139- Title: ^{31}P-NMR Assignments in Some New Diazaphosphorinanes and Diazaphospholes

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Abstract:

Diazaphosphosphorinanes and diazaphospholes are important classes of phosphoramidate compounds due to their biological significance[1]. We report here the synthesis of some diazaphosphorinanes and benzodiazaphospholes with formula 4-F-$C_6H_4C(O)NHP(O)(NH)_2C_6H_4$ **1**, 4-$CH_3C_6H_4NHP(O)(NH)_2X$; X=C_6H_4 **2**, $C_{10}H_6$ **3**, $CH_2C_6H_4$ **4**, $CH_2C(CH_3)_2CH_2$ **5**. Synthesis of compounds **1-5** were performed by the reaction of 4-F-$C_6H_4C(O)NHP(O)Cl_2$ and 4-$CH_3C_6H_4NHP(O)Cl_2$ with the corresponding diamines. The products were characterized by ^{1}H, ^{1}H{^{31}P}, ^{13}C, ^{31}P, ^{31}P{^{1}H} NMR and IR spectroscopy and elemental analysis. The phosphorus chemical shift $\delta\{^{31}P\}$ of these compounds in the range from -10.39ppm (in **3**) to 13.1ppm (in**1**). ^{31}P nuclei in compounds **1** and **2** (diazaphospholes) are deshieled relative to those of other compounds that is due to the increase of ring size in diamino compounds **3**-**5**. ^{31}P-NMR chemical shift in compound **3** involving the diamino naphthalene group was at lower field as compared to **4** and **5** that involving $CH_2C_6H_4$ and aliphatic diamino groups respectively.

References:

[1] J.D.Boughton, R.D. Brown, R.Bryat, F.J.Burger, and C.M.Combs. ***J.Pharm.Sci.***, 1972, 61, 97.
[2] J.M.A.Al.Rawi, G.Q.Behnam, N.Ayed, and R.Kreamer, ***Magn.Res.Chem.***, 1985, 23, 728.
[3] K.Gholivand, M.Pourayoubi, and Z.Shariatinia, in press, ***Polyhedron.***
[4] K.Gholivand, M.Pourayoubi, S.Farshadian, S.Molani and Z.Shariatinia, ***Analytical Sciences****:* X-ray Structure Analysis Online, 2005, 21(3), x55.