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Characterization of normal and inverted sapphyrins and rubyrins

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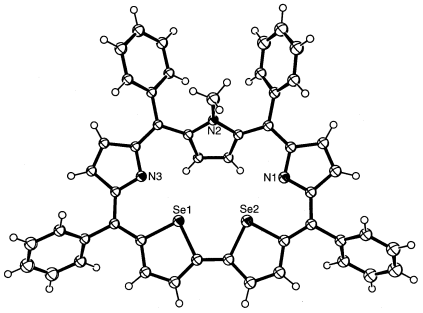
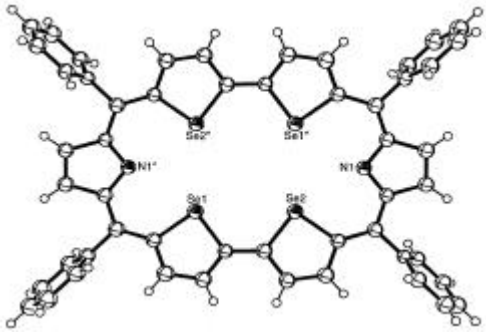
Research on the development of easy and efficient methods for the synthesis of expanded porphyrins, particularly sapphyrins and rubyrins, is receiving attention in view of their diverse applications in Photodynamic Therapy (PDT), as contrasting agents for Magnetic Resonance Imaging (MRI) and as anion receptors. Both sapphyrins and rubyrins show diverse structures [1]. An inverted structure of sapphyrin is characterized by rotation of the heterocyclic ring opposite to bipyrrole/bithiophene/biselenophene unit **1**, while an inverted rubyrin structure shows rotation of both heterocyclic rings connected to two bipyrrole units. The normal structures of sapphyrins and rubyrins do not show any ring inversion. An example of normal rubyrin is shown in **2**. In this work, an attempt has been made to rationalize this structural diversity on the basis of X-ray crystal structural data of both sapphyrins and rubyrins.



1



2

Reference

1. Srinivasan A, Anand V G, Narayanan S J P, Pushpan S K, Kumar M R, Chandrashekar T K, Sugiura K-I and Sakata Y 1999 *J. Org. Chem.* **64** 8693