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Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713618290>

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Online publication date: 27 October 2010

To cite this Article Goto, Kei , Kobayashi, Junji , Kawashima, Takayuki , Schmidt, Michael W. and Nagase, Shigeru(2002) 'Bonding Properties of 5-Carbaphosphatranes', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 177: 8, 2037 – 2038

To link to this Article: DOI: 10.1080/10426500213414

URL: <http://dx.doi.org/10.1080/10426500213414>

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BONDING PROPERTIES OF 5-CARBAPHOSPHATRANES

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(Received July 29, 2001; accepted December 25, 2001)

Recently we have reported the synthesis and structure of 5-carbaphosphatranes, the first example of main group atranes bearing a 1-5 covalent bond.¹ It is very intriguing how the properties of their transannular bonding are different from usual phosphatranes bearing a N→P dative bond. Here we report the theoretical studies on the bonding properties of 5-carbaphosphatranes along with the analysis of their vibrational spectra. In contrast to phosphatranes, for which the calculated transannular distances largely depend on the basis sets, the calculations on 5-carbaphosphatrane **1** at RHF/6-31G(d), MP2/6-31 G(d), and B3LYP/6-31 G(d) levels gave very similar results for the transannular P–C distances. These results are in good agreement with the crystal structure of **2** (1.921(2) Å), hinting that the transannular bond of a

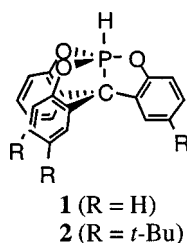


FIGURE 1

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5-carbaphosphatrane possesses a steeper potential well than a phosphatrane. The calculations on the force constants and bond orders indicated that the transannular bond of a 5-carbaphosphatrane is about twice stronger than that of a phosphatrane, with a substantially covalent character.

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- [1] J. Kobayashi, K. Goto, and T. Kawashima, *J. Am. Chem. Soc.*, **123**, 3387–3388 (2001).