Electronic Supplementary Material (ESI) for Dalton Transactions.

Rigid, Yet Flexible: Formation of the Unprecedented Silver MB-DIPY Dimers with Orthogonal Chromophore Geometry

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SUPPORTING INFORMATION

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EXPERIMENTAL SECTION

Materials. Solvents were purified using standard approaches: THF, 1,4-dioxane were dried over sodium metal and benzophenone, DCM, MeCN, DMF were dried over phosphorus(V) oxide. Compounds **1a** and **1b** were synthesized as described before [1]. Silver nitrate was purchased from Sigma Aldrich.

Spectroscopy Measurements. Jasco-V770 spectrophotometer was used to collect UV-Vis data. Electrochemical cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were conducted using a CHI-620 C electrochemical analyzer utilizing a three-electrode scheme with platinum working, auxiliary and Ag/AgCl reference electrodes. DCM was used as solvent and 0.1 M solution of tetrabutylammonium perchlorate (TBAP). In all cases, experimental redox potentials were corrected using decamethylferrocene (Fc*H) as an internal standard. NMR spectra were recorded a Bruker Avance instrument with a 300 MHz frequency for protons. Chemical shifts are reported in parts per million (ppm) and referenced to the residual proton resonance of the deuterated solvent ($CDCl_3$ = δ 7.26). High-resolution mass spectra of all new compounds were recorded using a Bruker micrOTOF-QIII. All exact mass measurements showed an error of less than 5 ppm.

Computational Details. The starting geometries of MB-$DIPY_2Ag_2$ **2a** and **2b** were optimized using a hybrid B3LYP exchange-correlation functional [2]. Solvent effects were calculated using the polarized continuum model (PCM) [3]. In all calculations, DCM was used as the solvent. In PCM-TDDFT calculations, the first 50 states were calculated. In all calculations 20s16p9d2f1g full-electron basis set [4] was utilized for silver atoms, while all other atoms were modeled using 6-31G(d) basis set [5]. Gaussian 09 software was used in all calculations [6]. QMForge program was used for molecular orbital analysis [7].

X-ray Experimental Details.

A dark purple, multi-faceted block of suitable size (0.082 x 0.055 x 0.032 mm) and quality was selected from a representative sample of crystals of the same habit using an optical microscope and mounted onto a MiTiGen loop. X-ray data were obtained on a Bruker D8 QUEST ECO CMOS diffractometer (Mo sealed X-ray tube, K_α = 0.71073 Å) at 150 K. All diffractometer manipulations, including data collection, integration and scaling were carried out using the Bruker APEX3 software suite.[8] An absorption correction was applied using SADABS.[8] The space group was determined on the basis of systematic absences and intensity statistics and the structure was solved by direct methods and refined by full-matrix least squares on F^2. The structure was solved in the monoclinic space group *P*-1 using XS[9] (incorporated in SHELXTL). No obvious missed symmetry was reported by PLATON.[10] “Flip”-type disorder[11] was observed for two thiophenyl side chains, wherein different types of atoms (sulfur and

carbon) occupy positions that are close to each other. This influences their thermal parameters, which were therefore equated for each pair of disordered atoms in the disordered rings. All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms, including those on disordered atoms, were placed in idealized positions and refined using a riding model. The structure was refined (weighted least squares refinement on F^2) and the final least-squares refinement converged to R_1 = 0.0554 ($I > 2\sigma(I)$, 7340 data) and wR_2 = 0.1482 (F^2, 11041 data, 671 parameters).

General procedure for synthesis of compounds 2a and 2b

The solution of compounds **1a**, **1b** (0.1 mmol) in dry acetonitrile (10 mL) was treated with the solution of $AgNO_3$ (0.11 mmol, 19 mg) in acetonitrile (3 mL). The resulting solution was stirred for 40 min at room temperature. The resulting precipitate was collected by vacuum filtration and air-dried to give pure silver complexes **2a** and **2b**.

Compound 2a. Yield 54 mg (90 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 – 7.37 (m, 18H), 7.22 – 7.16 (m, 6H), 7.03 (s, 4H), 6.37 (s, 4H); HRMS (APCI-TOF) m/z: $[M+H]^+$ Calcd for $C_{56}H_{32}N_6O_4S_4Ag_2$ 1196.9542; Found 1196.9532.

Compound 2b. Yield 48 mg (83 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 – 7.28 (m, 28H), 7.20 – 7.13 (m, 8H), 6.46 (s, 4H); HRMS (APCI-TOF) m/z: $[M+H]^+$ Calcd for $C_{64}H_{40}N_6O_4Ag_2$ 1173.1291; Found 1173.1314.

ACKNOWLEDGEMENT

Generous support from the Minnesota Supercomputing Institute, NSERC, CFI, University of Manitoba, and WestGrid Canada to VN is greatly appreciated. We wish to acknowledge Gabriel Cohen for the help with some experimental work.

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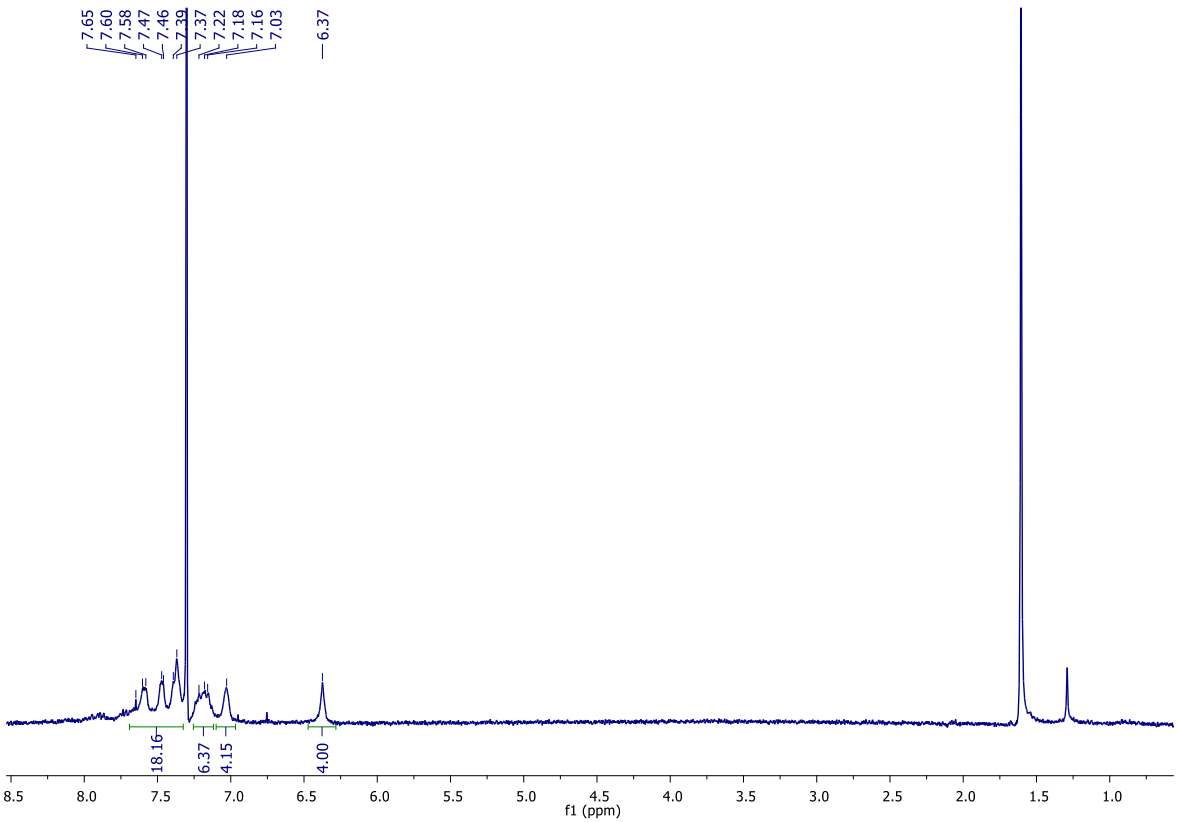

