Complementary Hydrogen Bonding in a New Tridentate Schiff Base Ligand: X-Ray, DFT, and Solution NMR Studies

Orde Q. Munro,* Sandra D. Strydom, and Craig D. Grimmer

School of Chemical and Physical Sciences, University of Natal, Pietermaritzburg, Private Bag X01, Scottsville, 3209, South Africa. Fax: 27 33 260 5009; Tel: 27 33 260 5009; E-mail: <u>munroo@nu.ac.za</u>



Fig. S1. Stereo view of the unit cell contents of the crystal structure of N-[(1*E*)-1*H*-pyrrol-2-ylmethylene]-benzene-1,2-diamine.



Fig. S2. ¹H NMR spectra of a 10 mg sample of *N*-[(1*E*)-1*H*-pyrrol-2-ylmethylene]benzene-1,2-diamine dissolved in 500 μ L CDCl₃ as a function of the volume of added distilled water. Only the ArNH₂ ($\delta_{\rm H} = 4.16$ ppm) and pyrrole NH proton ($\delta_{\rm H} = 9.7(2)$ ppm) regions of the spectra have been shown for clarity.