1,3,2-Diazaphospha-[3]ferrocenophanes. Molecular Structures and Multinuclear Magnetic Resonance Studies

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

2-Phenoxy-1,3,2-diazaphospha-[3]ferrocenophane and related derivatives (oxide, sulfide, selenide) were prepared, characterized in solution by multinuclear magnetic resonance methods (1D and 2D ^{1}H, ^{13}C, ^{15}N and ^{31}P NMR) and in the solid state by X-ray structural analysis. The conformation of the 2-phenoxy derivative differs from that of the 2-*tert*-butyl compound. For further comparison, 2-R-2,3-dihydro-*1H*-1,3,2-diazaphospha-phenalene derivatives R = ^{t}Bu, PhO were prepared and studied by the same NMR techniques. The molecular structure of a selenide was determined, and together with the NMR evidence, it was concluded that the conformation of these heterocycles is independent of the respective substituent at the phosphorus atom.

Key words: Aminophosphanes, 1,1′-Diaminoferrocene, [3]Ferrocenophanes, NMR Spectroscopy, Crystal Structure