Figure S1. ^{1}H NMR spectrum of compound **2a** in $CDCl_3$

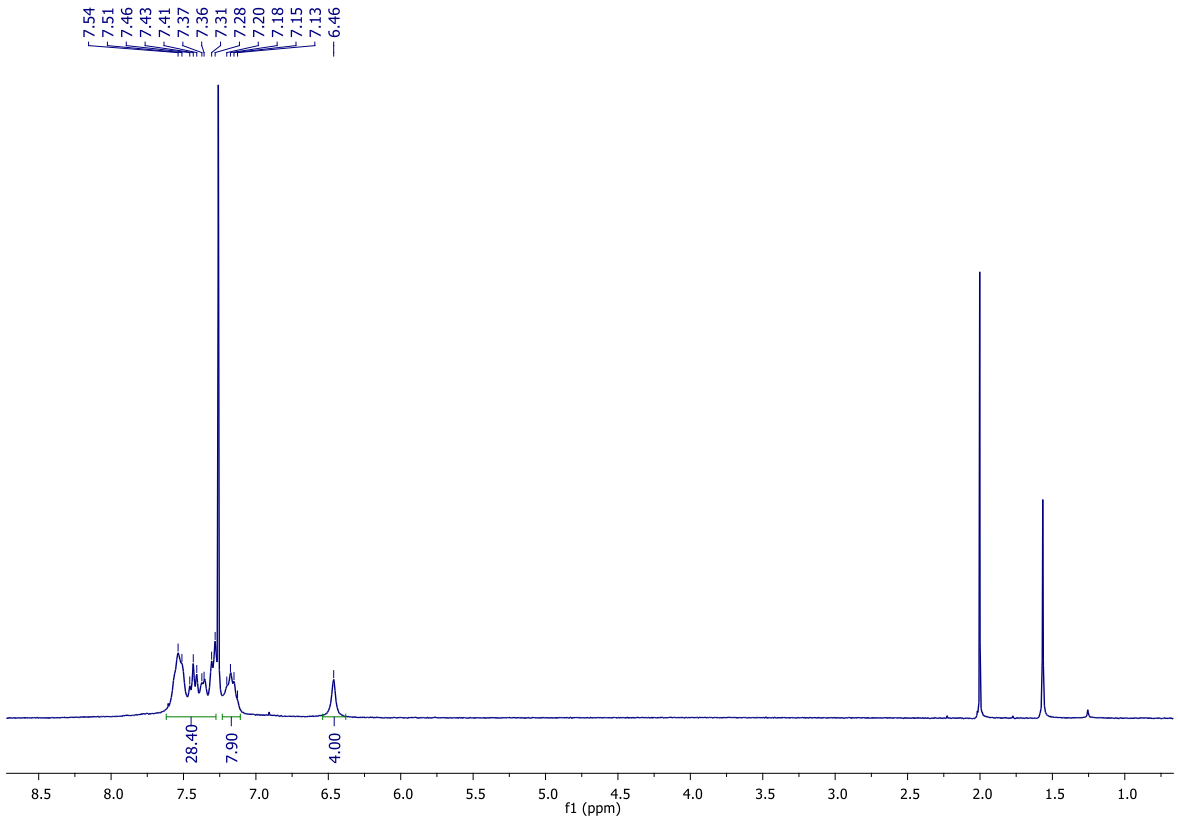

Figure S2. ^{1}H NMR spectrum of compound **2b** in $CDCl_3$

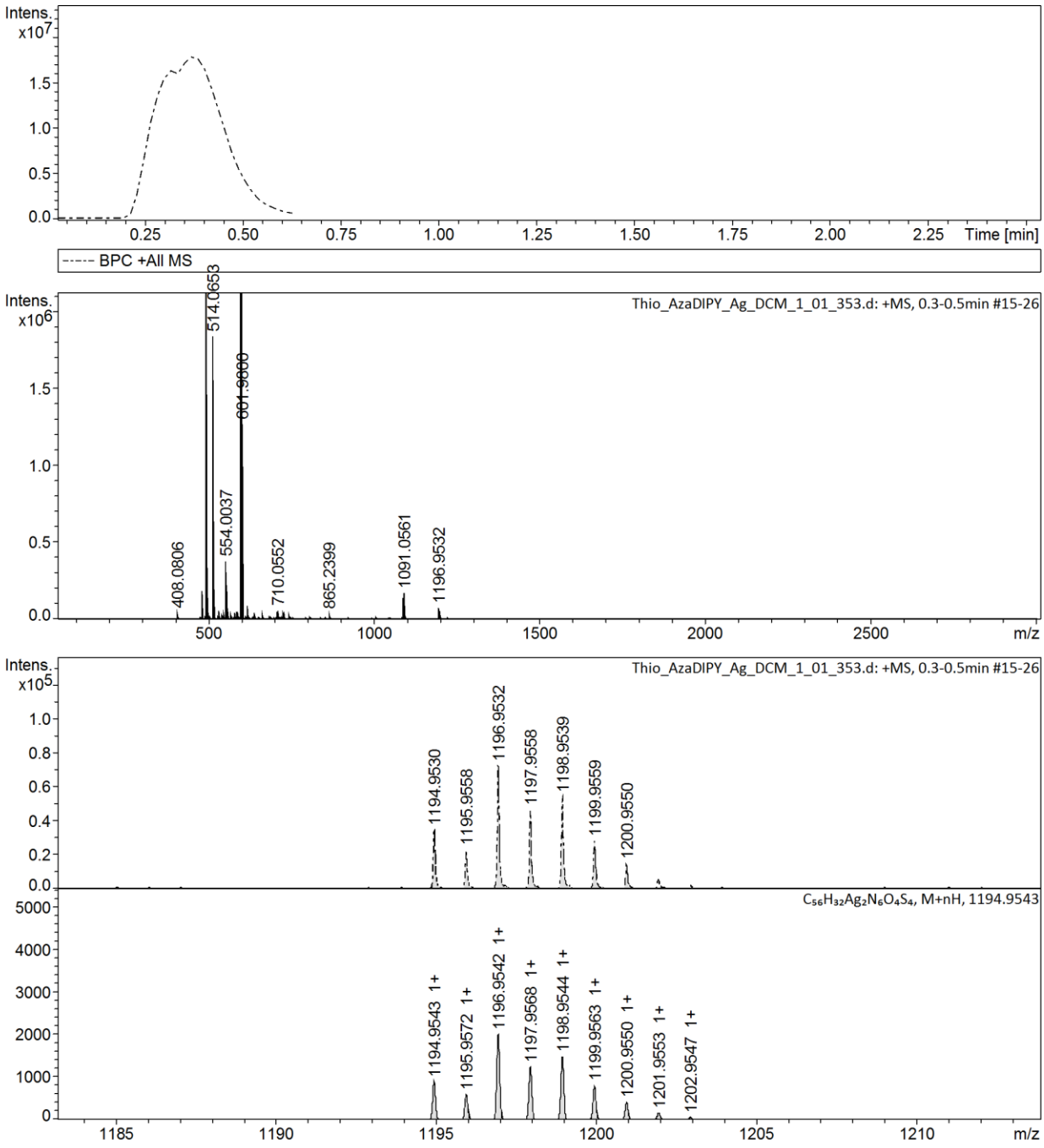

Figure S3. APCI high-resolution mass spectrum of compound **2a**

