

## Bioactive Ag(I) coordination complexes as dopants for castor oil plasticized ethylcellulose films

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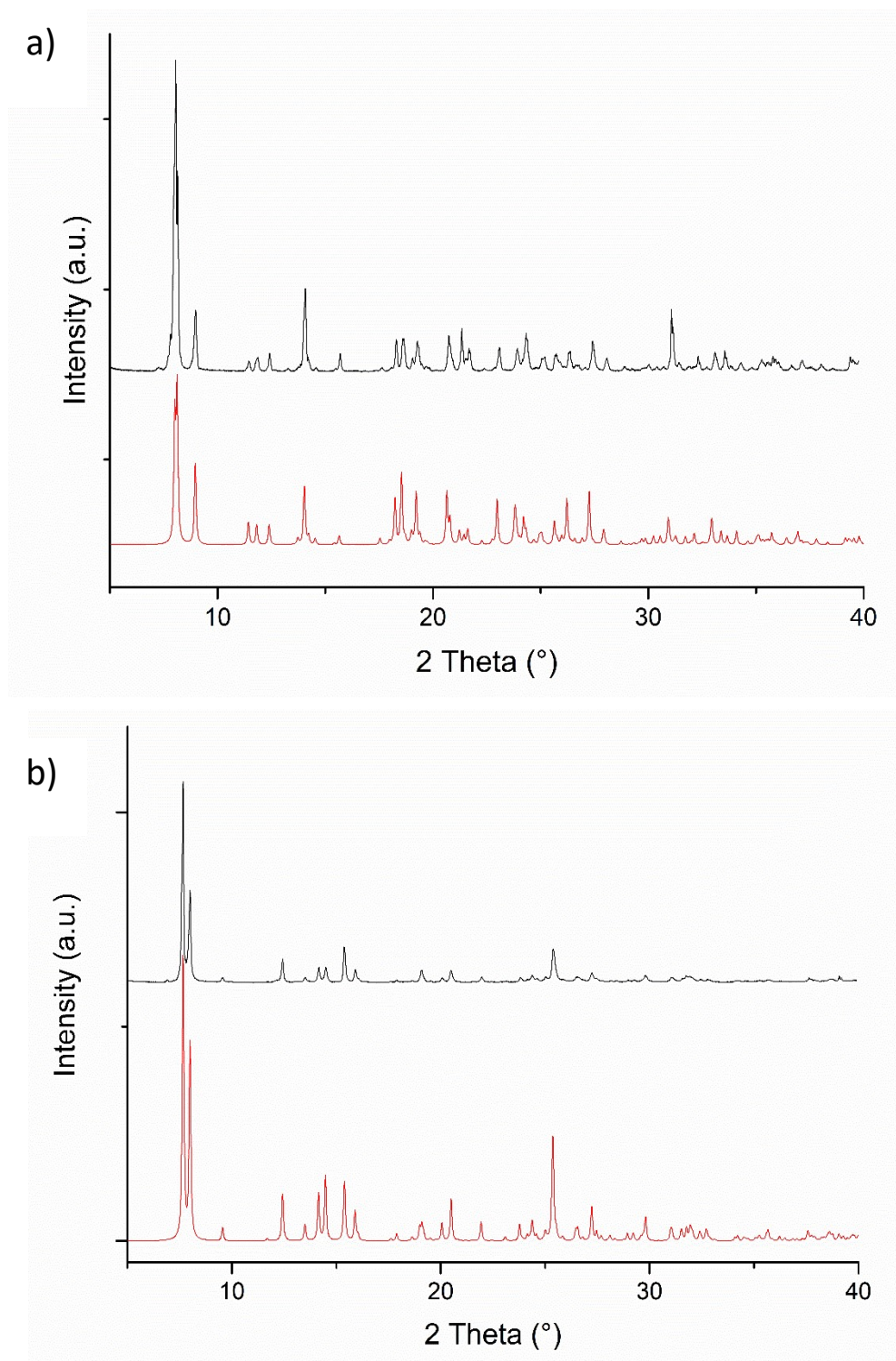
