

1. Compound codes and abbreviations:

L1 = (\pm)-2,7,12-trimethoxy-3,8,13-*tris*(4-pyridylcarboxy)-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclononene

FL1 = (\pm)-2,7,12-trimethoxy-3,8,13-*tris*(3-fluoro-4-pyridylcarboxy)-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclononene

L2 = (\pm)-2,7,12-trimethoxy-3,8,13-*tris*(methylbenzimidazol-1-yl)-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclononene

CTG = cyclotriguaiacylene

dppp = bis(diphenylphosphino)propane

en = ethylenediamine

OTf = triflate

NO₃ = nitrate

Pd = palladium

Cl = chloride

MeCN/CD₃CN = D₃-acetonitrile

MeNO₂/CD₃NO₂ = D₃-nitromethane

DMSO = D₆-dimethylsulfoxide

CDCl₃ = D₁-chloroform

2. Data Deposited

NMR.zip

NMR data as fid or mnova files for L1, FL1, L2, complexes [Pd₃(dppp)₃(L1)₂] \cdot 6OTf, [Pd₃(dppp)₃(FL1)₂] \cdot 6OTf, starting material [Pd(dppp)(OTf)₂], mixtures of Pd(en)(NO₃)₂ with L1/FL1, mixtures of PdCl₂ with L2.

Xray.zip

L2, L2-CTG, [Pd₃(dppp)₃(FL1)₂] \cdot 6(OTf) and [Pd₃Cl₆(L2)₂]

Final refinement files .res (shelx results file); .hkl data files (pre and post-SQUEEZE); crystallographic information file (.cif) and structure factors (.fcf); raw data and integration details

Powder diffraction pattern for L2-CTG

Analysis.zip

Mass spectra, infrared spectra, CHN analysis