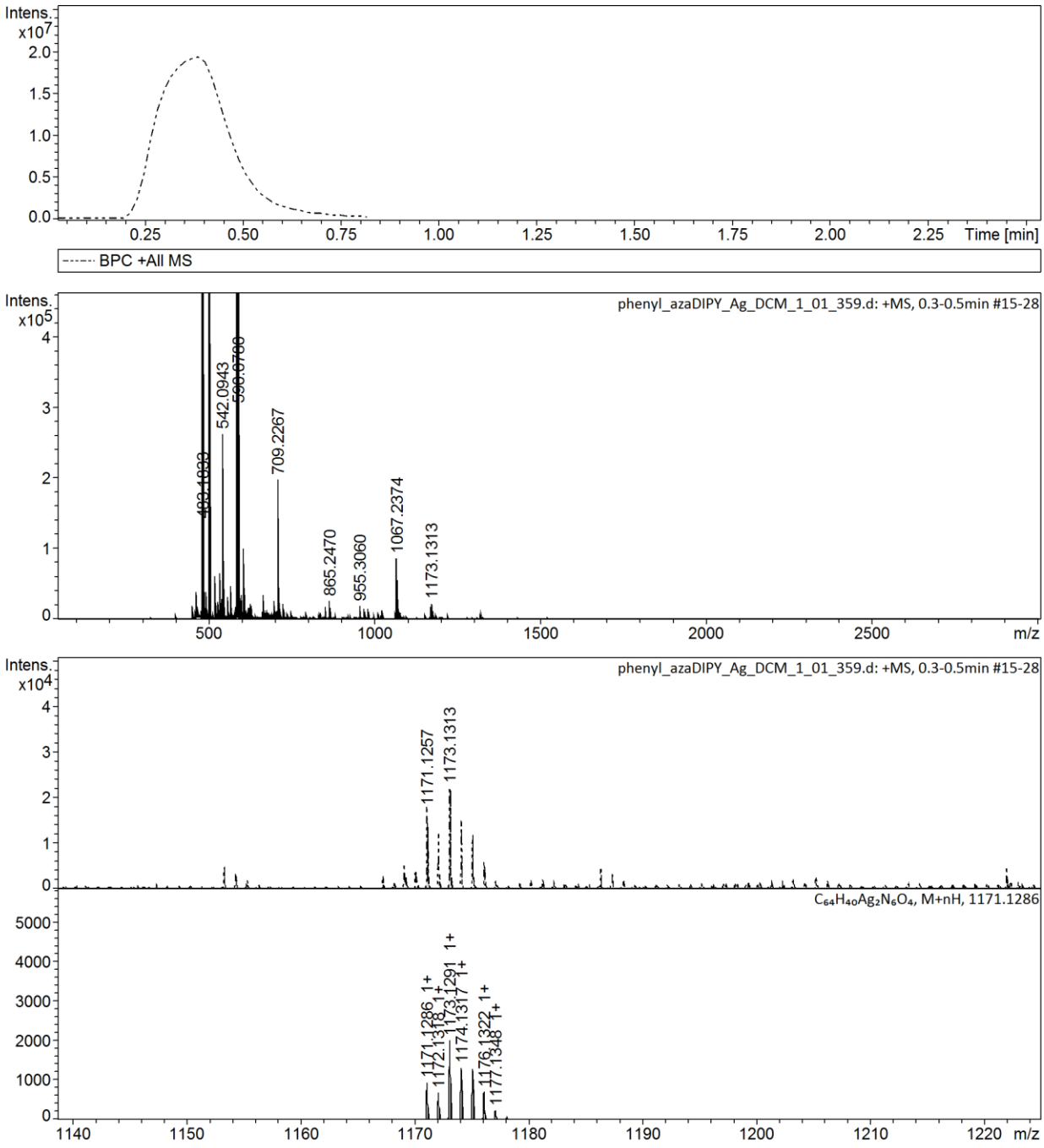

Figure S4. APCI high-resolution mass spectrum of compound **2b**

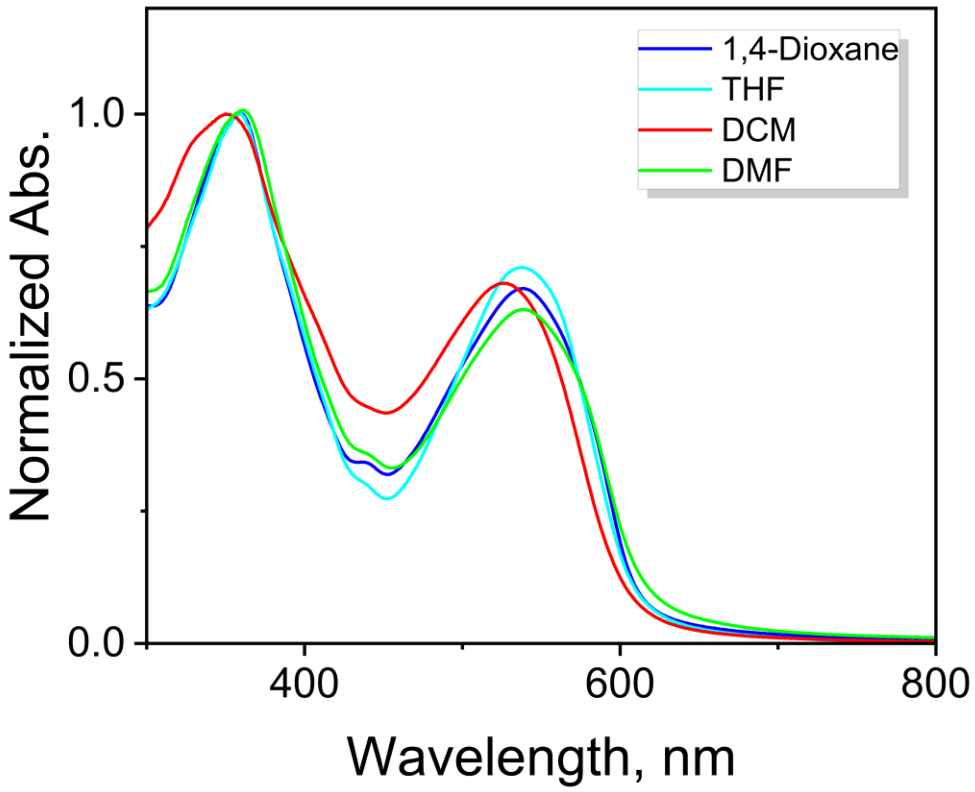

Figure S5. Normalized UV-vis absorption spectra of MB-DIPY$_2$Ag$_2$ **2b** in different solvents.