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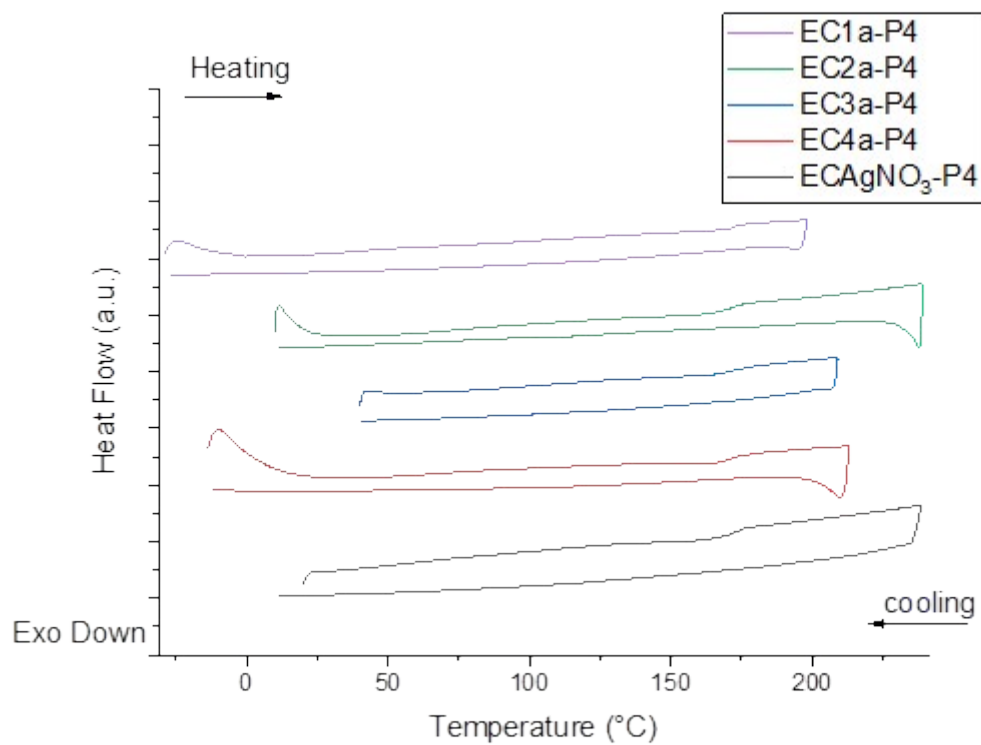
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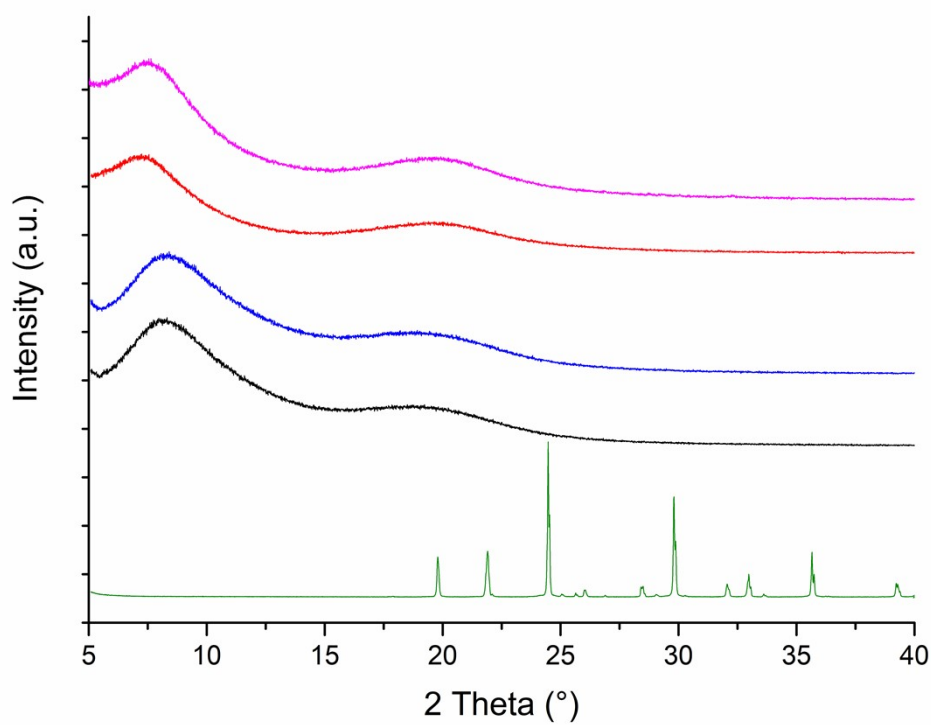
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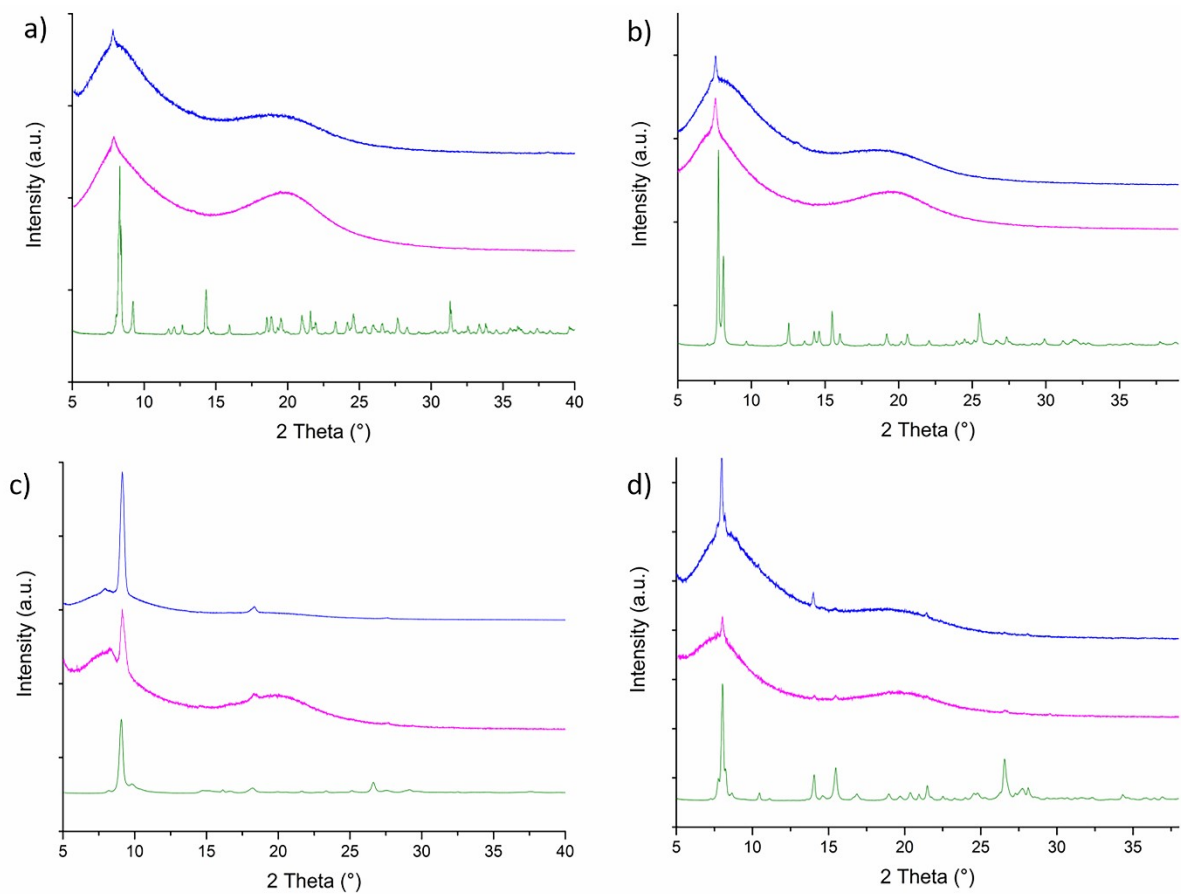
**Figure S1.** Comparison between the PXR D patterns calculated from single crystal data (red lines) and those measured on powder samples (black lines) for complex **1** (a) and complex **2** (b).



