

# Large meso-Pentafluorophenyl-Substituted Expanded Porphyrins

## Introduction

Porphyrin analogs having five or more pyrrole rings is referred to as a ring-extended porphyrins. They have been found to have a variety of interesting properties diverting from those of porphyrin. Whilst porphyrin has a planar structure, the ring extended porphyrins take on a twisted structure due to both its flexibility and by the presence of hydrogen bonds among NH groups. The flexibility of the structure increases with increasing ring size meaning that structures of these large twisted compound are difficult to predict. Precise structure can only be determined by way of single crystal X-ray structure analysis. The three-dimensional structural of compounds having more than ten pyrrole rings has rarely been reported, because structure analysis of such a huge twisted aromatic compounds are generally cumbersome.

## Measurement and results

Figures 1 and 2 denote the structural formula and diffraction patterns, respectively. As shown in Figure 2, large reciprocal space must be covered when using Cu radiation to achieve high resolution and data completeness simultaneously. Software controlling a Rigaku XtaLAB Synergy uses an advanced data collection strategy routine that generates a series of scans most efficiently covers the reciprocal space by taking crystal orientation and symmetry into account. The shutterless mode of the Hybrid Photon Counting detector eliminates overhead time and errors that exists in conventional integration type X-ray image sensors such as CCD and CMOS based detectors. Figure 3 shows the structure of this ring-expanded porphyrin and Table 1 summaries crystallographic data.

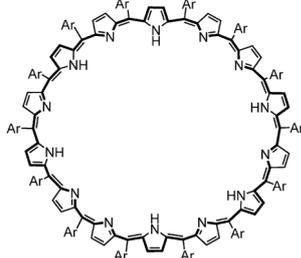


Figure 1. Structural formula of the large expanded porphyrin.

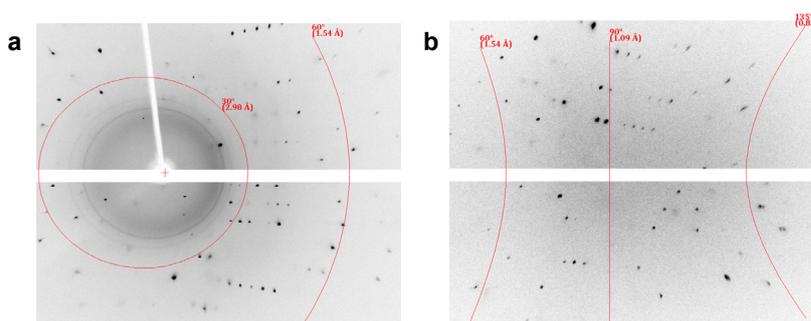


Figure 2. Diffraction images at (a) Low angle and (b) high angle diffraction images.

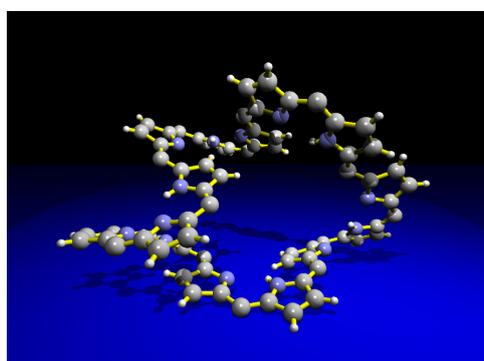


Figure 3. Molecular structure of the large expanded porphyrins. (Pentafluorophenyl groups are not shown for clarity)

Table 1. Crystallographic data

Sample	meso-Pentafluorophenyl-Substituted [62]Tetradecaphyrin(1.1.1.1.1.1.1.1.1.1.1.1)
Formula, MW	C <sub>154</sub> H <sub>36</sub> F <sub>70</sub> N <sub>14</sub> , 3411.96
Space group	<i>P</i> -1
Unit cell	$a = 14.339(2)\text{Å}$ , $b = 18.854(3)\text{Å}$ , $c = 27.328(6)\text{Å}$ $\alpha = 88.026(16)^\circ$ , $\beta = 87.803(19)^\circ$ , $\gamma = 72.875(9)^\circ$
X-ray source	CuK $\alpha$

Samples provided by: Professor Osuka, Kyoto University

Recommended equipment  
 ▶ XtaLAB Synergy series

(P1228en)