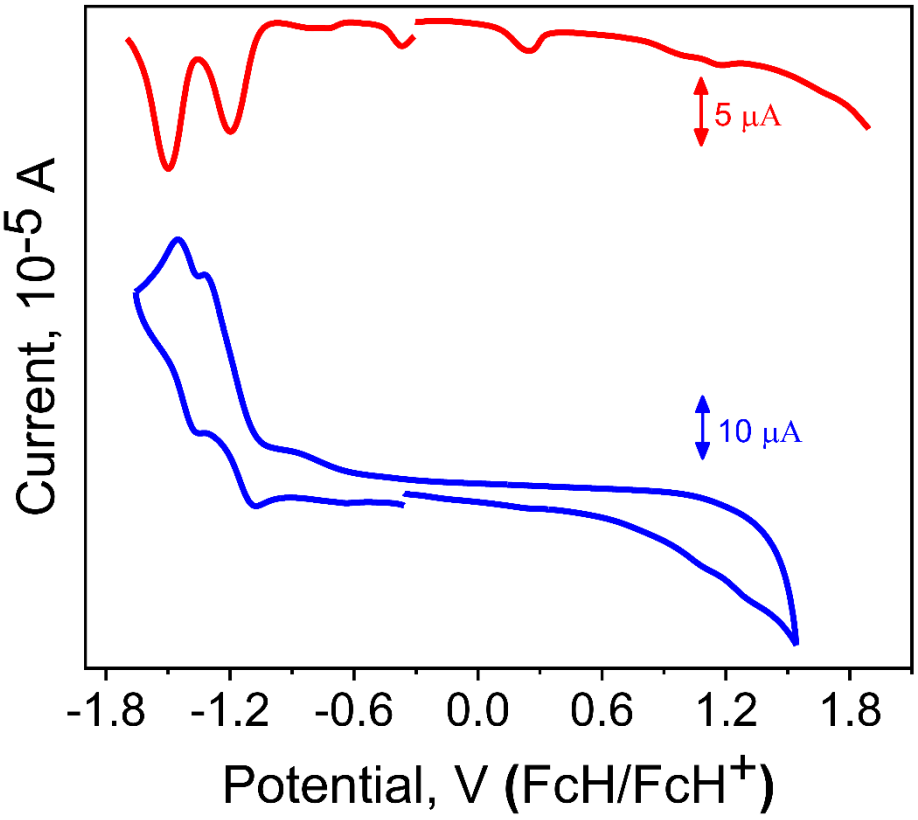

Figure S6. CV (bottom) and DPV (top) spectra of MB-DIPY$_2$Ag$_2$ **2a** in the deoxygenated 0.1 M TBAP/DCM system.

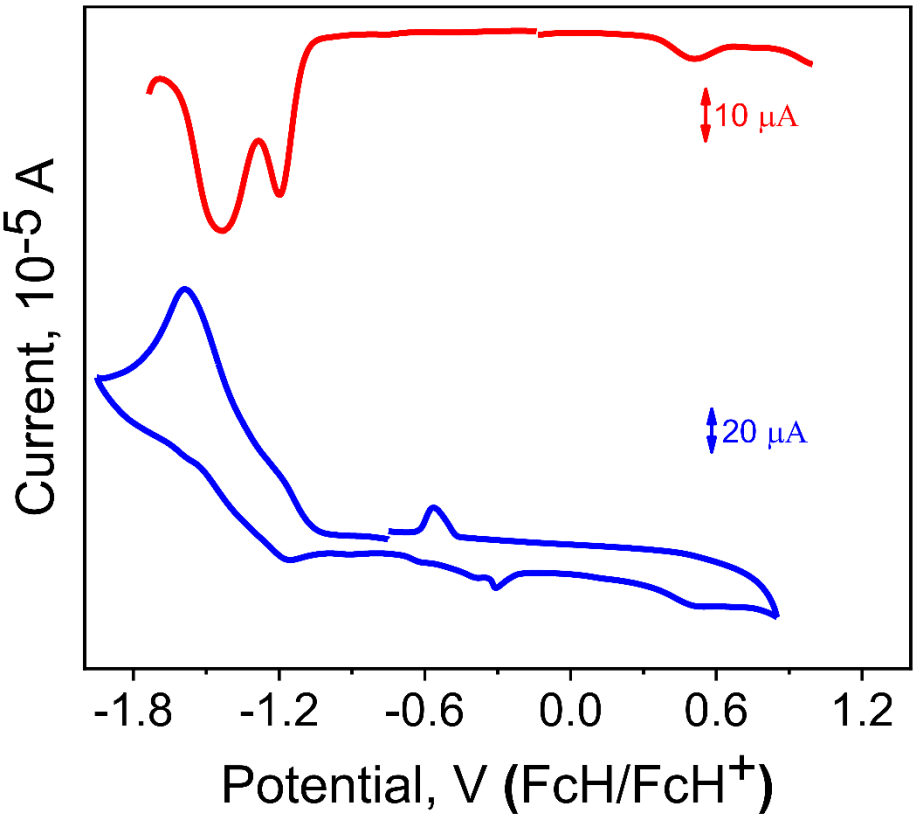

Figure S7. CV (bottom) and DPV (top) spectra of MB-DIPY$_2$Ag$_2$ **2b** in the deoxygenated 0.1 M TBAP/DCM system.

Table S1. DFT-optimized coordinates of **2a.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.025673	-1.139206	0.977277
2	47	0	0.027841	1.132125	-0.974180
3	6	0	3.223628	-1.812842	1.728056
4	6	0	3.520381	-2.073088	0.331605
5	6	0	2.669218	-2.126488	-0.738248
6	6	0	3.131496	-2.509227	-2.096369
7	6	0	4.375709	-2.828497	-2.627539
8	6	0	4.443210	-3.173391	-3.980718
9	6	0	3.294458	-3.203741	-4.778712
10	6	0	2.044652	-2.885198	-4.241813
11	6	0	1.990436	-2.538189	-2.899613
12	6	0	0.866449	-2.136926	-2.028351
13	6	0	-1.465610	-1.478194	-2.263112
14	6	0	-2.796824	-2.062241	-2.531362
15	6	0	-3.193278	-3.345646	-2.878986
16	6	0	-4.559785	-3.577556	-3.052910
17	6	0	-5.486522	-2.542395	-2.887556
18	6	0	-5.075163	-1.250761	-2.545969
19	6	0	-3.715269	-1.024423	-2.365571
20	6	0	-2.917606	0.182402	-2.028914
21	6	0	-3.491289	1.417707	-1.883482
22	6	0	-2.847988	2.698430	-1.663827
23	6	0	3.221441	1.817852	-1.732453
24	6	0	3.521495	2.074955	-0.336142
25	6	0	2.672308	2.126562	0.735433
26	6	0	3.136787	2.507218	2.093424
27	6	0	4.381805	2.825959	2.623094
28	6	0	4.451294	3.170053	3.976342
29	6	0	3.303665	3.200045	4.776007
30	6	0	2.053083	2.881967	4.240677
31	6	0	1.996889	2.535706	2.898371
32	6	0	0.871454	2.135780	2.028138
33	6	0	-1.461014	1.478580	2.264699
34	6	0	-2.791665	2.064531	2.531558
35	6	0	-3.186707	3.348734	2.877784
36	6	0	-4.553129	3.582612	3.050148
37	6	0	-5.481072	2.548574	2.884711
38	6	0	-5.071123	1.256099	2.544541
39	6	0	-3.711381	1.027823	2.365616
40	6	0	-2.914886	-0.180459	2.031389
41	6	0	-3.489715	-1.415383	1.887142
42	6	0	-2.847159	-2.697469	1.673628
43	7	0	1.304023	-1.893055	-0.774607
44	7	0	-0.372349	-2.171282	-2.466474
45	7	0	-1.581850	-0.166961	-1.947120
46	7	0	1.307346	1.893225	0.773550
47	7	0	-0.366758	2.170189	2.467665
48	7	0	-1.578695	0.167175	1.950219
49	8	0	2.091638	-1.582658	2.188096

