

The Janus-like behaviour of sulphur in substituted diquinoline inclusion crystal structures

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SUPPLEMENTARY DATA:

Experimental

¹H NMR data (400 MHz) were recorded using a Bruker instrument. Melting points were measured using a Büchi B-540 instrument, and IR spectra as KBr discs using an Excalibur Series Biorad FTS3000MX.

8,16-Diphenyl-6,7,14,15-tetrahydro-6,14-thiacycloocta[1,2-*b*:5,6-*b'*]diquinoline 9

IR $\nu_{\max}$ 3148, 3057, 1612, 1567, 1556, 1500, 1486, 1440, 1424, 1398, 1356, 1273, 1218, 1156, 1146 cm^{-1} ; ¹H NMR (CDCl_3) δ 3.60 and 3.65 (d, $J_{\text{AB}} = 20$ Hz, 2H), 3.81 and 3.85 (dd, $J_{\text{AB}} = 20$ Hz, $J_{\text{BX}} = 6.4$ Hz, 2H), 6.03 (d, $J = 6.4$ Hz, 2H), 7.11-7.24 (m, 4H), 7.51 (d, $J = 8.4$ Hz, 2H), 7.58-7.69 (m, 8H), 7.96-8.00 (t, 2H), 8.92 (d, $J = 8.8$ Hz, 2H).

7 α ,15 α -Dibromo-8,16-diphenyl-6,7,14,15-tetrahydro-6 α ,14 α -thiacycloocta[1,2-*b*:5,6-*b'*]diquinoline 10

IR $\nu_{\max}$ 3197, 3056, 3022, 2960, 1612, 1566, 1556, 1502, 1485, 1441, 1398, 1352, 1316, 1265, 1233, 1214, 895, 868, 810, 765, 698 cm^{-1} ; ¹H NMR (CD_3SOCD_3) δ 4.88 (d, $J = 3$ Hz, 2H), 5.55 (d, $J = 3$ Hz, 2H), 7.15 (d, $J = 8.4$ Hz, 2H), 7.31-7.35 (t, 2H), 7.40 (d, $J = 7.6$ Hz, 2H), 7.49-7.63 (m, 6H), 7.60-7.63 (t, 2H), 7.82-7.86 (m, 2H), 8.10 (d, $J = 8.4$ Hz, 2H).