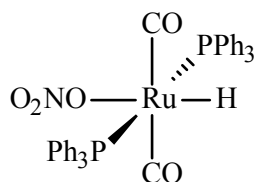


Created by Kristy L. Mardis (Chicago State University), Robert J. LeSuer (Chicago State University) and Chip Nataro (Lafayette College) (kmardis@csu.edu, rlesuer@csu.edu and nataroc@lafayette.edu) and posted on VIPER (www.ionicviper.org) on May 16, 2013. Copyright Kristy L. Mardis, Robert J. LeSuer and Chip Nataro 2013. This work is licensed under the Creative Commons Attribution Non-commercial Share Alike License. To view a copy of this license visit <http://creativecommons.org/about/license/>.

The synthesis and characterization of $[\text{RuH}(\text{ONO}_2)(\text{CO})_2(\text{PPh}_3)_2]$ has been reported (Critchlow, P. B.; Robinson, S. D. *Inorg. Chem.* **1978**, *17*, 1896). The nitrate ligand bonds exclusively as a monodentate ligand through an oxygen atom and is drawn as ONO_2 to emphasize this coordination mode. There are eight possible octahedral isomers of this compound. One isomer is shown below. Sketch the remaining isomers (*Hint*: there are two pairs of enantiomers among the eight isomers).



The authors present the following data and rationale for determining that only one isomer was prepared in their synthesis. The data are accurate, but there is something wrong with the rationale. You can assume that the authors' presentation and interpretation of the NMR spectra is correct.

Three absorptions, one attributable to ν_{RuH} and two to ν_{CO} (1940, 1977 and 2058 cm^{-1}) are observed in the infrared spectra of the product. In addition, one ^1H NMR triplet ($\tau_{\text{RuH}} = 13.9$)* and one ^{31}P singlet ($\delta = 42.25$ ppm) indicative of two magnetically equivalent phosphorus nuclei were observed.

The presence of two strong infrared frequencies attributable to ν_{CO} enables the structure shown above to be eliminated. The exceptionally low values of the hydridic NMR resonance reveal a relatively deshielded proton, thus virtually excluding the possibility of hydride *trans* to nitrate but rather suggesting the removal of electron density by a *trans* ligand with high π acidity.

Where did the authors err in their reasoning? Based on the information provided, determine the isomer formed and provide its name.

C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$	
A_1	1	1	1	1	z
A_2	1	1	-1	-1	R_z
B_1	1	-1	1	-1	x, R_y
B_2	1	-1	-1	1	y, R_x

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C_s	E	σ_h	
A'	1	1	x, y, R_z
A''	1	-1	z, R_x , R_y

* τ is an older scale for reporting ^1H NMR shifts that is no longer used. The chemical shift of tetramethylsilane is 0.00 ppm which would correspond to 10.00 τ . A chemical shift of 10.00 ppm would correspond to 0.00 τ . The shift of the hydridic proton in this compound occurs at -3.9 ppm. Although the τ scale is no longer used, the effects of this scale still impact us today. Many students find the terms upfield and downfield with respect to chemical shifts to be confusing, because a downfield shift is to higher numbers in ppm. However, in the τ scale, a downfield shift is to lower values of τ .