50	8	0	-1.620620	2.871563	-1.559420
51	8	0	2.087720	1.592932	-2.190990
52	8	0	-1.619221	-2.873094	1.579279
53	1	0	4.556035	-2.287314	0.102564
54	1	0	5.277504	-2.813859	-2.025330
55	1	0	5.403323	-3.422884	-4.419478
56	1	0	3.377375	-3.479070	-5.824449
57	1	0	1.147180	-2.909125	-4.849583
58	1	0	-2.465781	-4.138852	-3.009265
59	1	0	-4.908372	-4.569101	-3.320347
60	1	0	-6.542742	-2.745721	-3.028145
61	1	0	-5.808442	-0.460556	-2.426640
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63	1	0	4.557772	2.287833	-0.108736
64	1	0	5.282782	2.811234	2.019632
65	1	0	5.412005	3.419469	4.413842
66	1	0	3.388122	3.474639	5.821808
67	1	0	1.156472	2.905666	4.849755
68	1	0	-2.458263	4.141015	3.008317
69	1	0	-4.900683	4.574894	3.316221
70	1	0	-6.537149	2.753368	3.024235
71	1	0	-5.805376	0.466835	2.425014
72	1	0	-4.567270	-1.435314	1.984581
73	6	0	-3.724293	-3.881395	1.585524
74	6	0	-5.095549	-4.016677	1.640636
75	16	0	-2.959322	-5.440158	1.367660
76	6	0	-5.532853	-5.358951	1.510348
77	1	0	-5.776969	-3.185691	1.767414
78	6	0	-4.490348	-6.235085	1.357356
79	1	0	-6.572208	-5.662178	1.529300
80	1	0	-4.536170	-7.308105	1.238798
81	6	0	4.357863	-1.846200	2.670616
82	6	0	5.707993	-2.055469	2.478590
83	16	0	4.009826	-1.577949	4.364300
84	6	0	6.459652	-2.002465	3.678872
85	1	0	6.157030	-2.240850	1.511632
86	6	0	5.675272	-1.753881	4.775163
87	1	0	7.532123	-2.143008	3.729039
88	1	0	5.984674	-1.664321	5.806580
89	6	0	4.354175	1.848090	-2.676953
90	6	0	5.705300	2.052831	-2.487145
91	16	0	4.002320	1.582026	-4.370208
92	6	0	6.454709	1.998124	-3.688769
93	1	0	6.156571	2.236313	-1.520866
94	6	0	5.667652	1.752705	-4.783848
95	1	0	7.527542	2.135232	-3.740705
96	1	0	5.975000	1.662575	-5.815828
97	6	0	-3.723688	3.883846	-1.580907
98	6	0	-5.094095	4.021877	-1.648719
99	16	0	-2.957897	5.440626	-1.351973
100	6	0	-5.530120	5.364648	-1.519218
101	1	0	-5.775818	3.192561	-1.784459
102	6	0	-4.487465	6.238406	-1.354140
103	1	0	-6.568677	5.669898	-1.547280
104	1	0	-4.532396	7.311197	-1.233176

Table S2. DFT-optimized coordinates of **2b.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.082969	-1.231033	0.847571
2	47	0	0.144226	1.170841	-0.924666
3	6	0	3.094210	-2.042463	1.592673
4	6	0	3.393228	-2.248684	0.185926
5	6	0	2.553002	-2.210419	-0.893718
6	6	0	3.011756	-2.557886	-2.262690
7	6	0	4.243285	-2.924432	-2.792811
8	6	0	4.311480	-3.207230	-4.160462
9	6	0	3.175743	-3.129350	-4.973845
10	6	0	1.938442	-2.763021	-4.438015
11	6	0	1.883609	-2.480176	-3.080742
12	6	0	0.772711	-2.053503	-2.205032
13	6	0	-1.500756	-1.226255	-2.437819
14	6	0	-2.864999	-1.682401	-2.778243
15	6	0	-3.351158	-2.903389	-3.223384
16	6	0	-4.725754	-3.011016	-3.448494
17	6	0	-5.571919	-1.917001	-3.237281
18	6	0	-5.070039	-0.688394	-2.797875
19	6	0	-3.702945	-0.586436	-2.566359
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21	6	0	-3.299004	1.796570	-1.922969
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23	6	0	3.405540	1.783406	-1.441348
24	6	0	3.617412	1.956158	-0.015219
25	6	0	2.705954	1.954674	1.006389
26	6	0	3.100375	2.211810	2.414941
27	6	0	4.321560	2.438943	3.038474
28	6	0	4.321522	2.670022	4.417446
29	6	0	3.130168	2.679440	5.150497
30	6	0	1.903546	2.453087	4.521028
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32	6	0	0.833427	1.929050	2.191073
33	6	0	-1.528323	1.321423	2.297600
34	6	0	-2.853232	1.922476	2.561818
35	6	0	-3.230647	3.195960	2.962550
36	6	0	-4.595494	3.447369	3.122487
37	6	0	-5.539001	2.440089	2.892516
38	6	0	-5.146598	1.157396	2.498087
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40	6	0	-3.008191	-0.295469	1.955667
41	6	0	-3.606486	-1.512443	1.750790
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45	7	0	-1.523080	0.066512	-2.035330
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47	7	0	-0.427489	1.976493	2.558789
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55	1	0	5.261797	-3.493183	-4.598490
56	1	0	3.258701	-3.358120	-6.030849
57	1	0	1.050816	-2.703540	-5.057863
58	1	0	-2.685432	-3.742817	-3.390390
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68	1	0	-2.490732	3.967673	3.143129
69	1	0	-4.929432	4.432442	3.429904
70	1	0	-6.593528	2.657691	3.025011
71	1	0	-5.892829	0.388365	2.329974
72	1	0	-4.685976	-1.508060	1.820509
73	6	0	4.234317	-2.135187	2.568455
74	6	0	5.574310	-1.926207	2.210322
75	6	0	3.930771	-2.413579	3.909388
76	6	0	6.582490	-1.998858	3.168743
77	1	0	5.840282	-1.677184	1.189870
78	6	0	4.938475	-2.502382	4.862298
79	1	0	2.894207	-2.561269	4.186975
80	6	0	6.268881	-2.294599	4.494292
81	1	0	7.613220	-1.823524	2.879078
82	1	0	4.688745	-2.731381	5.893007
83	1	0	7.056317	-2.359564	5.238008
84	6	0	-3.890260	-4.001331	1.408232
85	6	0	-3.439281	-5.120848	0.693508
86	6	0	-5.129405	-4.073902	2.060884
87	6	0	-4.213271	-6.272680	0.613875
88	1	0	-2.475809	-5.067981	0.201280
89	6	0	-5.897643	-5.234094	1.994869
90	1	0	-5.491109	-3.239783	2.650497
91	6	0	-5.446018	-6.333000	1.266013
92	1	0	-3.856020	-7.125661	0.046291
93	1	0	-6.848052	-5.279876	2.516179
94	1	0	-6.048833	-7.233505	1.209801
95	6	0	-3.332791	4.286807	-1.478269
96	6	0	-2.657170	5.498288	-1.687179
97	6	0	-4.684004	4.325606	-1.104953
98	6	0	-3.316934	6.713736	-1.548108
99	1	0	-1.610295	5.467528	-1.964017
100	6	0	-5.341019	5.544127	-0.949721
101	1	0	-5.226033	3.409575	-0.902539
102	6	0	-4.662637	6.740194	-1.178052
103	1	0	-2.783459	7.641652	-1.726153
104	1	0	-6.383128	5.558235	-0.648224
105	1	0	-5.178094	7.688315	-1.064772

106	6	0	4.601791	1.908687	-2.343562
107	6	0	5.746166	2.646889	-2.007950
108	6	0	4.546830	1.282652	-3.597886
109	6	0	6.807984	2.751946	-2.903400
110	1	0	5.806063	3.171651	-1.061777
111	6	0	5.614025	1.372825	-4.483718
112	1	0	3.657492	0.723102	-3.860845
113	6	0	6.748589	2.109454	-4.138951
114	1	0	7.680592	3.338498	-2.636011
115	1	0	5.562033	0.871296	-5.444365
116	1	0	7.579973	2.185742	-4.832041

Table S3. Crystal data and structure refinement for **2a**.