**Figure S2.** DSC traces of EC1a-P4 (violet line), EC2a-P4 (green line), EC3a-P4 (blue line), EC-4a (red line) and ECAgNO<sub>3</sub>a-P4 (black line) obtained at a heating rate of 5°C/ min.



**Figure S3.** PXRD pattern of AgNO<sub>3</sub> (green line), EC0 (black line), ECAgNO<sub>3</sub>a (blue line), EC-P4 (red line), ECAgNO<sub>3</sub>a-P4 (pink line).



**Figure S4.** PXRD patterns of a) complex **1**, EC1a, and EC1a-P4; b) complex **2**, EC2a and EC2a-P4; c) complex **3**, EC3a and EC3a-P4; d) complex **4**, EC4a and EC4a-P4. In all patterns: complexes: green lines; ECn-P4 and ECn: pink and blue lines.

**Table S1.** Summary of crystal data and structure refinement for complexes **1** and **2**.

	<b>1</b>	<b>2</b>
Formula	C <sub>21</sub> H <sub>17</sub> F <sub>3</sub> N <sub>5</sub> O <sub>2</sub> Ag	C <sub>18</sub> H <sub>19</sub> F <sub>3</sub> N <sub>5</sub> O <sub>2</sub> Ag
<i>F<sub>w</sub></i> / g mol <sup>-1</sup>	536.27	839.06
<i>T</i> /K	298	298
Crystal system	Monoclinic	Triclinic
Space group	<i>C2/c</i>	<i>P</i> -1
<i>a</i> /Å	25.799(5)	7.7583(10)
<i>b</i> /Å	12.7842(17)	11.6991(15)
<i>c</i> /Å	15.510(4)	11.9243(15)
<i>α</i> /°		104.268(6)
<i>β</i> /°	122.528(14)	91.117(6)
<i>γ</i> /°		102.264(6)
<i>V</i> /Å <sup>3</sup>	4313.0(15)	1022.0(2)
<i>Z</i>	8	2
<i>D<sub>c</sub></i> /g cm <sup>-3</sup>	1.652	1.632
<i>F</i> (000)	2144	504
<i>μ</i> (Mo-Kα)/mm <sup>-1</sup>	0.989	1.036
Refl. Collected	86714	43304
Refl. Indep. [ <i>R</i> int]	4112 [0.0285]	4031 [0.0400]
Reflec. Obs. [ <i>I</i> >2σ( <i>I</i> )]	3638	3089
Restraints/parameters	0 / 290	0 / 264
<i>G</i> OO <i>F</i>	1.070	1.001
<i>R</i> <sub>1</sub> [ <i>I</i> >2σ( <i>I</i> )] (all)	0.0280 (0.0702)	0.0320 (0.0749)
<i>wR</i> <sub>2</sub> [ <i>I</i> >2σ( <i>I</i> )] (all)	0.0328 (0.0746)	0.0499 (0.0843)
Largest diff. peak/hole /eÅ <sup>-3</sup>	0.534, -0.899	0.408, -0.322

