

Electronic Supplementary Information (ESI)

Planarity Takes Over in the $C_xH_xP_{6-x}$ ($x = 0-6$) Series at $x = 4$

Timur R. Galeev and Alexander I. Boldyrev*

Department of Chemistry and Biochemistry, Utah State University, Old Main Hill 0300, Logan, UT 84322-0300, USA. Fax: +1 435-797-3390, Tel: +1 435 7971630; E-mail: a.i.boldyrev@usu.edu

Complete reference 33

- 33 *Gaussian 03, Revision D.01*, 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, J. A. Pople, Gaussian, Inc., Wallingford, CT, 2004.

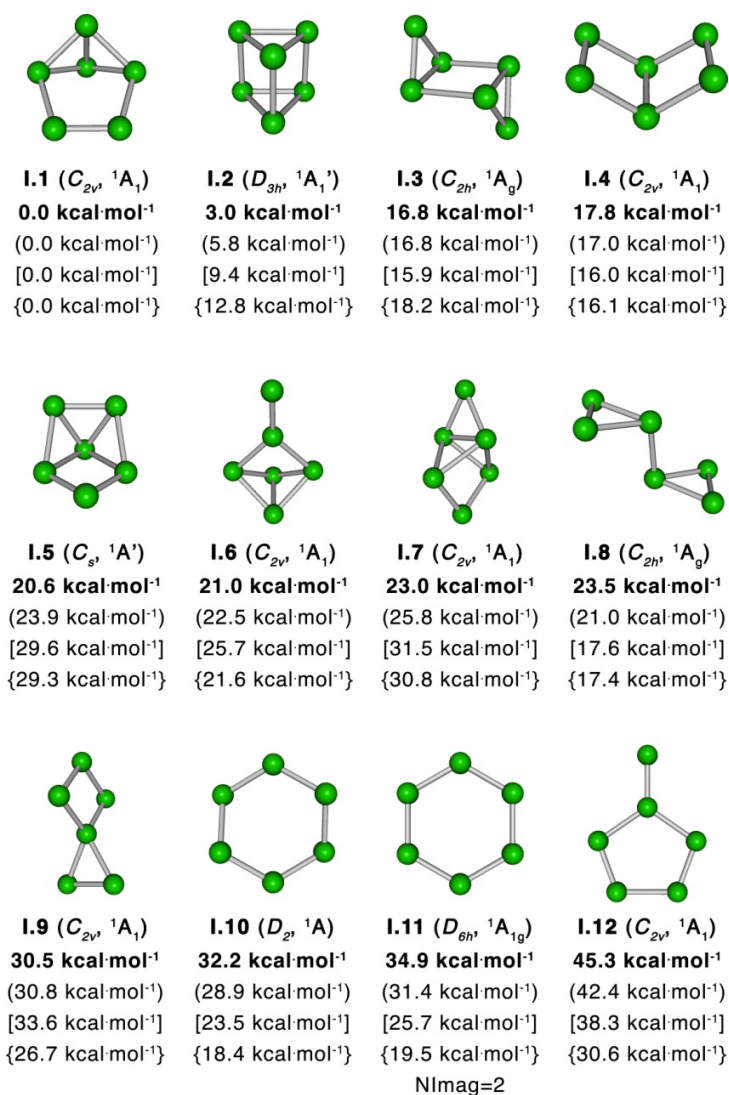


Fig. S1 Lowest-lying structures of P_6 , their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311+G* (curly brackets), all at B3LYP/6-311+G* optimized geometries

