

Syntheses and Spectroscopic Studies of Some New Diazaphospholes and Diazaphosphorinanes. Crystal Structure of 4-F-C₆H₄C(O)N(H)P(O)(NHC₆H₄NH)

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New diazaphospholes and diazaphosphorinanes with formula
4-F-C₆H₄C(O)NHP(O)(NHC₆H₄NH) (**1**), 4-CH₃-C₆H₄NHP(O)(NHC₆H₄NH) (**2**),
4-CH₃-C₆H₄NHP(O)(NHC₁₀H₆NH) (**3**), 4-CH₃-C₆H₄NHP(O)(NHCH₂C₆H₄NH) (**4**),
4-F-C₆H₄C(O)NHP(O)(NHCH₂C₆H₄NH) (**5**), CCl₃C(O)NHP(O)(NHCH₂C₆H₄NH) (**6**)
and 4-CH₃-C₆H₄NHP(O)(NHCH₂C(CH₃)₂CH₂NH) (**7**) were synthesized and characterized by ¹H,
¹³C, ³¹P NMR and IR spectroscopy and elemental analysis. The structure of compound **1** has been
determined by X-ray crystallography. A one-dimensional polymeric chain was observed in the crys-
talline lattice produced by intermolecular -P=O...H-N- and -C=O...H-N-hydrogen bonds. Com-
pounds **1** and **2** contain five-membered rings and show high values for ²J(PNH) and ²J(P,C) cou-
pling constants due to the ring strain. These constants are reduced seriously in compounds with
six-membered rings. In compound **6** with CCl₃C(O)NH moiety, all phosphorus-hydrogen couplings
are zero.

Key words: X-Ray Crystallography, NMR Spectroscopy, Diazaphosphorinane, Diazaphosphole