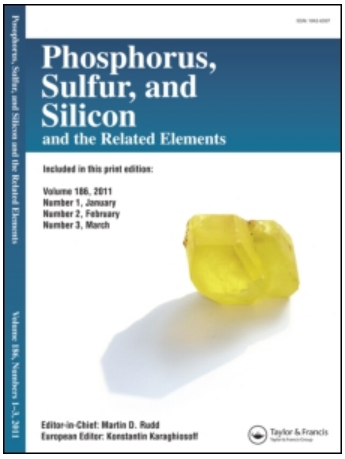

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THE PREPARATION AND PROPERTIES OF SOME NOVEL GUANIDINOPHOSPHONIC ACIDS

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The following poster abstract was omitted between pages 824 and 825, Vol. 30, 3–4 (1987).

ω-Guanidinoalkylaminoalkanephosphonic acids, $(HO)_2P(O)(CH_2)_mNH(CH_2)_nNHC(:NH)NH_2$, have been prepared by reaction of the corresponding ω-amino compounds with *S*-methylisothiouronium chloride in the presence of alkali. The amino compounds were obtained in good yield by reaction of an excess of the corresponding α,ω-diamine $H_2N(CH_2)_nNH_2$ ($n = 2 - 12$) with chloromethanephosphonic acid (or other ω-halogenoalkanephosphonic acid) in water. Reactions were carried out by heating under reflux for 20 hours and the aminophosphonic acids were isolated as dihydrates. In the subsequent reaction with *S*-methylisothiouronium chloride, cyclisation occurred when $n = 2$, leading to the alternative formation of 1-phosphonomethyl-2-iminoimidazolidine. The ω-amino and ω-guanidinophosphonic acids were fully characterised by elemental analysis, ^1H, ^{13}C, and ^{31}P nmr spectroscopy, and by fast atom bombardment mass spectrometry which gave a base peak at $[M + H]^+$ in all cases. The compounds are zwitterionic and show variations in the phosphorus chemical shift and in certain phosphorus-carbon coupling constants according to the acidity of the medium. δ_P values thus fall at 7–8 ppm in D_2O but 13–15 ppm in acid solution, whilst the J_{PC} value for the guanidino derivative ($m = 1$, $n = 8$) is increased from 132.2 to 149.9 upon acidification. Fragmentations in the FAB mass spectra show that initial loss of H_3PO_3 or of ammonia in the case of the amino compounds, and of H_3PO_3 or cyanamide in the case of the guanidines. These new guanidinophosphonic acids show activity against a number of fungal organisms.

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