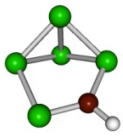
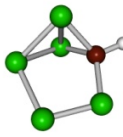
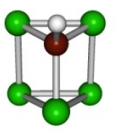
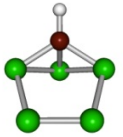
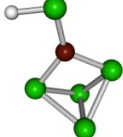
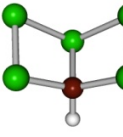
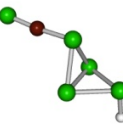
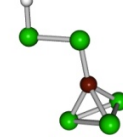
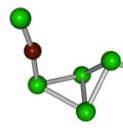
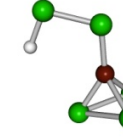
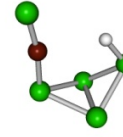
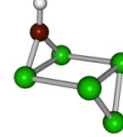
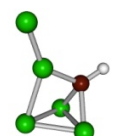
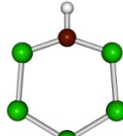
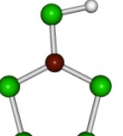
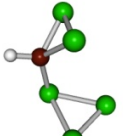
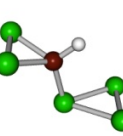
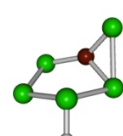
						
II.1 (C_s , $^1A'$) 0.0 kcal·mol⁻¹ (0.0 kcal·mol ⁻¹) [0.0 kcal·mol ⁻¹] {0.0 kcal·mol ⁻¹ }	II.2 (C_s , $^1A'$) 3.7 kcal·mol⁻¹ (3.0 kcal·mol ⁻¹) [2.0 kcal·mol ⁻¹] {1.8 kcal·mol ⁻¹ }	II.3 (C_s , $^1A'$) 11.5 kcal·mol⁻¹ (13.1 kcal·mol ⁻¹) [15.4 kcal·mol ⁻¹] {16.0 kcal·mol ⁻¹ }	II.4 (C_s , $^1A'$) 12.6 kcal·mol⁻¹ (11.8 kcal·mol ⁻¹) [10.8 kcal·mol ⁻¹] {9.4 kcal·mol ⁻¹ }	II.5 (C_s , $^1A'$) 12.8 kcal·mol⁻¹ (12.3 kcal·mol ⁻¹) [12.2 kcal·mol ⁻¹] {10.0 kcal·mol ⁻¹ }	II.6 (C_s , $^1A'$) 20.4 kcal·mol⁻¹ (19.2 kcal·mol ⁻¹) [17.6 kcal·mol ⁻¹] {16.8 kcal·mol ⁻¹ }	II.7 (C_s , $^1A'$) 21.5 kcal·mol⁻¹ (20.0 kcal·mol ⁻¹) [18.3 kcal·mol ⁻¹] {17.6 kcal·mol ⁻¹ }
						
II.8 (C_s , $^1A'$) 21.8 kcal·mol⁻¹ (19.7 kcal·mol ⁻¹) [16.7 kcal·mol ⁻¹] {16.1 kcal·mol ⁻¹ }	II.9 (C_s , $^1A'$) 21.9 kcal·mol⁻¹ (19.6 kcal·mol ⁻¹) [16.5 kcal·mol ⁻¹] {16.2 kcal·mol ⁻¹ }	II.10 (C_s , $^1A'$) 22.9 kcal·mol⁻¹ (21.4 kcal·mol ⁻¹) [20.2 kcal·mol ⁻¹] {18.3 kcal·mol ⁻¹ }	II.11 (C_s , $^1A'$) 24.4 kcal·mol⁻¹ (22.2 kcal·mol ⁻¹) [18.9 kcal·mol ⁻¹] {19.1 kcal·mol ⁻¹ }	II.12 (C_s , $^1A'$) 25.8 kcal·mol⁻¹ (24.2 kcal·mol ⁻¹) [22.9 kcal·mol ⁻¹] {21.2 kcal·mol ⁻¹ }	II.13 (C_s , $^1A'$) 26.8 kcal·mol⁻¹ (24.3 kcal·mol ⁻¹) [20.8 kcal·mol ⁻¹] {20.5 kcal·mol ⁻¹ }	II.14 (C_s , $^1A'$) 27.1 kcal·mol⁻¹ (26.5 kcal·mol ⁻¹) [25.1 kcal·mol ⁻¹] {26.5 kcal·mol ⁻¹ }
						