Identification code	**2a**	
Empirical formula	C57 H36 Ag2 N6 O5 S4	
Formula weight	1228.90	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.2065(8) Å	a= 69.848(3)°.
	b = 14.1626(10) Å	b= 85.511(3)°.
	c = 16.1136(11) Å	g = 87.425(3)°.
Volume	2393.1(3) $Å^3$	
Z	2	
Density (calculated)	1.705 Mg/m^3	
Absorption coefficient	1.054 mm^{-1}	
F(000)	1236	
Crystal size	0.082 x 0.055 x 0.032 mm^3	
Theta range for data collection	2.340 to 27.590°.	
Index ranges	-14<=h<=14, -18<=k<=18, -20<=l<=20	
Reflections collected	65682	
Independent reflections	11041 [R(int) = 0.1058]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6678	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11041 / 0 / 671	
Goodness-of-fit on F^2	1.028	

Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.1286
R indices (all data)	R1 = 0.1032, wR2 = 0.1482
Extinction coefficient	n/a
Largest diff. peak and hole	2.176 and -1.057 e.Å^{-3}

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	3078(1)	2340(1)	3789(1)	22(1)
Ag(2)	4802(1)	3939(1)	3080(1)	23(1)
C(1)	2618(6)	1168(5)	8275(4)	30(1)
C(2)	3771(6)	835(5)	8350(4)	39(2)
S(1A)	2217(1)	1569(1)	7224(1)	31(1)
C(3A)	4408(6)	900(4)	7525(3)	51(2)
C(3B)	2217(1)	1569(1)	7224(1)	31(1)
S(1B)	4408(6)	900(4)	7525(3)	51(2)
C(4)	3597(5)	1277(4)	6833(4)	21(1)
C(5)	3798(5)	1447(4)	5890(3)	20(1)
C(6)	4956(5)	1113(4)	5600(3)	20(1)
C(7)	5387(4)	1196(4)	4770(3)	17(1)
C(8)	6594(4)	805(4)	4591(3)	18(1)
C(9)	7470(5)	282(4)	5138(4)	22(1)
C(10)	8491(5)	-13(4)	4745(4)	27(1)
C(11)	8649(5)	231(4)	3829(4)	27(1)
C(12)	7772(5)	755(4)	3283(4)	23(1)
C(13)	6735(5)	1028(4)	3679(4)	21(1)
C(14)	5615(5)	1533(4)	3325(3)	19(1)
C(15)	4775(4)	2495(4)	1952(3)	19(1)
C(16)	4174(5)	2378(4)	1209(3)	19(1)
C(17)	4015(5)	1546(4)	970(4)	27(1)
C(18)	3382(5)	1687(4)	236(4)	28(1)
C(19)	2941(6)	2623(4)	-252(4)	30(1)
C(20)	3098(5)	3456(4)	-8(4)	26(1)
C(21)	3720(4)	3314(4)	735(3)	18(1)
C(22)	4068(4)	4010(4)	1181(3)	18(1)
C(23)	3800(5)	5010(4)	878(4)	22(1)
C(24)	4102(5)	5759(4)	1241(4)	25(1)

C(25)	3655(5)	6795(4)	809(4)	30(1)
C(26)	3121(5)	7235(4)	5(4)	31(1)
C(27)	2872(6)	8264(5)	-155(6)	49(2)
C(28)	3187(7)	8572(5)	496(6)	58(2)
C(29)	10007(5)	2465(5)	5168(5)	35(2)
C(30)	9460(6)	2466(6)	5947(5)	49(2)
C(31)	8223(5)	2717(5)	5900(4)	35(2)
C(32)	7859(5)	2931(4)	5056(4)	20(1)
C(33)	6698(4)	3278(4)	4693(4)	19(1)
C(34)	5748(5)	3476(4)	5294(3)	19(1)
C(35)	4623(5)	3808(4)	5136(3)	19(1)
C(36)	3755(5)	3986(4)	5816(4)	20(1)
C(37)	3873(5)	3928(4)	6676(4)	24(1)
C(38)	2876(5)	4195(4)	7127(4)	27(1)
C(39)	1818(5)	4508(4)	6722(4)	30(1)
C(40)	1700(5)	4573(4)	5850(4)	26(1)
C(41)	2699(5)	4317(4)	5402(4)	21(1)
C(42)	2929(5)	4348(4)	4491(4)	20(1)
C(43)	1835(4)	4509(4)	3210(4)	20(1)
C(44)	1251(4)	5237(4)	2452(4)	20(1)
C(45)	1014(5)	6258(4)	2221(4)	27(1)
C(46)	422(5)	6730(4)	1456(4)	34(2)
C(47)	79(5)	6193(4)	938(4)	33(1)
C(48)	320(5)	5177(4)	1174(4)	28(1)
C(49)	923(5)	4704(4)	1937(3)	20(1)
C(50)	1306(5)	3644(4)	2382(3)	20(1)
C(51)	1078(5)	2894(4)	2065(4)	22(1)
C(52)	1328(5)	1848(4)	2427(4)	25(1)
C(53)	975(5)	1191(4)	1935(4)	26(1)
C(54A)	178(4)	1452(4)	1184(3)	42(2)
S(4A)	1509(2)	-10(1)	2262(2)	40(1)
S(4B)	178(4)	1452(4)	1184(3)	42(2)
C(54B)	1509(2)	-10(1)	2262(2)	40(1)
C(55)	158(7)	527(6)	979(5)	48(2)
C(56)	802(6)	-264(6)	1500(6)	50(2)
C(57)	2162(6)	6497(6)	8047(5)	46(2)
N(1)	4846(4)	1614(3)	3979(3)	18(1)
N(2)	5380(4)	1753(3)	2482(3)	24(1)
N(3)	4692(4)	3464(3)	1920(3)	20(1)
N(4)	4057(4)	4060(3)	4334(3)	19(1)

N(5)	2156(4)	4774(3)	3852(3)	25(1)
N(6)	1858(4)	3577(3)	3138(3)	18(1)
O(5)	2779(4)	5793(4)	8673(3)	50(1)
O(1)	2991(3)	1850(3)	5402(2)	25(1)
O(2)	4717(5)	5592(3)	1880(3)	42(1)
O(3)	6570(3)	3390(3)	3917(2)	26(1)
O(4)	1825(4)	1424(3)	3131(3)	38(1)
S(2)	3809(2)	7648(1)	1330(1)	50(1)
S(3)	9033(1)	2792(1)	4350(1)	33(1)

Table S5. Bond lengths [Å] and angles [°] for **2a**.

Ag(1)-N(1)	2.184(4)
Ag(1)-N(6)	2.187(4)
Ag(1)-O(1)	2.443(4)
Ag(1)-O(4)	2.473(4)
Ag(1)-Ag(2)	2.9043(6)
Ag(2)-N(4)	2.184(4)
Ag(2)-N(3)	2.208(4)
Ag(2)-O(3)	2.430(4)
Ag(2)-O(2)	2.473(4)
C(1)-C(2)	1.356(9)
C(1)-C(3B)	1.681(6)
C(1)-S(1A)	1.681(6)
C(1)-H(1)	0.9500
C(2)-S(1B)	1.434(8)
C(2)-C(3A)	1.434(8)
C(2)-H(2)	0.9500
S(1A)-C(4)	1.712(6)
C(3A)-C(4)	1.434(8)
C(3A)-H(3AA)	0.9500
C(3B)-C(4)	1.712(6)
C(3B)-H(3BA)	0.9500
S(1B)-C(4)	1.434(8)
C(4)-C(5)	1.455(7)
C(5)-O(1)	1.232(6)
C(5)-C(6)	1.459(7)

