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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, $(\text{HO})_2\text{P}(\text{O})(\text{CH}_2)_m\text{NH}(\text{CH}_2)_n\text{NHC}(\text{:NH})\text{NH}_2$, have been prepared by reaction of the corresponding ω -amino compounds with *S*-methylisothiuronium 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 $\text{H}_2\text{N}(\text{CH}_2)_n\text{NH}_2$ ($n = 2 - 12$) 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*-methylisothiuronium 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 $[\text{M} + \text{H}]^+$ 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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