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THE ^{14}N QUADRUPOLE BROADENING OF THE HYDRIDE ^{1}H NMR PATTERN IN *trans*-[PtH(NCS)(PEt$_3$)$_2$]

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Summary

One of the sets of hydride ^{1}H NMR patterns for the isothiocyanato/thiocyanato mixture *trans*-[PtH(SCN)(PEt$_3$)$_2$] is broad. Previously there had been disagreement on the cause of this broadening. It is now shown to be due to the ^{14}N quadrupole by double resonance.

In 1965 we showed by NMR spectroscopy that *trans*-[PtH(SCN)(PEt$_3$)$_2$] is present in CDCl$_3$ solution as a mixture of the *S*-bonded (thiocyanato) and *N*-bonded (isothiocyanato) isomers [1]. One set of resonances was broad and

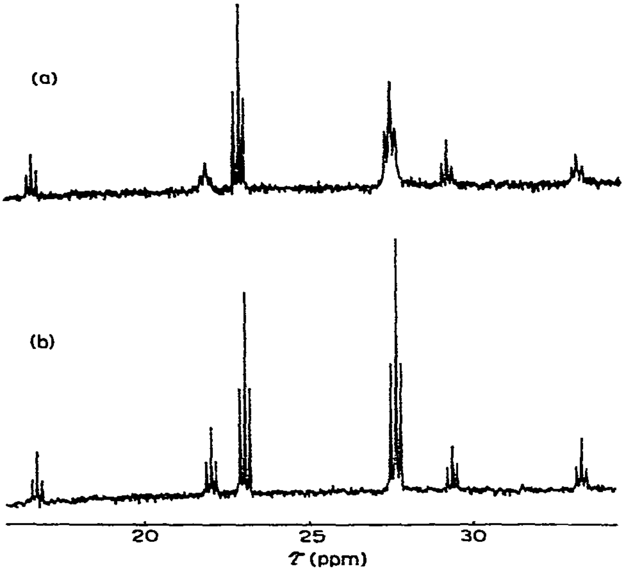

Fig. 1. (a) The hydride ^{1}H NMR patterns for the mixture of *S*- and *N*-bonded isomers of *trans*-[PtH(SCN)-(PEt$_3$)$_2$]. Measured at 99.99429 MHz and ca. 23° in CDCl$_3$. (b) As for (a) with the ^{14}N nuclei decoupled by irradiation at 7.224419 MHz with noise modulation.

the other sharp. The broadening was attributed to coupling with the ^{14}N nucleus which is partially relaxed and this set of resonances was assigned to the *N*-bonded isomer. Our interpretation has been criticised by Adlard and Socrates who attributed the broadening to exchange of triethylphosphine and considered that we had assigned the resonances correctly by a fortunate coincidence [2—4]. Recently Pidcock [5] has presented strong but indirect evidence supporting our interpretation. We have now demonstrated unequivocally by double irradiation that the broadening is due to coupling with the ^{14}N nucleus.

On decoupling the ^{14}N by irradiation at 7.224419 MHz, with noise modulation, the ^{1}H NMR pattern which had been originally broad becomes sharp (as sharp as the other pattern). The spectra were measured at 99.99429 MHz and ca. 23° in $CDCl_3$.

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