Supplementary Materials: Synthesis of New Polyether Ether Ketone Derivatives with Silver Binding Site and Coordination Compounds of Their Monomers with Different Silver Salts

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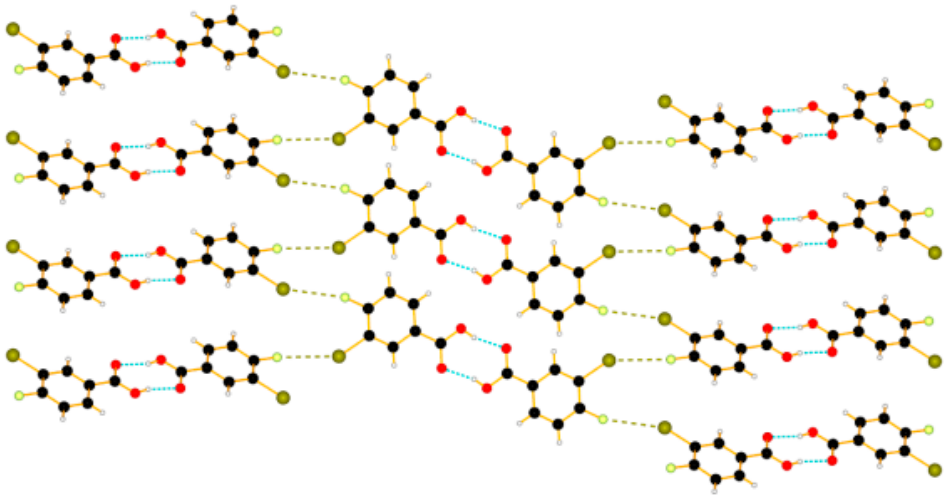

Figure S1. Packing structure of compound **2**.

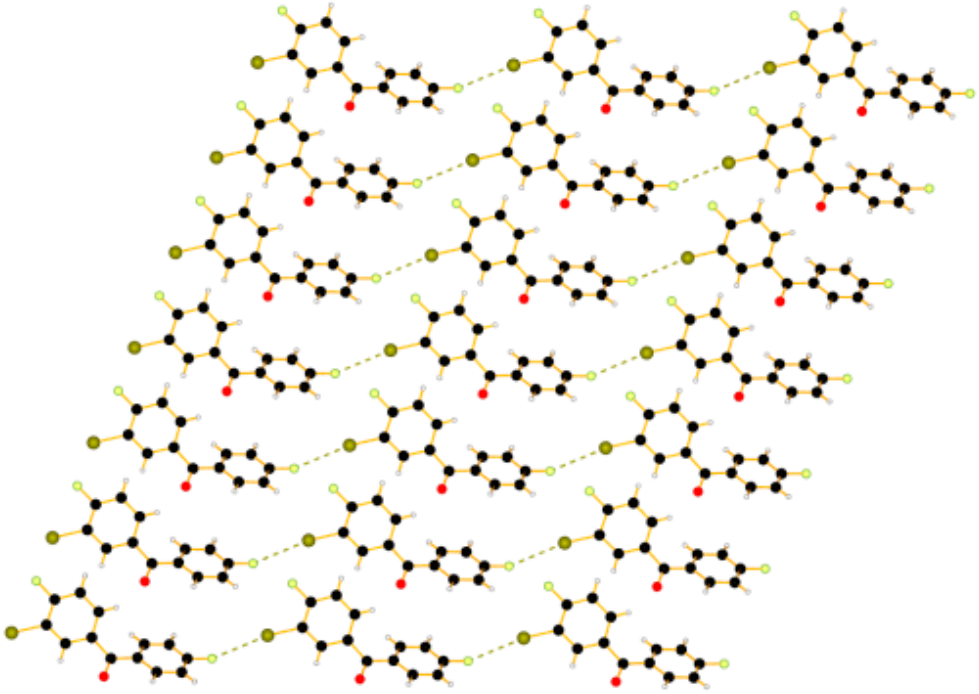

Figure S2. Packing structure of compound **3**.

