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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 Chen, Zhong-Zhou, Tan, Bo, Li, Yan-Mei and Zhao, Yu-Fen(2010) 'Comparing the Penta-Coordinate Phosphoric Intermediates from N-Dimethylphosphoryl L-Aspartic Acid', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 177: 8, 2073 – 2074

To link to this Article: DOI: 10.1080/10426500213453

URL: <http://dx.doi.org/10.1080/10426500213453>

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COMPARING THE PENTA-COORDINATE PHOSPHORIC INTERMEDIATES FROM N-DIMETHYLPHOSPHORYL L-ASPARTIC ACID

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

Phosphorus plays an important role in biological process through phosphorylation and dephosphorylation. The structures and the properties of penta-coordinate phosphoric intermediates were very important in the study of many biochemical processes, such as phosphorylation.¹

Two types of penta-coordinate phosphoric intermediates might be formed from N-dimethylphosphoryl L-aspartic acid. These isomers were further optimized at the HF/6-31G** and B3LYP/6-31G** level, their geometries were shown in Figure 1. It was found that the intermediates **3** with six-membered ring in apical-equatorial spanning arrangement was more stable than **3'** with di-equatorial spanning arrangement and the intermediates **2** were more stable than intermediates **3**. These results were in agreement with that predicted by the reference and experiments.^{2,3}

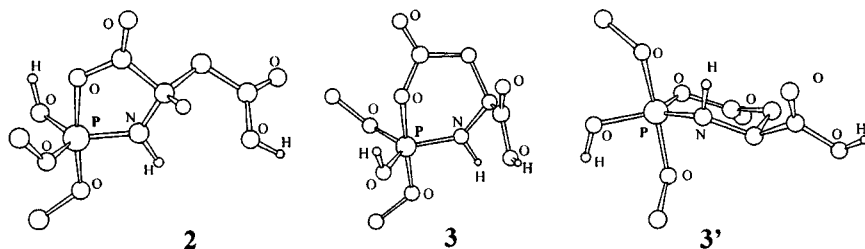


FIGURE 1 The geometry of **2**, **3**, and **3'** at B3LYP/6-31G** level.

The authors would like to thank the financial supports from the National Natural Science Foundation of China (No. 20072023).

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REFERENCES

- [1] F. Ramirez, J. F. Marecek, and H. Okazaki, *J. Am. Chem. Soc.*, 5310 (1976).
- [2] R. R. Holmes, *J. Am. Chem. Soc.*, **97**, 5379 (1975).
- [3] R. R. Holmes, *Phosphorus, Sulfur and Silicon*, **98**, 89 (1995).