II.15 (C_s , $^1A'$) 28.1 kcal·mol⁻¹ (28.9 kcal·mol ⁻¹) [31.1 kcal·mol ⁻¹] {27.8 kcal·mol ⁻¹ }	II.16 (C_{2v} , 1A_1) 28.2 kcal·mol⁻¹ (24.8 kcal·mol ⁻¹) [19.4 kcal·mol ⁻¹] {13.9 kcal·mol ⁻¹ }	II.17 (C_s , $^1A'$) 30.3 kcal·mol⁻¹ (25.9 kcal·mol ⁻¹) [19.5 kcal·mol ⁻¹] {16.8 kcal·mol ⁻¹ }	II.18 (C_s , $^1A'$) 31.2 kcal·mol⁻¹ (28.1 kcal·mol ⁻¹) [23.8 kcal·mol ⁻¹] {26.1 kcal·mol ⁻¹ }	II.19 (C_s , $^1A'$) 32.0 kcal·mol⁻¹ (28.8 kcal·mol ⁻¹) [24.6 kcal·mol ⁻¹] {25.5 kcal·mol ⁻¹ }	II.20 (C_s , $^1A'$) 33.7 kcal·mol⁻¹ (30.6 kcal·mol ⁻¹) [26.6 kcal·mol ⁻¹] {24.9 kcal·mol ⁻¹ }	II.21 (C_s , $^1A'$) 35.4 kcal·mol⁻¹ (32.3 kcal·mol ⁻¹) [28.1 kcal·mol ⁻¹] {25.9 kcal·mol ⁻¹ }

Fig. S2 Lowest-lying structures of CHP_5 , their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