C(6)-C(7)	1.354(7)
C(6)-H(6)	0.9500
C(7)-N(1)	1.383(6)
C(7)-C(8)	1.484(7)
C(8)-C(9)	1.381(7)
C(8)-C(13)	1.390(7)
C(9)-C(10)	1.382(8)
C(9)-H(9)	0.9500
C(10)-C(11)	1.393(8)
C(10)-H(10)	0.9500
C(11)-C(12)	1.383(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.386(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.470(7)
C(14)-N(2)	1.329(7)
C(14)-N(1)	1.342(7)
C(15)-N(2)	1.305(7)
C(15)-N(3)	1.354(7)
C(15)-C(16)	1.479(7)
C(16)-C(21)	1.380(7)
C(16)-C(17)	1.381(7)
C(17)-C(18)	1.378(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.380(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(8)
C(19)-H(19)	0.9500
C(20)-C(21)	1.383(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.486(7)
C(22)-C(23)	1.357(7)
C(22)-N(3)	1.397(6)
C(23)-C(24)	1.440(7)
C(23)-H(23)	0.9500
C(24)-O(2)	1.233(7)
C(24)-C(25)	1.474(8)
C(25)-C(26)	1.399(9)
C(25)-S(2)	1.713(6)
C(26)-C(27)	1.409(9)

C(26)-H(26)	0.9500
C(27)-C(28)	1.343(12)
C(27)-H(27)	0.9500
C(28)-S(2)	1.689(9)
C(28)-H(28)	0.9500
C(29)-C(30)	1.353(10)
C(29)-S(3)	1.704(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.417(8)
C(30)-H(30)	0.9500
C(31)-C(32)	1.379(8)
C(31)-H(31)	0.9500
C(32)-C(33)	1.463(7)
C(32)-S(3)	1.719(5)
C(33)-O(3)	1.224(6)
C(33)-C(34)	1.466(7)
C(34)-C(35)	1.338(7)
C(34)-H(34)	0.9500
C(35)-N(4)	1.411(7)
C(35)-C(36)	1.487(7)
C(36)-C(37)	1.377(7)
C(36)-C(41)	1.386(7)
C(37)-C(38)	1.394(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.379(8)
C(38)-H(38)	0.9500
C(39)-C(40)	1.392(8)
C(39)-H(39)	0.9500
C(40)-C(41)	1.386(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.456(7)
C(42)-N(4)	1.342(7)
C(42)-N(5)	1.356(7)
C(43)-N(5)	1.296(7)
C(43)-N(6)	1.363(7)
C(43)-C(44)	1.476(7)
C(44)-C(49)	1.378(7)
C(44)-C(45)	1.382(7)
C(45)-C(46)	1.389(9)
C(45)-H(45)	0.9500

C(46)-C(47)	1.391(9)
C(46)-H(46)	0.9500
C(47)-C(48)	1.376(8)
C(47)-H(47)	0.9500
C(48)-C(49)	1.393(7)
C(48)-H(48)	0.9500
C(49)-C(50)	1.483(7)
C(50)-C(51)	1.370(7)
C(50)-N(6)	1.381(6)
C(51)-C(52)	1.415(8)
C(51)-H(51)	0.9500
C(52)-O(4)	1.248(7)
C(52)-C(53)	1.498(8)
C(53)-S(4B)	1.494(7)
C(53)-C(54A)	1.494(7)
C(53)-C(54B)	1.694(6)
C(53)-S(4A)	1.694(6)
C(54A)-C(55)	1.459(8)
C(54A)-H(54A)	0.9500
S(4A)-C(56)	1.657(8)
S(4B)-C(55)	1.459(8)
C(54B)-C(56)	1.657(8)
C(54B)-H(54B)	0.9500
C(55)-C(56)	1.362(11)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(57)-O(5)	1.359(8)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
O(5)-H(5)	0.8400

N(1)-Ag(1)-N(6)	152.90(16)
N(1)-Ag(1)-O(1)	82.82(14)
N(6)-Ag(1)-O(1)	114.58(14)
N(1)-Ag(1)-O(4)	109.29(15)
N(6)-Ag(1)-O(4)	81.64(15)
O(1)-Ag(1)-O(4)	118.18(14)
N(1)-Ag(1)-Ag(2)	73.78(11)
N(6)-Ag(1)-Ag(2)	81.00(11)

O(1)-Ag(1)-Ag(2)	107.14(9)
O(4)-Ag(1)-Ag(2)	134.66(11)
N(4)-Ag(2)-N(3)	151.58(16)
N(4)-Ag(2)-O(3)	81.95(14)
N(3)-Ag(2)-O(3)	116.69(14)
N(4)-Ag(2)-O(2)	110.50(16)
N(3)-Ag(2)-O(2)	79.30(15)
O(3)-Ag(2)-O(2)	121.15(14)
N(4)-Ag(2)-Ag(1)	74.32(11)
N(3)-Ag(2)-Ag(1)	79.51(12)
O(3)-Ag(2)-Ag(1)	106.85(10)
O(2)-Ag(2)-Ag(1)	132.00(11)
C(2)-C(1)-C(3B)	112.9(5)
C(2)-C(1)-S(1A)	112.9(5)
C(2)-C(1)-H(1)	123.6
S(1A)-C(1)-H(1)	123.6
C(1)-C(2)-S(1B)	114.3(6)
C(1)-C(2)-C(3A)	114.3(6)
C(1)-C(2)-H(2)	122.8
C(3A)-C(2)-H(2)	122.8
C(1)-S(1A)-C(4)	92.4(3)
C(4)-C(3A)-C(2)	108.4(5)
C(4)-C(3A)-H(3AA)	125.8
C(2)-C(3A)-H(3AA)	125.8
C(1)-C(3B)-C(4)	92.4(3)
C(1)-C(3B)-H(3BA)	133.8
C(4)-C(3B)-H(3BA)	133.8
C(4)-S(1B)-C(2)	108.4(5)
S(1B)-C(4)-C(5)	129.6(5)
C(3A)-C(4)-C(5)	129.6(5)
S(1B)-C(4)-C(3B)	111.9(4)
C(5)-C(4)-C(3B)	118.5(4)
C(3A)-C(4)-S(1A)	111.9(4)
C(5)-C(4)-S(1A)	118.5(4)
O(1)-C(5)-C(4)	118.5(5)
O(1)-C(5)-C(6)	125.1(5)
C(4)-C(5)-C(6)	116.4(5)
C(7)-C(6)-C(5)	128.8(5)
C(7)-C(6)-H(6)	115.6
C(5)-C(6)-H(6)	115.6

C(6)-C(7)-N(1)	129.2(5)
C(6)-C(7)-C(8)	121.9(5)
N(1)-C(7)-C(8)	109.0(4)
C(9)-C(8)-C(13)	121.3(5)
C(9)-C(8)-C(7)	132.7(5)
C(13)-C(8)-C(7)	106.0(4)
C(8)-C(9)-C(10)	117.5(5)
C(8)-C(9)-H(9)	121.2
C(10)-C(9)-H(9)	121.2
C(9)-C(10)-C(11)	121.4(5)
C(9)-C(10)-H(10)	119.3
C(11)-C(10)-H(10)	119.3
C(12)-C(11)-C(10)	121.0(5)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	117.6(5)
C(11)-C(12)-H(12)	121.2
C(13)-C(12)-H(12)	121.2
C(12)-C(13)-C(8)	121.2(5)
C(12)-C(13)-C(14)	132.7(5)
C(8)-C(13)-C(14)	106.1(4)
N(2)-C(14)-N(1)	126.1(5)
N(2)-C(14)-C(13)	122.6(5)
N(1)-C(14)-C(13)	110.8(4)
N(2)-C(15)-N(3)	128.1(5)
N(2)-C(15)-C(16)	121.3(5)
N(3)-C(15)-C(16)	110.3(4)
C(21)-C(16)-C(17)	121.7(5)
C(21)-C(16)-C(15)	106.6(4)
C(17)-C(16)-C(15)	131.6(5)
C(18)-C(17)-C(16)	117.3(5)
C(18)-C(17)-H(17)	121.3
C(16)-C(17)-H(17)	121.3
C(17)-C(18)-C(19)	121.5(5)
C(17)-C(18)-H(18)	119.2
C(19)-C(18)-H(18)	119.2
C(18)-C(19)-C(20)	121.0(5)
C(18)-C(19)-H(19)	119.5
C(20)-C(19)-H(19)	119.5
C(21)-C(20)-C(19)	117.6(5)