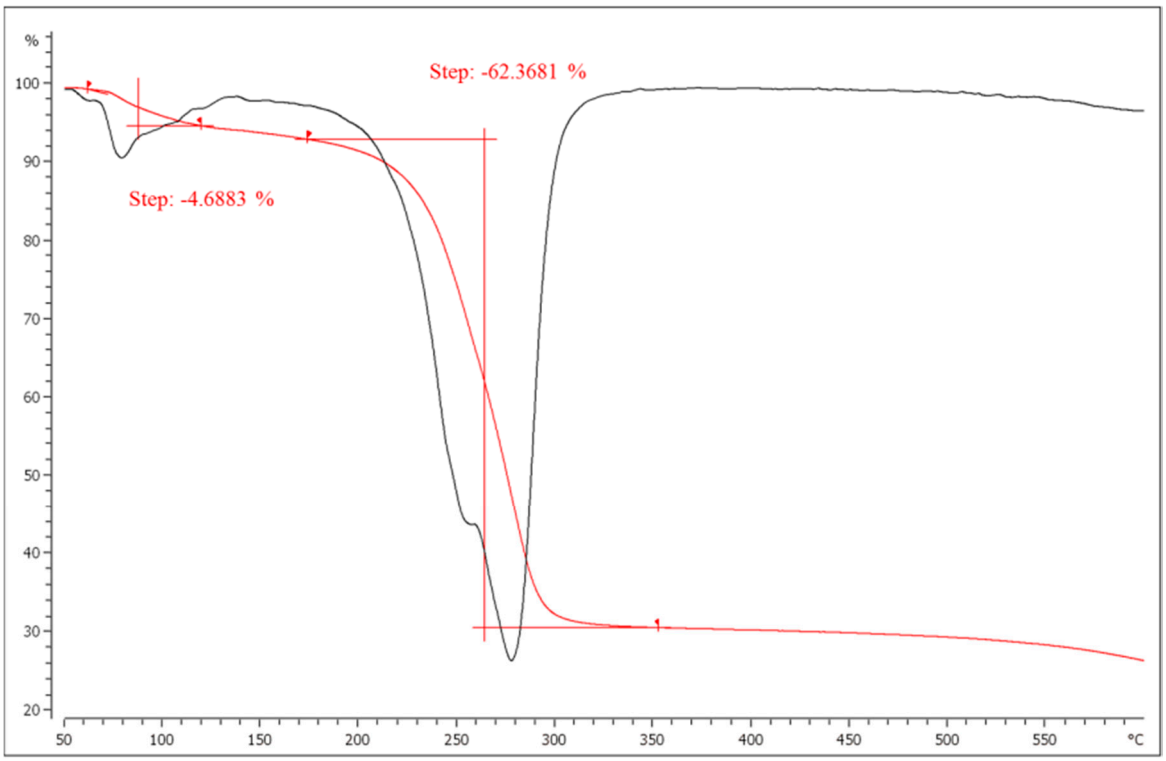

Figure S3. TGA of compound **4b**.

Table S1. Crystal data and structures refinement for X-ray structures.

