044	39	H	0.02203	62	H	0.15369	85	H	0.15482	108	C	-0.15353
19	B	0.00315	40	B	0.02706	63	C	-0.15343	86	C	-0.17195	109	H	0.16201
20	H	0.03970	41	H	0.02238	64	H	0.15388	87	H	0.16568	110	C	0.04089
21	B	-0.08408	42	B	-0.05905	65	C	-0.13437	88	C	0.05303			
			43	H	0.04003	66	H	0.15886	89	C	0.06389			
			44	B	0.00356	67	C	0.05435	90	C	0.04354			

Table S9 Calculated atomic charge for **9biAT** in S_1–optimized geometry in dichloromethane.

Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge
1	C	-0.31459	22	H	-0.00087	45	H	0.02935	68	C	0.05695	91	C	-0.15337
2	C	-0.30351	23	C	0.13111	46	B	0.04596	69	C	-0.16764	92	H	0.16220
3	B	0.01031	24	C	-0.12295	47	H	-0.01047	70	H	0.16371	93	C	-0.13427
4	H	0.07303	25	H	0.16404	48	B	-0.10649	71	C	-0.14401	94	H	0.16333
5	B	0.01929	26	C	-0.15294	49	H	-0.01062	72	H	0.15589	95	C	-0.14513
6	H	0.03272	27	H	0.15788	50	B	0.04563	73	C	-0.14554	96	H	0.16029
7	B	0.02158	28	C	-0.12228	51	H	-0.01061	74	H	0.15559	97	C	-0.13343
8	H	0.03208	29	H	0.15526	52	B	0.00365	75	C	-0.15227	98	H	0.16170
9	B	0.01033	30	C	-0.15850	53	H	0.02902	76	H	0.15446	99	C	0.08516
10	H	0.07303	31	H	0.15773	54	B	-0.08058	77	C	0.07455	100	C	-0.13880
11	B	0.00437	32	C	-0.12593	55	H	-0.01113	78	C	-0.11415	101	C	0.08413
12	H	0.03897	33	H	0.16472	56	C	0.12434	79	C	0.07713	102	C	-0.13304
13	B	-0.00803	34	C	-0.28336	57	C	-0.13443	80	C	-0.15341	103	H	0.16061
14	H	0.00032	35	C	-0.26703	58	H	0.15851	81	H	0.15648	104	C	-0.14360
15	B	-0.09790	36	B	-0.05836	59	C	-0.15282	82	C	-0.14166	105	H	0.15174
16	H	-0.00030	37	H	0.03939	60	H	0.15399	83	H	0.14790	106	C	-0.13443
17	B	-0.00786	38	B	0.02785	61	C	-0.12565	84	C	-0.14232	107	H	0.16302
18	H	0.00027	39	H	0.02196	62	H	0.15446	85	H	0.15557	108	C	-0.15389
19	B	0.00274	40	B	0.02703	63	C	-0.15418	86	C	-0.17263	109	H	0.16219
20	H	0.04014	41	H	0.02221	64	H	0.15451	87	H	0.16622	110	C	0.04055
21	B	-0.08460	42	B	-0.05905	65	C	-0.13498	88	C	0.05257			
			43	H	0.04017	66	H	0.15914	89	C	0.06361			
			44	B	0.00328	67	C	0.05397	90	C	0.04374			

Table S10 Calculated atomic charge for **9biAT** in S_1–optimized geometry in acetone.

Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge	Tag	Atom	Charge
1	C	-0.31409	22	H	-0.00192	45	H	0.03061	68	C	0.05698	91	C	-0.15471
2	C	-0.30356	23	C	0.13060	46	B	0.04445	69	C	-0.16958	92	H	0.16274
3	B	0.00978	24	C	-0.12565	47	H	-0.01121	70	H	0.16491	93	C	-0.13462
4	H	0.07443	25	H	0.16543	48	B	-0.10816	71	C	-0.14451	94	H	0.16522
5	B	0.01900	26	C	-0.15454	49	H	-0.01201	72	H	0.15764	95	C	-0.14601
6	H	0.03303	27	H	0.15995	50	B	0.04403	73	C	-0.14649	96	H	0.16235
7	B	0.02052	28	C	-0.12413	51	H	-0.01123	74	H	0.15743	97	C	-0.13453
8	H	0.03266	29	H	0.15799	52	B	0.00269	75	C	-0.15350	98	H	0.16281
9	B	0.00965	30	C	-0.15866	53	H	0.03047	76	H	0.15560	99	C	0.08670
10	H	0.07480	31	H	0.16008	54	B	-0.08198	77	C	0.07520	100	C	-0.14051
11	B	0.00345	32	C	-0.12700	55	H	-0.01240	78	C	-0.11499	101	C	0.08529
12	H	0.04047	33	H	0.16590	56	C	0.12370	79	C	0.07740	102	C	-0.13411
13	B	-0.00919	34	C	-0.28267	57	C	-0.13628	80	C	-0.15494	103	H	0.16069
14	H	-0.00005	35	C	-0.26724	58	H	0.15958	81	H	0.15634	104	C	-0.14401
15	B	-0.09923	36	B	-0.05854	59	C	-0.15410	82	C	-0.14235	105	H	0.15454
16	H	-0.00144	37	H	0.04048	60	H	0.15629	83	H	0.14999	106	C	-0.13482
17	B	-0.00876	38	B	0.02721	61	C	-0.12731	84	C	-0.14324	107	H	0.16518
18	H	-0.00010	39	H	0.02198	62	H	0.15728	85	H	0.15755	108	C	-0.15511
19	B	0.00223	40	B	0.02609	63	C	-0.15464	86	C	-0.17335	109	H	0.16269
20	H	0.04122	41	H	0.02233	64	H	0.15678	87	H	0.16689	110	C	0.04094
21	B	-0.08552	42	B	-0.05908	65	C	-0.13653	88	C	0.05292			
			43	H	0.04111	66	H	0.16002	89	C	0.06405			
			44	B	0.00249	67	C	0.05407	90	C	0.04368			