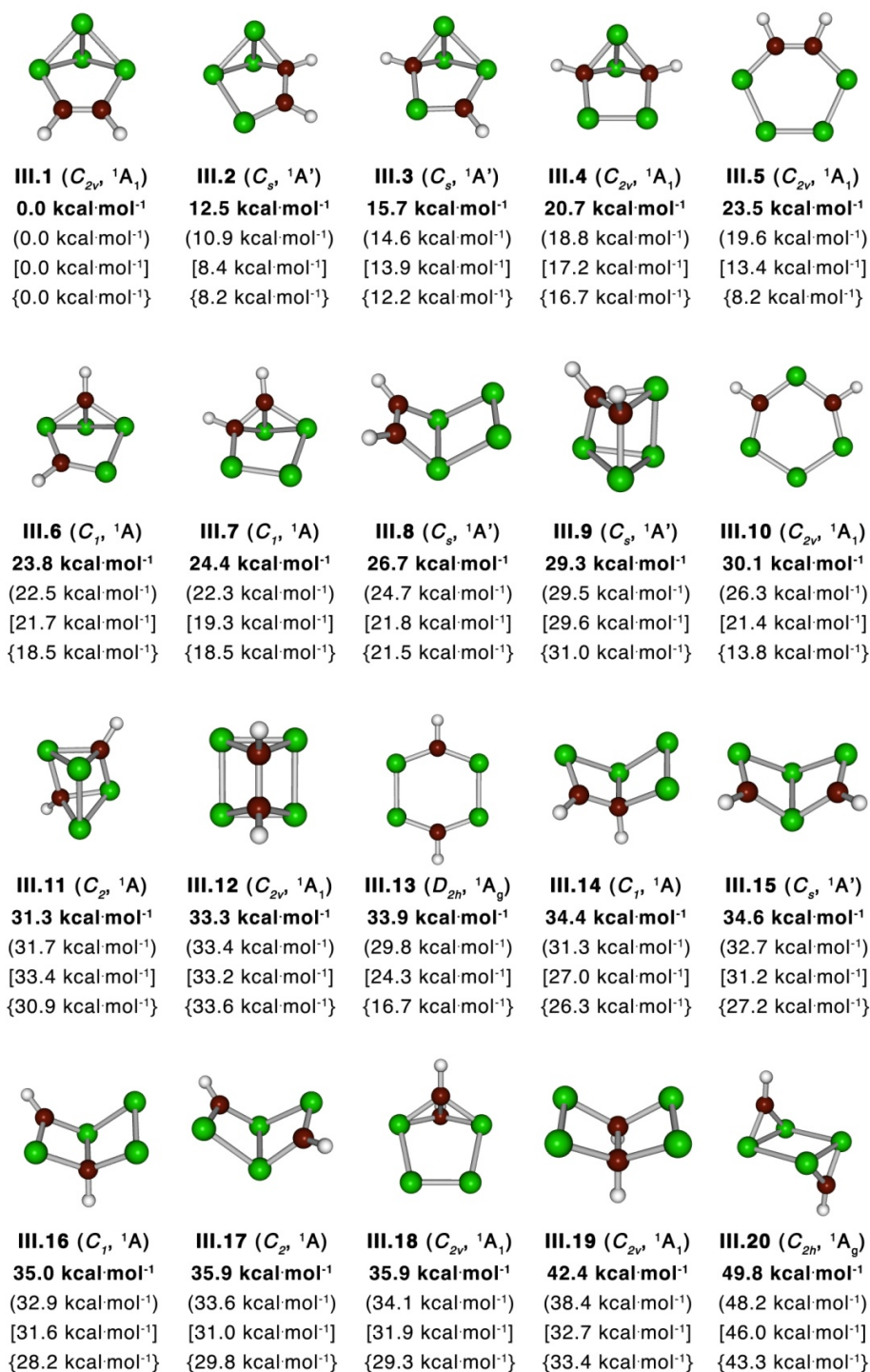


Fig. S3 Selected structures of $C_2H_2P_4$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