Compound	**2**	**3**	**4**	**4a**	**4b**	**5a**
CCDC number	CCDC-1411840	CCDC-1411841	CCDC-1411842	CCDC-1411843	CCDC-1411844	CCDC-1411845
Empirical formula	$C_7H_4BrFO_2$	$C_{13}H_7BrF_2O$	$C_{18}H_{11}F_2NO$	$C_{37}H_{18}AgF_7N_2O_5S$	$C_{37}H_{25}AgF_4N_2O_3$	$C_{37}H_{26}AgF_4N_3O_6$
Formula weight (g·mol^{-1})	219.01	297.10	295.28	843.47	729.46	792.48
Temperature	200(2) K	200(2) K	200(2) K	200(2) K	200(2) K	200(2) K
Wavelength	0.71073 Å	1.54186 Å	0.71073 Å	0.71073 Å	1.54186 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P* 2$_1$/n	*P*2$_1$/c	*P* 2$_1$/c	*C* 2/c	*P* 2$_1$/c	*P* 2$_1$/n
Unit cell dimensions	*a* = 4.6710(10) Å *b* = 5.8829(13) Å *c* = 26.760(5) Å β = 93.320(17)°	*a* = 6.2091(8) Å *b* = 14.4523(13) Å *c* = 12.2712(13) Å β = 93.510(10)°	*a* = 14.5724(8) Å *b* = 12.5173(14) Å *c* = 7.5171(15) Å β = 101.958(8)°	*a* = 38.964(3) Å *b* = 7.9942(5) Å *c* = 23.6965(14) Å β = 113.452(4)°	*a* = 24.301(2) Å *b* = 3.8259(3) Å *c* = 34.880(3) Å β = 92.941(7)°	*a* = 7.5262(4) Å *b* = 12.1802(4) Å *c* = 35.5300(17) Å β = 96.000(4)°
Volume	734.1(3) Å^3	1,099.1(2) Å^3	1,341.4(3) Å^3	6,771.3(7) Å^3	3,238.6(5) Å^3	3,239.2(3) Å^3
Z	4	4	4	8	4	4
Density (calculated) (Mg/m^3)	1.982	1.795	1.462	1.655	1.496	1.625
F(000)	424	584	608	3,360	1,472	1,600
Crystal size (mm^3)	0.2 × 0.07 × 0.05	0.25 × 0.05 × 0.03	0.180 × 0.120 × 0.050	0.220 × 0.10 × 0.030	0.36 × 0.04 × 0.02	0.250 × 0.117 × 0.040
Theta range for data collection	3.05° to 25.00°	4.73° to 62.72°	1.43° to 25.00°	1.76° to 25.00°	1.82° to 55.00°	1.77° to 25.00°
Index ranges	$-5 \le h \le 5$ $-6 \le k \le 6$ $-31 \le l \le 31$	$-6 \le h \le 6$ $0 \le k \le 16$ $0 \le l \le 14$	$-17 \le h \le 17$ $-14 \le k \le 14$ $-8 \le l \le 8$	$-46 \le h \le 46$ $-9 \le k \le 9$ $-27 \le l \le 28$	$-22 \le h \le 25$ $-3 \le k \le 4$ $-37 \le l \le 37$	$-8 \le h \le 8$ $-14 \le k \le 14$ $-42 \le l \le 42$
Reflections collected	7,325	1,563	16,600	63,084	20,891	38,973
Independent reflections	1,271 [*R*(int) = 0.1760]	1,563 [*R*(int) = 0.000]	2,346 [*R*(int) = 0.1828]	5,917 [*R*(int) = 0.1197]	4,025 [*R*(int) = 0.0952]	5,551 [*R*(int) = 0.0775]
Absorption correction	Empirical	Integration	None	None	Integration	Integration
Max. and min. transmission	0.7245 and 0.2754	0.9943 and 0.8995	/	/	0.7674 and 0.2321	0.9420 and 0.8631
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	1,271/0/101	1,563/0/154	2,346/0/199	5,917/0/505	4,025/0/425	5,551/0/443
Goodness-of-fit on F^2	1.140	0.990	1.021	1.037	0.981	1.055
Final *R* indices [I > 2σ(I)]	*R*1 = 0.0755 *wR*2 = 0.1412	*R*1 = 0.0464 *wR*2 = 0.1118	*R*1 = 0.0700 *wR*2 = 0.1392	*R*1 = 0.0711 *wR*2 = 0.1836	*R*1 = 0.0778 *wR*2 = 0.2226	*R*1 = 0.0987 *wR*2 = 0.2496
R indices (all data)	*R*1 = 0.0898 *wR*2 = 0.1478	*R*1 = 0.0799 *wR*2 = 0.1274	*R*1 = 0.1168 *wR*2 = 0.1565	*R*1 = 0.0955 *wR*2 = 0.1981	*R*1 = 0.0944 *wR*2 = 0.2399	*R*1 = 0.1394 *wR*2 = 0.2752
Largest diff. peak and hole	0.859 and −0.537 e·Å^{-3}	0.506 and −0.531 e·Å^{-3}	0.191 and −0.205 e·Å^{-3}	1.409 and −1.211 e·Å^{-3}	2.482 and −1.217 e·Å^{-3}	0.804 and −1.017 e·Å^{-3}