Compound naming schemes

 



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| Filename | Data type | Subfolder | Contents |
| NMR.zip | Nuclear magnetic resonance | Ligands | LazOEt and LazOPr nuclear magnetic resonance raw data and processed files including 1H; 13C; HSQC: HMBC; COSY |
|  |  | Cages | cage C1, C2 and C3 nuclear magnetic resonance raw data and processed files including 1H; 13C; HSQC: HMBC; COSY; DOSY; NOESY |
|  |  | Host-guest studies | cage C1, C2 and C3 and guest SOS or nap nuclear magnetic resonance raw data and processed files including 1H; DOSY; NOESY; ROESY and spreadsheets of 1H chemical shift changes |
| UV.zip | UV-visible (electronic) spectroscopy |  | Excel spreadsheets with UV-visible data (wavelength vs absorption including photoswitching for Laz-OMe; Laz-OEt; Laz-OPr |
| MS.zip | Mass spectrometry |  | Electro-spray mass spectra for Laz-OEt, Laz-OPr, cages C1 and C2; ion-mobility C1 before and after irradiation |
| Xray.zip | Single crystal X-ray diffraction |  | Crystal structures of Laz-OEt and Laz-OPr⋅CHCl3Crystallographic information files with embedded data (name.cif)Datafiles (name.hkl)Final refinement files (name.res)Solvent masks used in refinements |