

Summary of data/files

Compound identification

(±)-tris-(4-methylthiazolyl)cyclotriguaiacylene = L

[Ag₁₂(L)₈]·12ReO₄·n(dimethylformamide) = complex 1

[Ag₁₂(L)₈]·12BF₄·n(dimethylformamide) = complex 2

spectra.zip

File	Content
L NMR spectra.pdf	¹ H NMR, ¹ H- ¹ H COSY NMR, HMBC, HMQC, ¹³ C NMR and DEPT-135 spectra for ligand L
L NMR spectra.mnova	Mestrelab Mnova data files
L + AgBF ₄ in DMF.pdf	¹ H NMR for mixture of AgBF ₄ and L in dimethylformamide
L + AgBF ₄ in DMF.mnova	Mestrelab Mnova data files
ESI_MS ligand L.pdf	High resolution electrospray ionisation mass spectrum of ligand L
ESI_MS complex 1.pdf	High resolution electrospray ionisation mass spectrum of complex 1
IR_ligand L.pdf	Infrared spectrum of ligand L
IR_complex 1.pdf	Infrared spectrum of complex 1
IR_complex 2.pdf	Infrared spectrum of complex 2

Crystal.zip

1. X-Ray crystal structure data and refinement files, all readable as text files.

Crystallographic Information Files (prefix.CIF)

Final refinement files (prefix.RES)

Datafiles: Observed and calculated structure factors (prefix.FCF)

Original hkl data before use of SQUEEZE procedure (complex#_presqueeze.hkl)

Compound	Filename prefix
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L·4(H ₂ O)	Lhydrate
L·3(CH ₃ NO ₂)	Lnitro
[Ag ₁₂ (L) ₈]·12ReO ₄ ·n(dimethylformamide)	complex1
[Ag ₁₂ (L) ₈]·12BF ₄ ·n(dimethylformamide)	complex2

2. Powder XRD data readable in Excel

Compound	Filename
1	pXRDcomplex1.xlsx
2	pXRDcomplex2.xlsx

Analysis.zip

File	Content
EDX.pdf	SEM-EDX results for complexes 1 and 2
TGA complex 1.png	Thermal Gravimetric Analysis complex 1
TGA complex 2.png	Thermal Gravimetric Analysis complex 2
EA_Complex 1.pdf	Elemental analysis results complex 1
EA_Complex 2.pdf	Elemental analysis results complex 2
EA_L.pdf	Elemental analysis results L
EA_L HCl.pdf	Elemental analysis results L with HCl contamination