

ERRATUM | OCTOBER 01 1976

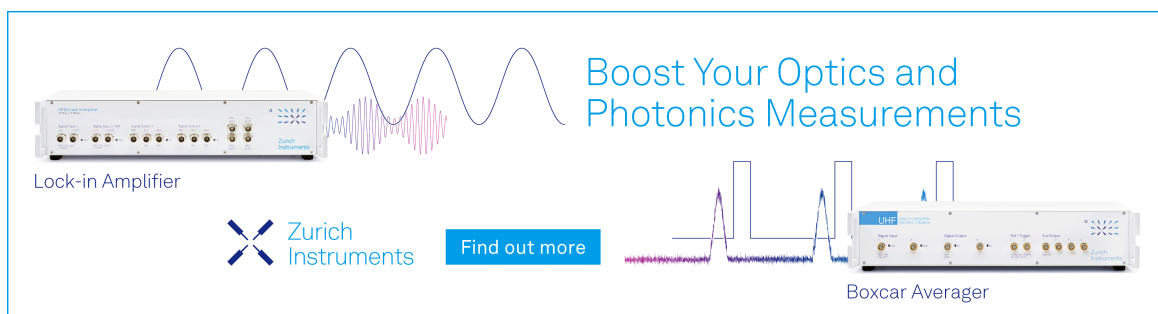
Erratum: ^{31}P NMR chemical shielding tensors of $\alpha\text{-Ca}_2\text{P}_2\text{O}_7$ **FREE**

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J. Chem. Phys. 65, 2922 (1976)

<https://doi.org/10.1063/1.433602>



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TABLE II. Observed relative absorbance of ^{14}N species to ^{15}N species compared with that expected for 54.6 atom% ^{15}N .

$\bar{\nu}$ (cm $^{-1}$) of ^{14}N Species	Absorbance ratio ^a		Identity
	Obs	Calc ^b	
1050.9 ₃	0.70	0.70	UN ₂
1000.9 ₇	0.84	0.84	UN
995.5 ₂	0.86	0.84	UN
991.9 ₀	0.86	0.84	UN
983.7 ₀	0.83	0.84	X-UN

^a ^{14}N species to ^{15}N species.

^bWith 54.6 atom% ^{15}N .

where X represents the probable presence of one or more additional atoms. To determine whether a carbon impurity might be responsible for X-UN, CO₂ was purposely added to the sputtering gas mixture, but no increase in the X-UN peak relative to the UN triplet was observed. Analysis of the U metal showed negligible amounts of metallic impurities. No correlation of the X-UN absorbance with that of any other spectral feature could be detected. Thus, X-UN remains unidentified.

The peak observed at 1050.9₃ cm $^{-1}$ [spectrum (A) in Fig. 1] has two counterparts (1040.7₄ and 1019.3₉ cm $^{-1}$) in the presence of ^{15}N [spectrum (B)]. The number of peaks and their frequencies are consistent with their assignment to the ν_3 modes of linear N-U-N isotopomers

(force constants $f = 8.215$ m dyn \AA^{-1} , $f' = 0.062$ m dyn \AA^{-1}). The weakness of the U $^{14}\text{N}_2$ peak in the experiment with 0.05% N₂ as compared with the experiment with 0.13% N₂ is consistent with this assignment. The assignment to linear UN₂ is tentative due to the overlap of the observed UN peaks with the calculated frequency of the ν_1 mode of ^{14}N -U- ^{15}N preventing observation of this mode and, thus, confirmation of the assignment.

Support for all assignments is obtained from the relative absorbances shown in Table II. The three peaks assigned to U ^{14}N and the X-U ^{14}N peak all have absorbances relative to their ^{15}N counterparts, which are consistent with 54.6 atom% ^{15}N enrichment. Using this value, the peak assigned to U $^{14}\text{N}_2$ has an absorbance relative to the peak assigned to U $^{15}\text{N}_2$, which is consistent only with the presence of two N atoms in the absorber.

*This work was sponsored, in part, by the Defense Nuclear Agency under Subtask Code S99QAXH1002 and Work Unit 28 and, in part, by the U. S. Energy Research and Development Administration.

¹D. W. Green, S. D. Gabelnick, and G. T. Reedy, *J. Chem. Phys.* **64**, 1697 (1976).

²A similar device has been described previously [D. H. W. Carstens, J. F. Kozlowski, and D. M. Gruen, *High Temp. Sci.* **4**, 301 (1972)].

³A Fourier transform spectrometer was used to record spectra. Further details of experimental methods are described in Ref. 1.

⁴S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, *J. Chem. Phys.* **58**, 4468 (1973).

ERRATA

Erratum: A model potential for chemisorption: H₂ + W(001) [*J. Chem. Phys.* **63**, 2340 (1975)]

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In Table I the entry for z_0 at the 5CN site should read 0.056. The correct value was used in the calculations.

Erratum: ^{31}P NMR chemical shielding tensors of α -Ca₂P₂O₇ [*J. Chem. Phys.* **64**, 4451 (1976)]

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The scale in Fig. 6 is mislabeled by a factor of 10; the proper values are -40, 0, 40, 80, and 120 ppm.

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