A New Class of Non-Racemic Chiral Macrocycles: A Conformational and Synthetic Study

Susan E. Gibson,[a] Nello Mainolfi,[a] S. Barret Kalindjian,[b] Paul T. Wright,[b] and Andrew J.P. White[c]

[a] Prof. S.E. Gibson, N. Mainolfi
Department of Chemistry, Imperial College London,
South Kensington Campus, London SW7 2AY (UK)
Fax: (+44) 207 594 5804
E-mail: s.gibson@imperial.ac.uk

[b] Dr S.B. Kalindjian, Dr P.T. Wright
James Black Foundation, 68 Half Moon Lane,
London SE24 9JE (UK)

[c] Dr A.J.P. White
Department of Chemical Crystallography, Imperial College London,
South Kensington Campus, London SW7 2AY (UK)
Supplementary crystallographic data for m$_2$-4v(Bn)p

The crystal structure shows disorder in the C(25) to C(32) region (ring B its adjacent -CH$_2$-CH$_2$- unit). This was resolved into two partial occupancy orientations of ca. 58 and 42% occupancy (shown in Figs S1 and S2 respectively). An overlay of these two orientations is shown in Fig. S3, and clearly shows the different angles of the two positions of the aromatic rings.

**Fig. S1.** The molecular structure of m$_2$-4v(Bn)p showing the major occupancy (ca. 58%) orientation for the "upper" aromatic ring.

**Fig. S2.** The molecular structure of m$_2$-4v(Bn)p showing the minor occupancy (ca. 42%) orientation for the "upper" aromatic ring.

**Fig. S3.** The molecular structure of m$_2$-4v(Bn)p showing an overlay of both the major (filled bonds, ca. 58% occupancy) and minor (open bonds, ca. 42% occupancy) orientations.