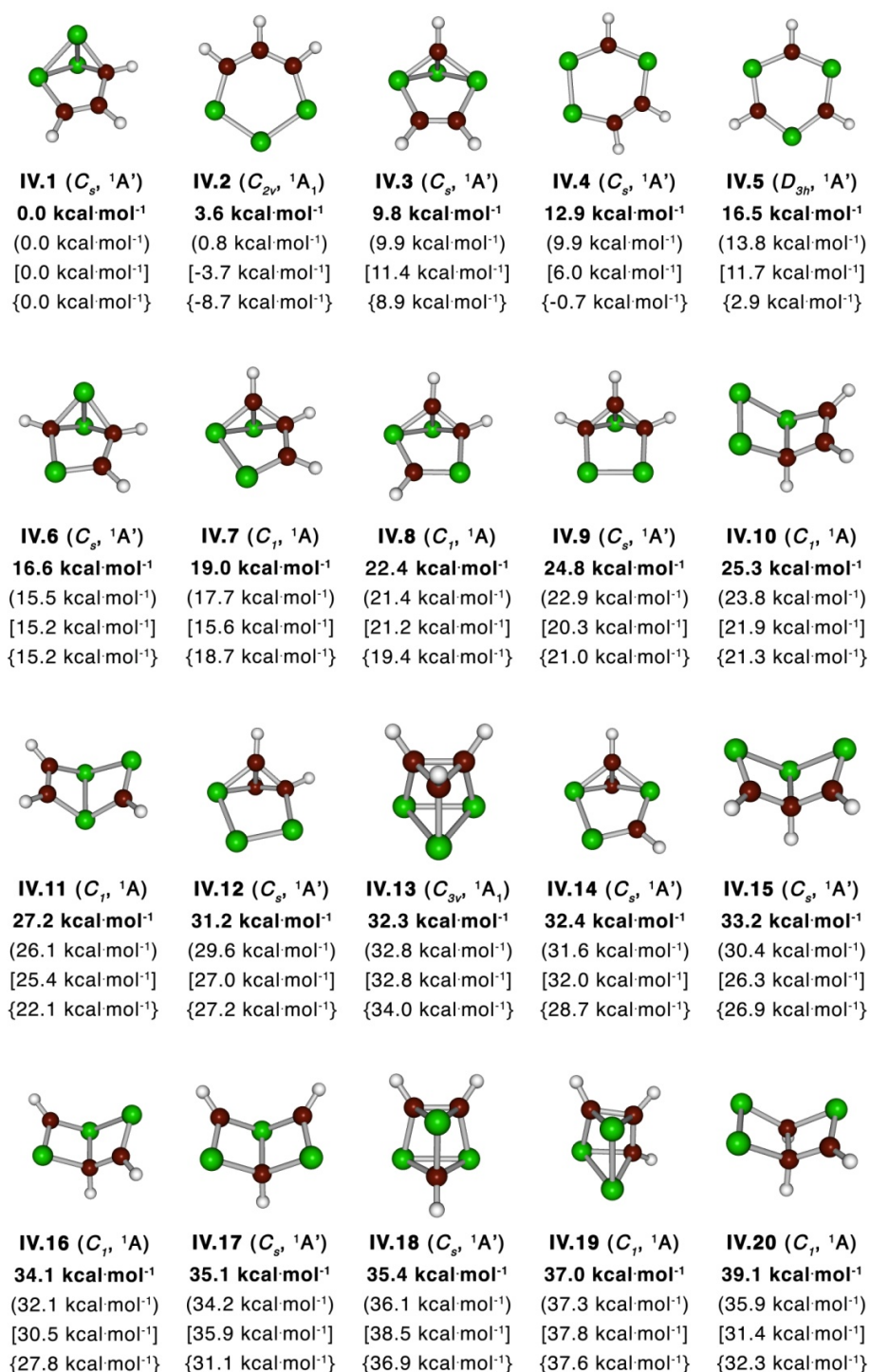


Fig. S4 Selected isomers of $C_3H_3P_3$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

