Remarkably Large ^{15}N, ^{13}C and ^{18}O Isotope NMR Shifts of the Mono-coordinate Phosphorus Atoms in the Compounds $(Me_3Si)^iPrNCP$, $K^+[^iPrNCP]^-$ and KOCP · 2 DME (DME = 1,2-Dimethoxyethane)

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Dedicated to Professor Ekkehard Fluck on the occasion of his 70th birthday

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Aminomethylidynephosphane, Phosphantriylmethylamide, Isotope Shifts

The ^{31}P and ^{13}C NMR spectra of the heteroatom-substituted λ^3-phosphaalkynes (Me_3Si)-^iPrNCP (**1**), $K^+[^iPrNCP]^-$ (**2**) and KOCP · 2 DME (**3**) are described (Me = methyl; ^iPr = isopropyl). In addition, ^{15}N NMR data of **1** and **2** as well as further NMR results of all accessible nuclei of **1** to **3** are reported. The absolute values of the coupling constants $^1J(^{31}P^{13}C)$ of **1**, **2** and **3**, 18.2, 45.7 and 57.2 Hz, respectively, are considerably different; the geminal coupling constants $^2J(^{31}P^{15}N)$ of the first two compounds show a decrease in the reverse order, 15.1 and 3.3 Hz. ^{13}C, ^{29}Si, ^{15}N, and ^{18}O isotope effects on the nuclear shielding of the ^{31}P nucleus in the non isotope-enriched compounds **1**, **2** or **3** are presented and discussed. The [mono-^{13}C]isotopomers of **1**, **2** and **3** exhibit extremely negative $^{31}P^{13}C$ one-bond isotope shifts varying from –211 to –223 ppb. Remarkably, for **1** and **2** large two-bond $^{31}P^{15}N$ isotope shifts of –32 and –84 ppb, respectively, are observed. An unexpectedly large two-bond $^{31}P^{18}O$ isotope effect of –124 ppb was assigned to the [mono-^{18}O]isotopomer of compound **3**. A three-bond $^{31}P^{13}C$ isotope shift of –27 ppb was found in **2**.