Supplementary Material (ESI) for New Journal of Chemistry

Supplementary Information

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Title: Structurally diverse penta- and hexa-coordinate phosphorus compounds from the reaction of diethyl- or diisopropyl- azodicarboxylates with phosphorus(III) compounds

We have optimized the structures of the compounds presented in the following table at B3LYP/6-31G* level[1] using Gaussian 03 program package.[2]

Table S1: Energies (au) of the optimized structures for **2**, **15**, **16** and **18**

Input structure[a]	Total Optimized Energies of the Compounds			
	2	**15**	**16**	**18**
I	-2603.48652	-2642.81688	-2929.11876	-2694.53156
II	-2603.47500	-2642.79752	-2929.12508	-2694.51646
III	-2603.49209	-2642.82621	-2929.12289	-2694.51646
V	-2603.49488	-2642.81895	-2929.12979	-2694.53748
VI	-2603.48600	-2642.81390	-2929.13438	-2694.53840
VII	-2603.50296	-2642.82358	Not applicable	Not applicable

[a] The coordinates from X-ray structures of **2**, **5**, **7**, **18** and **16** were used, respectively, for **I**, **II**, **III**, **V**, **VI** and **VII**. Modification of the substituents (like S replacing CH_2) was then effected and the structure was optimized for minimum energy.

Energy in atomic units: 1 a.u. = 627.50 kcal/mol

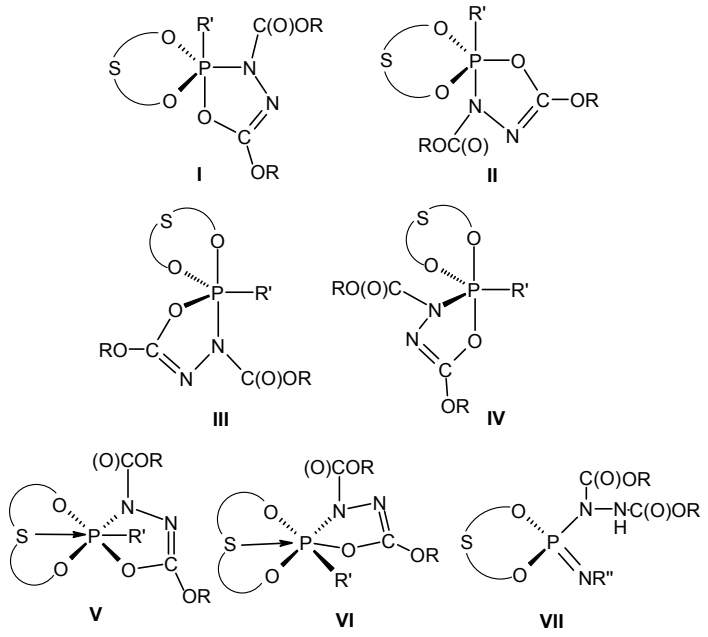

Chart. 5

1 a) A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 5648; b) A. D. Becke *Phys. Rev. A,* 1988, **38**, 2398; c) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785.

2. Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson,W. Chen,M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.