C(21)-C(20)-H(20)	121.2
C(19)-C(20)-H(20)	121.2
C(16)-C(21)-C(20)	120.8(5)
C(16)-C(21)-C(22)	106.4(4)
C(20)-C(21)-C(22)	132.8(5)
C(23)-C(22)-N(3)	128.4(5)
C(23)-C(22)-C(21)	122.7(5)
N(3)-C(22)-C(21)	108.9(4)
C(22)-C(23)-C(24)	127.9(5)
C(22)-C(23)-H(23)	116.0
C(24)-C(23)-H(23)	116.0
O(2)-C(24)-C(23)	124.3(5)
O(2)-C(24)-C(25)	118.2(5)
C(23)-C(24)-C(25)	117.5(5)
C(26)-C(25)-C(24)	130.6(5)
C(26)-C(25)-S(2)	111.6(4)
C(24)-C(25)-S(2)	117.8(5)
C(25)-C(26)-C(27)	110.7(6)
C(25)-C(26)-H(26)	124.7
C(27)-C(26)-H(26)	124.7
C(28)-C(27)-C(26)	113.1(7)
C(28)-C(27)-H(27)	123.4
C(26)-C(27)-H(27)	123.4
C(27)-C(28)-S(2)	113.4(5)
C(27)-C(28)-H(28)	123.3
S(2)-C(28)-H(28)	123.3
C(30)-C(29)-S(3)	111.4(5)
C(30)-C(29)-H(29)	124.3
S(3)-C(29)-H(29)	124.3
C(29)-C(30)-C(31)	113.6(6)
C(29)-C(30)-H(30)	123.2
C(31)-C(30)-H(30)	123.2
C(32)-C(31)-C(30)	111.8(6)
C(32)-C(31)-H(31)	124.1
C(30)-C(31)-H(31)	124.1
C(31)-C(32)-C(33)	130.7(5)
C(31)-C(32)-S(3)	110.8(4)
C(33)-C(32)-S(3)	118.5(4)
O(3)-C(33)-C(32)	119.2(5)
O(3)-C(33)-C(34)	123.8(5)

C(32)-C(33)-C(34)	117.0(5)
C(35)-C(34)-C(33)	129.5(5)
C(35)-C(34)-H(34)	115.3
C(33)-C(34)-H(34)	115.3
C(34)-C(35)-N(4)	128.0(5)
C(34)-C(35)-C(36)	123.5(5)
N(4)-C(35)-C(36)	108.5(4)
C(37)-C(36)-C(41)	121.8(5)
C(37)-C(36)-C(35)	132.0(5)
C(41)-C(36)-C(35)	106.2(5)
C(36)-C(37)-C(38)	117.3(5)
C(36)-C(37)-H(37)	121.4
C(38)-C(37)-H(37)	121.4
C(39)-C(38)-C(37)	121.1(5)
C(39)-C(38)-H(38)	119.5
C(37)-C(38)-H(38)	119.5
C(38)-C(39)-C(40)	121.7(5)
C(38)-C(39)-H(39)	119.2
C(40)-C(39)-H(39)	119.2
C(41)-C(40)-C(39)	117.0(5)
C(41)-C(40)-H(40)	121.5
C(39)-C(40)-H(40)	121.5
C(36)-C(41)-C(40)	121.2(5)
C(36)-C(41)-C(42)	106.5(5)
C(40)-C(41)-C(42)	132.3(5)
N(4)-C(42)-N(5)	124.2(5)
N(4)-C(42)-C(41)	111.9(5)
N(5)-C(42)-C(41)	123.0(5)
N(5)-C(43)-N(6)	129.1(5)
N(5)-C(43)-C(44)	120.9(5)
N(6)-C(43)-C(44)	109.7(4)
C(49)-C(44)-C(45)	121.3(5)
C(49)-C(44)-C(43)	106.6(4)
C(45)-C(44)-C(43)	132.2(5)
C(44)-C(45)-C(46)	117.8(5)
C(44)-C(45)-H(45)	121.1
C(46)-C(45)-H(45)	121.1
C(45)-C(46)-C(47)	121.1(5)
C(45)-C(46)-H(46)	119.5
C(47)-C(46)-H(46)	119.5

C(48)-C(47)-C(46)	120.6(6)
C(48)-C(47)-H(47)	119.7
C(46)-C(47)-H(47)	119.7
C(47)-C(48)-C(49)	118.3(5)
C(47)-C(48)-H(48)	120.8
C(49)-C(48)-H(48)	120.8
C(44)-C(49)-C(48)	120.9(5)
C(44)-C(49)-C(50)	106.7(4)
C(48)-C(49)-C(50)	132.5(5)
C(51)-C(50)-N(6)	128.8(5)
C(51)-C(50)-C(49)	122.4(5)
N(6)-C(50)-C(49)	108.8(4)
C(50)-C(51)-C(52)	129.5(5)
C(50)-C(51)-H(51)	115.3
C(52)-C(51)-H(51)	115.3
O(4)-C(52)-C(51)	125.0(5)
O(4)-C(52)-C(53)	116.8(5)
C(51)-C(52)-C(53)	118.2(5)
S(4B)-C(53)-C(52)	128.1(5)
C(54A)-C(53)-C(52)	128.1(5)
S(4B)-C(53)-C(54B)	114.3(4)
C(52)-C(53)-C(54B)	117.6(4)
C(54A)-C(53)-S(4A)	114.3(4)
C(52)-C(53)-S(4A)	117.6(4)
C(55)-C(54A)-C(53)	103.7(5)
C(55)-C(54A)-H(54A)	128.1
C(53)-C(54A)-H(54A)	128.1
C(56)-S(4A)-C(53)	92.2(4)
C(55)-S(4B)-C(53)	103.7(5)
C(56)-C(54B)-C(53)	92.2(4)
C(56)-C(54B)-H(54B)	133.9
C(53)-C(54B)-H(54B)	133.9
C(56)-C(55)-C(54A)	115.6(6)
C(56)-C(55)-S(4B)	115.6(6)
C(56)-C(55)-H(55)	122.2
C(54A)-C(55)-H(55)	122.2
C(55)-C(56)-S(4A)	114.2(5)
C(55)-C(56)-C(54B)	114.2(5)
C(55)-C(56)-H(56)	122.9
S(4A)-C(56)-H(56)	122.9

O(5)-C(57)-H(57A)	109.5
O(5)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
O(5)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(14)-N(1)-C(7)	108.1(4)
C(14)-N(1)-Ag(1)	124.8(3)
C(7)-N(1)-Ag(1)	127.0(3)
C(15)-N(2)-C(14)	131.6(5)
C(15)-N(3)-C(22)	107.8(4)
C(15)-N(3)-Ag(2)	124.1(3)
C(22)-N(3)-Ag(2)	123.4(3)
C(42)-N(4)-C(35)	107.0(4)
C(42)-N(4)-Ag(2)	125.3(3)
C(35)-N(4)-Ag(2)	127.7(3)
C(43)-N(5)-C(42)	131.8(5)
C(43)-N(6)-C(50)	108.2(4)
C(43)-N(6)-Ag(1)	125.4(3)
C(50)-N(6)-Ag(1)	123.0(3)
C(57)-O(5)-H(5)	109.5
C(5)-O(1)-Ag(1)	126.9(3)
C(24)-O(2)-Ag(2)	123.0(4)
C(33)-O(3)-Ag(2)	129.0(3)
C(52)-O(4)-Ag(1)	122.5(4)
C(28)-S(2)-C(25)	91.2(4)
C(29)-S(3)-C(32)	92.4(3)