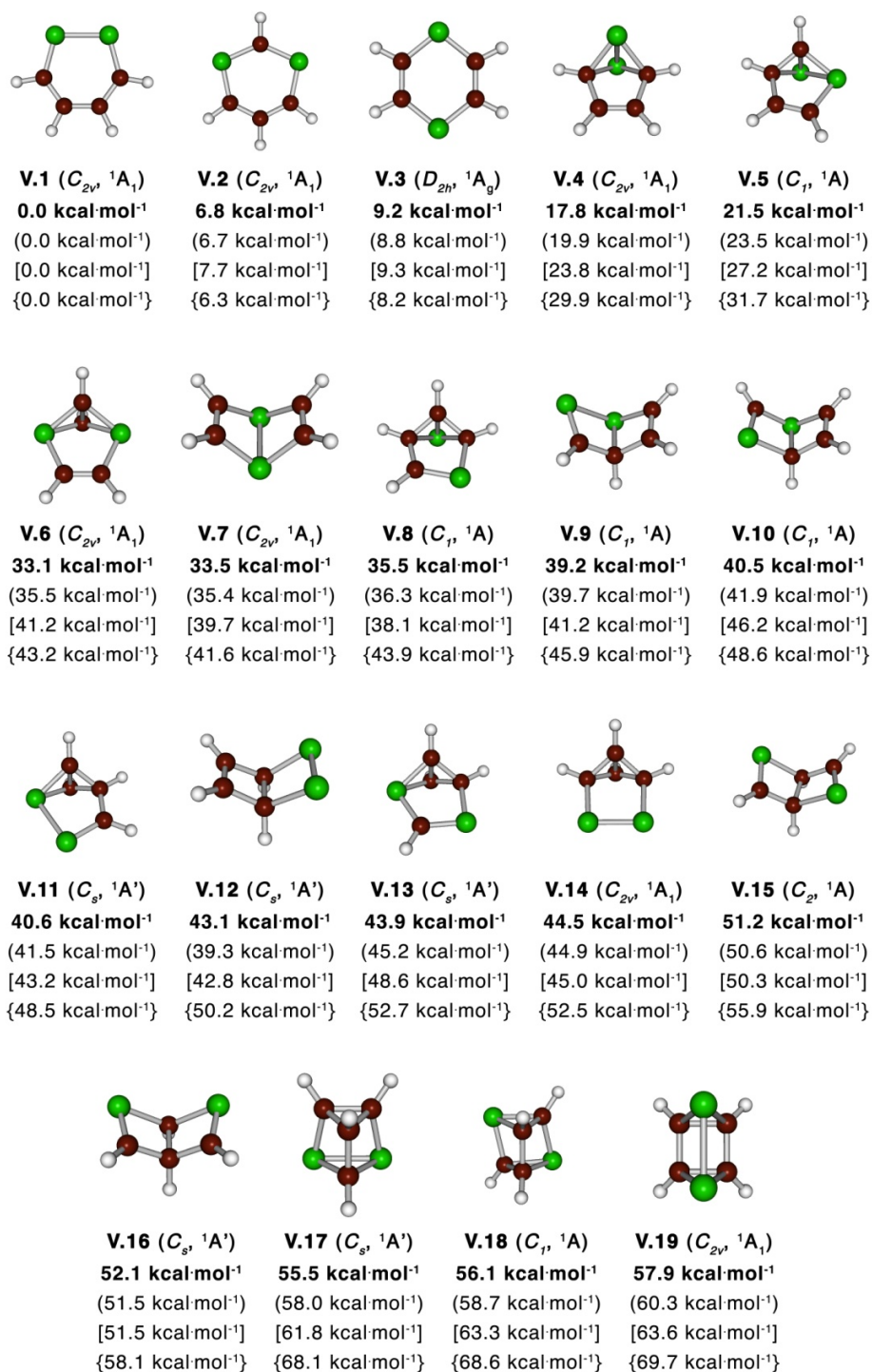


Fig. S5 Selected isomers of $C_4H_4P_2$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

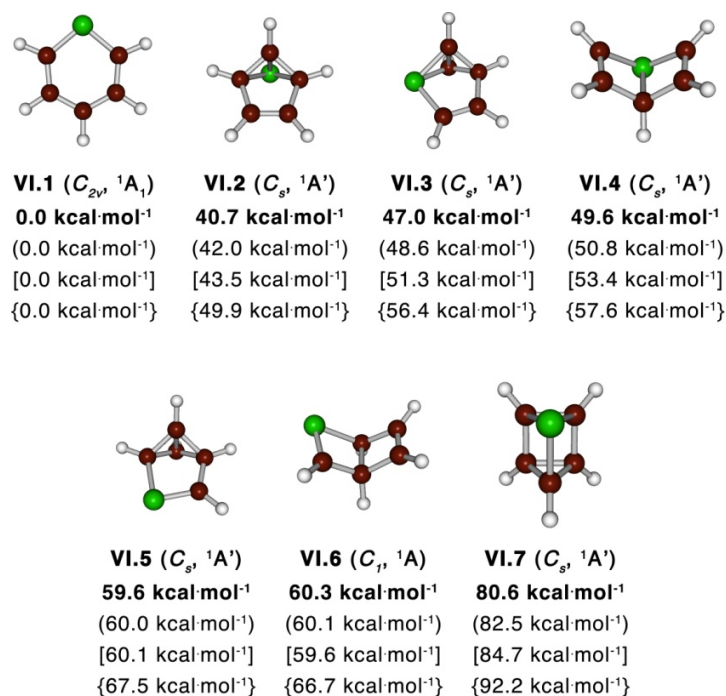


Fig. S6 Selected isomers of C_5H_5P , their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

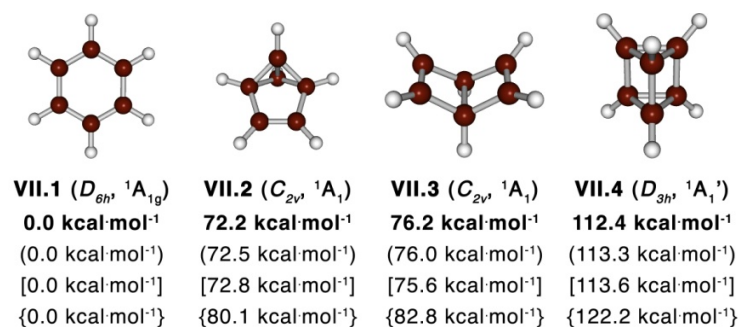


Fig. S7 Selected isomers of C_6H_6 , their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized geometries