**Table S2.** Mechanical properties of ECnx-P4 films.

Sample	Young Modulus (MPa)	Elongation at break (%)	Stress (MPa)
EC-P4	180 ± 8	18,6 ± 0,7	8,9 ± 0,5
EC1a-P4	292 ± 9	3,2 ± 0,1	6,9 ± 1,7
EC1b-P4	263 ± 10	4,8 ± 0,2	8,0 ± 0,9
EC1c-P4	418 ± 13	3,3 ± 0,1	13,3 ± 1,5
EC2a-P4	640 ± 20	4,0 ± 0,2	16,4 ± 1,5
EC2b-P4	418 ± 14	21,0 ± 0,8	18,0 ± 1,6
EC2c-P4	230 ± 9	20,0 ± 0,7	11,1 ± 0,8
EC3a-P4	537 ± 18	7,0 ± 0,3	16,0 ± 1,9
EC3b-P4	482 ± 15	8,0 ± 0,3	13,0 ± 1,5
EC3c-P4	367 ± 10	6,7 ± 0,4	9,4 ± 0,9
EC4a-P4	481 ± 17	6,9 ± 0,3	13,7 ± 1,4
EC4b-P4	474 ± 13	8,0 ± 0,1	13,8 ± 1,8
EC4c-P4	594 ± 19	10,1 ± 0,2	17,5 ± 1,3
ECAgNO <sub>3</sub> a-P4	303 ± 10	16,5 ± 0,6	13,6 ± 0,8
ECAgNO <sub>3</sub> b-P4	229 ± 11	11,0 ± 0,4	10,2 ± 1,2
ECAgNO <sub>3</sub> c-P4	198 ± 11	5,1 ± 0,2	5,7 ± 0,8

**Table S3.** Antibacterial activity of the ECnx-P4 as relative killing percentage (%), according to ISO standard.

	E. Coli (24 h) %
EC0-P4	0
EC1a-P4	100
EC1b-P4	95
EC1c-P4	68
EC2a-P4	100
EC2b-P4	84
EC2c-P4	35
EC3a-P4	100
EC3b-P4	100
EC3c-P4	39
EC4a-P4	100
EC4b-P4	74
EC4c-P4	26
EC-(AgNO <sub>3</sub> )a-P4	100
EC-(AgNO <sub>3</sub> )b-P4	100
EC-(AgNO <sub>3</sub> )c-P4	71

**Table S4.** Antibacterial activity of the ECnx as relative killing percentage (%), according to ISO standard.

	<b>E. Coli (24 h) %</b>
<b>EC0</b>	0
<b>EC1a</b>	100
<b>EC1b</b>	87
<b>EC1c</b>	59
<b>EC2a</b>	100
<b>EC2b</b>	75
<b>EC2c</b>	5
<b>EC3a</b>	100
<b>EC3b</b>	70
<b>EC3c</b>	18
<b>EC4a</b>	100
<b>EC4b</b>	99
<b>EC4c</b>	28
<b>EC-(AgNO<sub>3</sub>)a</b>	100
<b>EC-(AgNO<sub>3</sub>)b</b>	100
<b>EC-(AgNO<sub>3</sub>)c</b>	65

**Table S4** Specific Ag(I) migration from EC<sub>n</sub>-P4 square films, expressed in mg L<sup>-1</sup> release in several simulants by heating at 70 °C for 2 hours. Data represent mean of least three independent measurements.

Sample	Simulant A	Simulant B	Simulant C
EC0-P4	0	0	0
EC1a-P4	0.121	2.552	0.681
EC1b-P4	LOQ	LOQ	LOQ
EC1c-P4	LOQ	LOQ	LOQ
EC2a-P4	0.140	0.042	0.182
EC2b-P4	LOQ	LOQ	0.028
EC2c-P4	LOQ	LOQ	LOQ
EC3a-P4	0.891	1.052	1.961
EC3b-P4	0.072	0.092	0.121
EC3c-P4	0.042	0.071	0.082
EC4a-P4	0.912	0.751	1.971
EC4b-P4	0.061	0.071	0.052
EC4c-P4	LOQ	LOQ	LOQ
EC-(AgNO <sub>3</sub> )a-P4	0.581	0.791	0.841
EC-(AgNO <sub>3</sub> )b-P4	0.092	0.062	0.052
EC-(AgNO <sub>3</sub> )c-P4	0.039	0.032	0.015



**Table S5.** Specific Ag(I) migration from ECnx square films, expressed in mg L<sup>-1</sup> release in several simulants by heating at 70 °C for 2 hours. Data represent mean of least three independent measurements.

