Summary of data/files

Compound identification

(±)-tris(4-[4-methyl-2,2'-bipyridyl]methyl)-cyclotriguaiacylene = L1

(±)-tris(4-[4-methyl-2,2'-bipyridoyl])-cyclotriguaiacylene = L2

(±)-tris(4-[2,2',6',2''-terpyridyl]benzyl)cyclotriguaiacylene = L3

[{$Re(CO)_3Br$}$_3$(L1)] = complex **1**

[{$Re(CO)_3Br$}$_3$(L2)] = complex **2**

[{$Re(CO)_3Br$}$_3$(L3)] = complex **3**

Crystal.zip

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**
L1·(Et_2O)	ligandL1
[{$Re(CO)_3Br$}$_3$(L1)]·n(CH_3NO_2)	complex1_rebpy
[{$Re(CO)_3Br$}$_3$(L3)]·n($SOMe_2$)	complex3_retpy

NMR.zip

NMRspectra.pdf contains processed Nuclear Magnetic Resonance ^{1}H NMR, ^{1}H-^{1}H COSY NMR, ^{13}C NMR spectra for ligand L2, complexes **1**, **2**, **3**.

Compound name.mnova files are corresponding Mestrelab Mnova data files

IR.zip

As recorded Infrared Spectra

MS.zip

Filetype	Content
Compound name MS.pdf	Recorded mass spectra
Assigned MS spectra.pdf	Assigned MS spectra

EA.zip

CHN elemental analysis

Electronic.zip

Electronic spectroscopy.pdf shows absorption spectra, Emission and Excitation Spectra, Lifetime data for ligands and complexes.

Raw data file designations:

L1 – ligand 1; L2-ligand 2; L3 - ligand 3

C1 – complex 1; C2- complex 2; C3 – complex 3

UV – UV absorption data

EE – excitation and emission