Table S1 NICS_{zz} values (ppm) calculated at B3LYP/6-311++G**

Distance (Å)	P ₆	CHP ₅	C ₂ H ₂ P ₄			C ₃ H ₃ P ₃			C ₄ H ₄ P ₂			C ₅ H ₅ P	C ₆ H ₆
	I.11	II.16	III.5	III.10	III.13	IV.2	IV.4	IV.5	V.1	V.2	V.3	VI.1	VII.1
0.0	-23.7	-12.1	-9.0	-9.1	-9.0	-9.2	-9.2	-8.9	-10.4	-10.4	-10.2	-12.5	-14.5
0.1	-23.8	-12.3	-9.3	-9.4	-9.2	-9.5	-9.5	-9.2	-10.7	-10.7	-10.5	-12.9	-14.9
0.2	-24.2	-12.9	-10.0	-10.1	-10.0	-10.4	-10.3	-10.1	-11.7	-11.7	-11.5	-14.1	-16.3
0.3	-24.8	-13.9	-11.2	-11.3	-11.1	-11.8	-11.7	-11.5	-13.2	-13.3	-13.1	-15.8	-18.2
0.4	-25.5	-15.1	-12.7	-12.8	-12.5	-13.5	-13.4	-13.2	-15.1	-15.2	-14.9	-17.9	-20.6
0.5	-26.3	-16.6	-14.4	-14.4	-14.2	-15.3	-15.3	-15.0	-17.1	-17.2	-17.0	-20.1	-23.0
0.6	-27.2	-18.0	-16.0	-16.2	-15.8	-17.2	-17.2	-16.9	-19.1	19.2	-19.0	-22.3	-25.2
0.7	-28.0	-19.4	-17.7	-17.8	-17.5	-19.0	-19.0	-18.7	-21.0	-21.0	-20.9	-24.1	-27.0
0.8	-28.7	-20.7	-19.2	-19.3	-18.9	-20.6	-20.5	-20.2	-22.5	-22.6	-22.4	-25.5	-28.3
0.9	-29.3	-21.8	-20.5	-20.5	-20.1	-21.9	-21.7	-21.5	-23.6	-23.7	-23.5	-26.5	-29.1
1.0	-29.6	-22.7	-21.4	-21.5	-21.1	-22.8	-22.6	-22.3	-24.4	-24.4	-24.2	-27.0	-29.2
1.1	-29.8	-23.3	-22.1	-22.1	-21.7	-23.4	-23.1	-22.9	-24.7	-24.7	-24.6	-27.0	-28.9
1.2	-29.7	-23.6	-22.5	-22.4	-22.1	-23.6	-23.3	-23.0	-24.7	-24.7	-24.5	-26.6	-28.2
1.3	-29.5	-23.7	-22.6	-22.5	-22.1	-23.5	-23.2	-22.9	-24.4	-24.3	-24.2	-26.0	-27.2
1.4	-29.0	-23.6	-22.4	-22.3	-22.0	-23.2	-22.8	-22.6	-23.8	-23.7	-23.6	-25.0	-26.0
1.5	-28.4	-23.2	-22.0	-21.9	-21.6	-22.6	-22.2	-22.0	-23.0	-22.9	-22.8	-23.9	-24.6
1.6	-27.7	-22.7	-21.5	-21.3	-21.0	-21.9	-21.5	-21.3	-22.1	-21.9	-21.8	-22.7	-23.2
1.7	-26.8	-22.0	-20.9	-20.7	-20.4	-21.0	-20.6	-20.4	-21.1	-20.9	-20.8	-21.5	-21.7
1.8	-25.9	-21.3	-20.0	-19.8	-19.6	-20.1	-16.7	-19.4	-20.0	-19.8	-19.7	-20.2	-20.2
1.9	-24.9	-20.5	-19.2	-19.0	-18.8	-19.1	-18.7	-18.5	-18.9	-18.7	-18.6	-18.9	-18.8
2.0	-23.8	-19.6	-18.3	-18.1	-17.9	-18.1	-17.7	-17.5	-17.8	-17.6	-17.4	-17.6	-17.4