Sample	Simulant A	Simulant B	Simulant C
EC-0	0	0	0
EC-1a	0.160	3.950	0.408
EC-1b	LOQ	0.027	0.031
EC-1c	LOQ	0.016	0.017
EC-2a	0.240	1.012	0.253
EC-2b	0.031	LOQ	0.039
EC-2c	LOQ	LOQ	LOQ
EC-3a	1.180	0.047	2.100
EC-3b	LOQ	LOQ	LOQ
EC-3c	LOQ	LOQ	0.043
EC-4a	0.870	0.476	1.440
EC-4b	0.044	0.039	0.043
EC-4c	LOQ	LOQ	LOQ
EC-(AgNO <sub>3</sub> )a	0.330	0.186	0.286
EC-(AgNO <sub>3</sub> )b	0.041	LOQ	0.045
EC-(AgNO <sub>3</sub> )c	0.032	LOQ	0.008

**Table S6.** Specific Ag(I) migration from EC<sub>n</sub>-P4 square films, expressed in mg L<sup>-1</sup> release in several simulants by heating at 40 °C for 10 days. Data represent mean of least three independent measurements.

<b>Sample</b>	<b>Simulant A</b>	<b>Simulant B</b>	<b>Simulant C</b>
<b>EC0-P4</b>	0	0	0
<b>EC1a-P4</b>	0.131	0.012	1.651
<b>EC1b-P4</b>	LOQ	LOQ	LOQ
<b>EC1c-P4</b>	LOQ	LOQ	LOQ
<b>EC2a-P4</b>	0.440	0.023	0.815
<b>EC2b-P4</b>	LOQ	LOQ	LOQ
<b>EC2c-P4</b>	LOQ	LOQ	LOQ
<b>EC3a-P4</b>	0.871	2.922	2.722
<b>EC3b-P4</b>	0.061	0.092	0.081
<b>EC3c-P4</b>	0.042	0.052	0.071
<b>EC4a-P4</b>	0.742	1.361	2.872
<b>EC4b-P4</b>	0.081	0.052	0.081
<b>EC4c-P4</b>	0.034	0.032	0.051
<b>EC(AgNO<sub>3</sub>)a-P4</b>	0.881	0.962	1.122
<b>EC(AgNO<sub>3</sub>)b-P4</b>	0.097	0.131	0.452
<b>EC(AgNO<sub>3</sub>)c-P4</b>	0.042	0.072	0.091

**Table S7.** Specific Ag(I) migration from ECnx square films, expressed in mg L<sup>-1</sup> release in several simulants by heating at 40 °C for 10 days. Data represent mean of least three independent measurements.

Sample	Simulant A	Simulant B	Simulant C
EC-0	0	0	0
EC-1a	0.210	0.024	1.790
EC-1b	LOQ	LOQ	LOQ
EC-1c	LOQ	LOQ	LOQ
EC-2a	0.522	0.037	0.998
EC-2b	0.032	0.028	0.028
EC-2c	LOQ	LOQ	LOQ
EC-3a	1.012	2.001	1.640
EC-3b	0.052	0.035	0.046
EC-3c	LOQ	LOQ	LOQ
EC-4a	0.421	1.122	2.275
EC-4b	0.032	0.043	0.051
EC-4c	LOQ	LOQ	LOQ
EC-(AgNO <sub>3</sub> )a	0.532	0.053	0.108
EC-(AgNO <sub>3</sub> )b	0.044	LOQ	0.044
EC-(AgNO <sub>3</sub> )c	0.038	LOQ	0.027