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¹H, ¹³C, ³¹P, ¹⁵N, ¹⁷O-NMR Investigations of α-Sub-Stituted Aminophosphonates

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 1 H, 13 C, 31 P, 15 N, 17 O-NMR INVESTIGATIONS OF α -SUB-STITUTED AMINOPHOSPHONATES

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The reaction of aminomethanephosphonates $\underline{1}$ with dimethylsulfate in dioxan leads to the crystalline methosulfates $\underline{2}$ (1). Deprotonation of the salts $\underline{2}$ with aqueous potassium carbonate solution gives the very stable N-ylides $\underline{3}$ (1).

$$(Et0)_{2}P(0)CH-R$$

$$= 1 NMe_{2}$$

$$= (Et0)_{2}P(0)CH-R$$

$$= 1 NMe_{3} MeSO_{4}$$

$$= (Et0)_{2}P(0)$$

$$= 1 EtO$$

$$= 1 CO$$

$$= 1$$

The structures of the compounds 1-3 were unequivocally confirmed by NMR-spectroscopy of all atoms (H, C, P, N, O) contained in the molecule. Owing to the extensive NMR data (chemical shifts and coupling constants) exact statements can also be made now with regard to the charge distribution of the ylides 3. The delocalisation of the negative charge as defined by formula 3 could be unambigously confirmed by detailed NMR investigations in accordance with earlier publications (1).

(1) H. Groß, B. Costisella, Angew. Chem. <u>50</u> (1965) 445 B. Costisella, H. Groß, J. prakt. Chem. <u>324</u> (1982) 545