Table S2 NICS values (ppm) calculated at B3LYP/6-311++G**

Distance (Å)	P ₆	CHP ₅	C ₂ H ₂ P ₄			C ₃ H ₃ P ₃			C ₄ H ₄ P ₂			C ₅ H ₅ P	C ₆ H ₆
	I.11	II.16	III.5	III.10	III.13	IV.2	IV.4	IV.5	V.1	V.2	V.3	VI.1	VII.1
0.0	-9.7	-6.3	-5.7	-5.7	-5.0	-6.6	-5.9	-5.1	-6.7	-6.0	-6.0	-7.8	-8.0
0.1	-9.8	-6.4	-5.8	-5.8	-5.1	-6.7	-6.0	-5.2	-6.8	-6.1	-6.1	-7.9	-8.2
0.2	-9.9	-6.6	-6.0	-6.0	-5.3	-6.9	-6.3	-5.5	-7.1	-6.4	-6.4	-8.1	-8.5
0.3	-10.1	-6.9	-6.4	-6.3	-5.7	-7.2	-6.7	-5.9	-7.4	-6.9	-6.8	-8.5	-8.9
0.4	-10.4	-7.3	-6.8	-6.8	-6.1	-7.6	-7.1	-6.5	-7.9	-7.4	-7.3	-9.0	-9.4
0.5	-10.6	-7.7	-7.2	-7.2	-6.6	-8.1	-7.6	-7.0	-8.3	-7.9	-7.9	-9.5	-9.9
0.6	-10.9	-8.1	-7.7	-7.7	-7.1	-8.5	-8.1	-7.6	-8.7	-8.4	-8.4	-9.9	-10.2
0.7	-11.1	-8.5	-8.1	-8.1	-7.6	-8.8	-8.5	-8.0	-9.0	-8.8	-8.8	-10.1	-10.5
0.8	-11.3	-8.9	-8.4	-8.4	-7.9	-9.1	-8.8	-8.4	-9.3	-9.1	-9.0	-10.3	-10.6
0.9	-11.5	-9.1	-8.7	-8.7	-8.2	-9.3	-9.0	-8.6	-9.4	-9.2	-9.2	-10.3	-10.5
1.0	-11.5	-9.3	-8.8	-8.8	-8.4	-9.3	-9.1	-8.7	-9.4	-9.2	-9.2	-10.1	-10.2
1.1	-11.5	-9.4	-8.9	-8.8	-8.4	-9.3	-9.0	-8.7	-9.2	-9.1	-9.1	-9.8	-9.8
1.2	-11.3	-9.3	-8.8	-8.8	-8.4	-9.1	-8.9	-8.6	-9.0	-8.9	-8.8	-9.4	-9.3
1.3	-11.2	-9.2	-8.7	-8.6	-8.3	-8.9	-8.6	-8.3	-8.7	-8.5	-8.5	-8.9	-8.8
1.4	-10.9	-9.0	-8.5	-8.4	-8.1	-8.5	-8.3	-8.1	-8.3	-8.1	-8.1	-8.4	-8.2
1.5	-10.6	-8.8	-8.2	-8.1	-7.8	-8.2	-7.9	-7.7	-7.9	-7.7	-7.7	-7.9	-7.6
1.6	-10.2	-8.5	-7.9	-7.7	-7.5	-7.8	-7.5	-7.3	-7.4	-7.3	-7.2	-7.3	-7.0
1.7	-9.8	-8.1	-7.5	-7.4	-7.2	-7.4	-7.1	-6.9	-7.0	-6.8	-6.7	-6.8	-6.4
1.8	-9.4	-7.8	-7.1	-7.0	-6.8	-6.9	-6.7	-6.5	-6.5	-6.3	-6.3	-6.2	-5.8
1.9	-9.0	-7.4	-6.7	-6.6	-6.5	-6.5	-6.3	-6.1	-6.1	-5.9	-5.8	-5.7	-5.3
2.0	-8.5	-7.0	-6.4	-6.2	-6.1	-6.1	-5.8	-5.7	-5.6	-5.4	-5.4	-5.3	-4.8