Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

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.

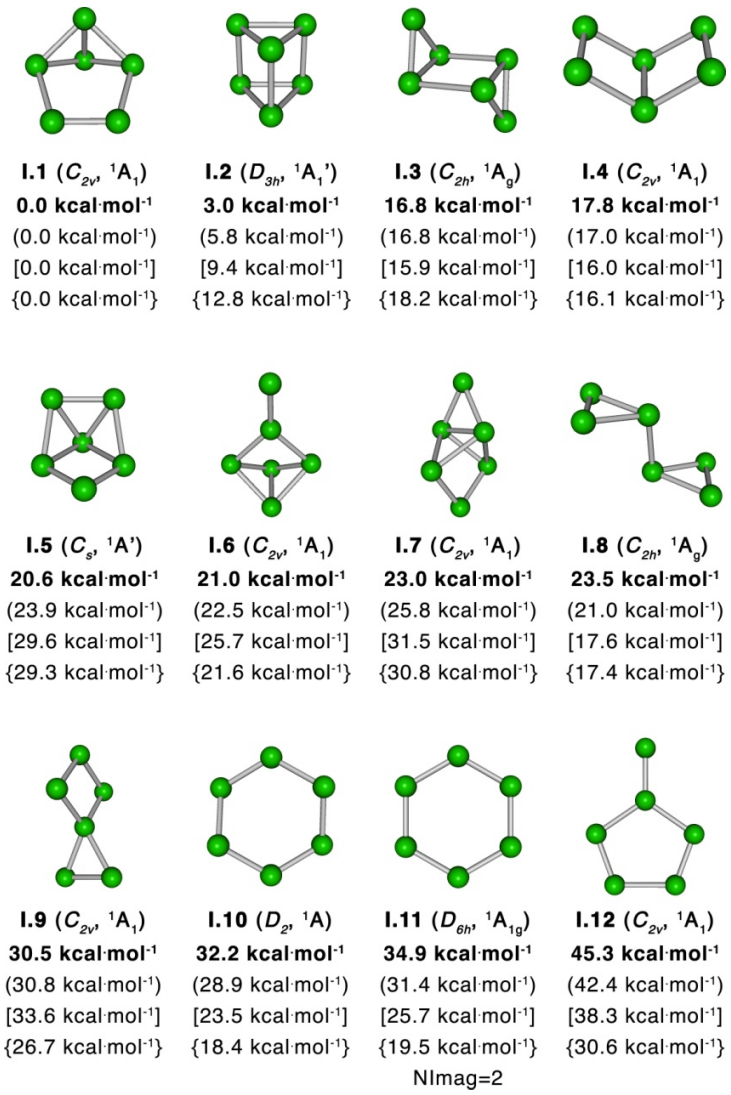

Fig. S1 Lowest-lying structures of P_6, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311+G* (curly brackets), all at B3LYP/6-311+G* optimized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

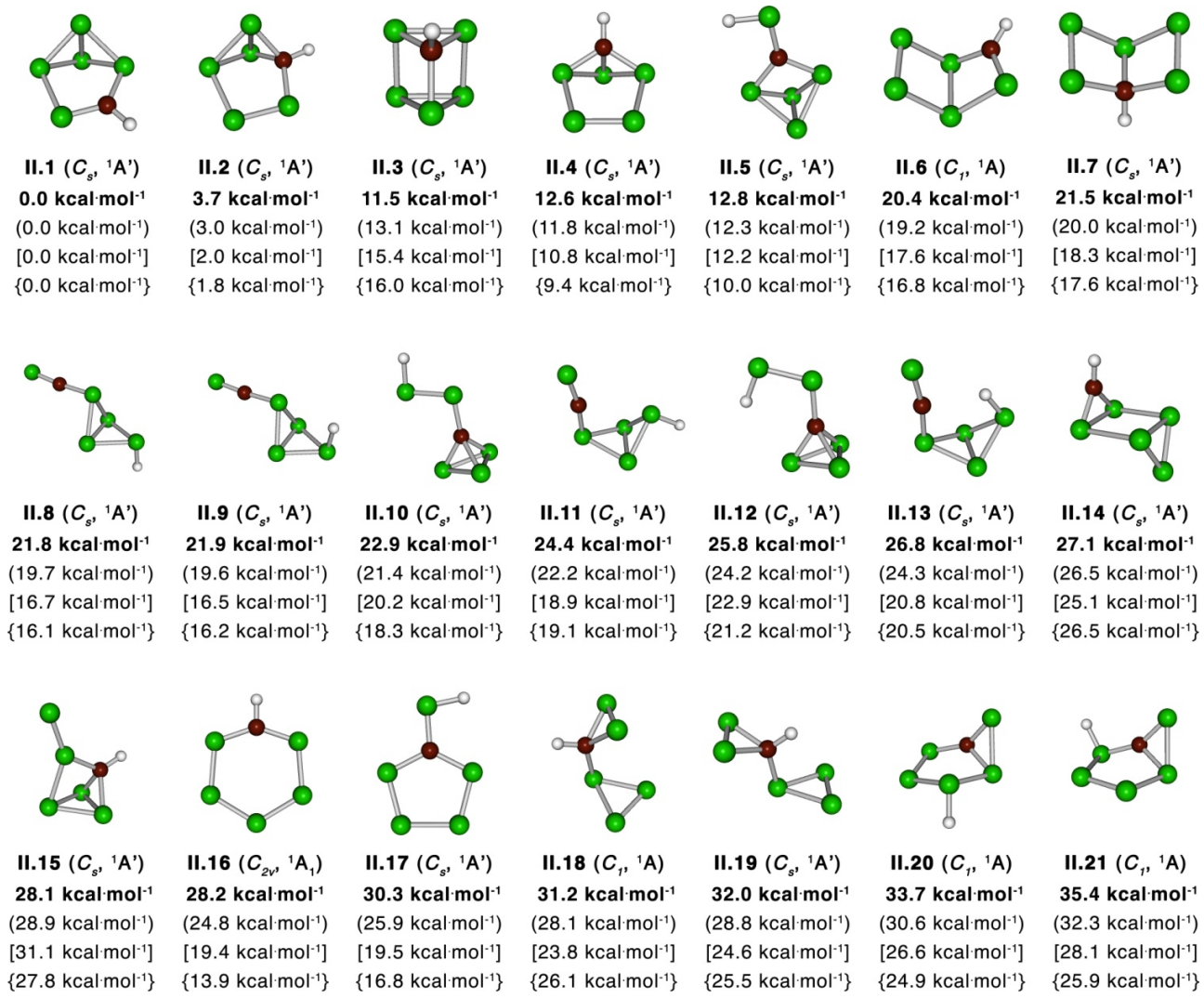

Fig. S2 Lowest-lying structures of CHP_5, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G**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

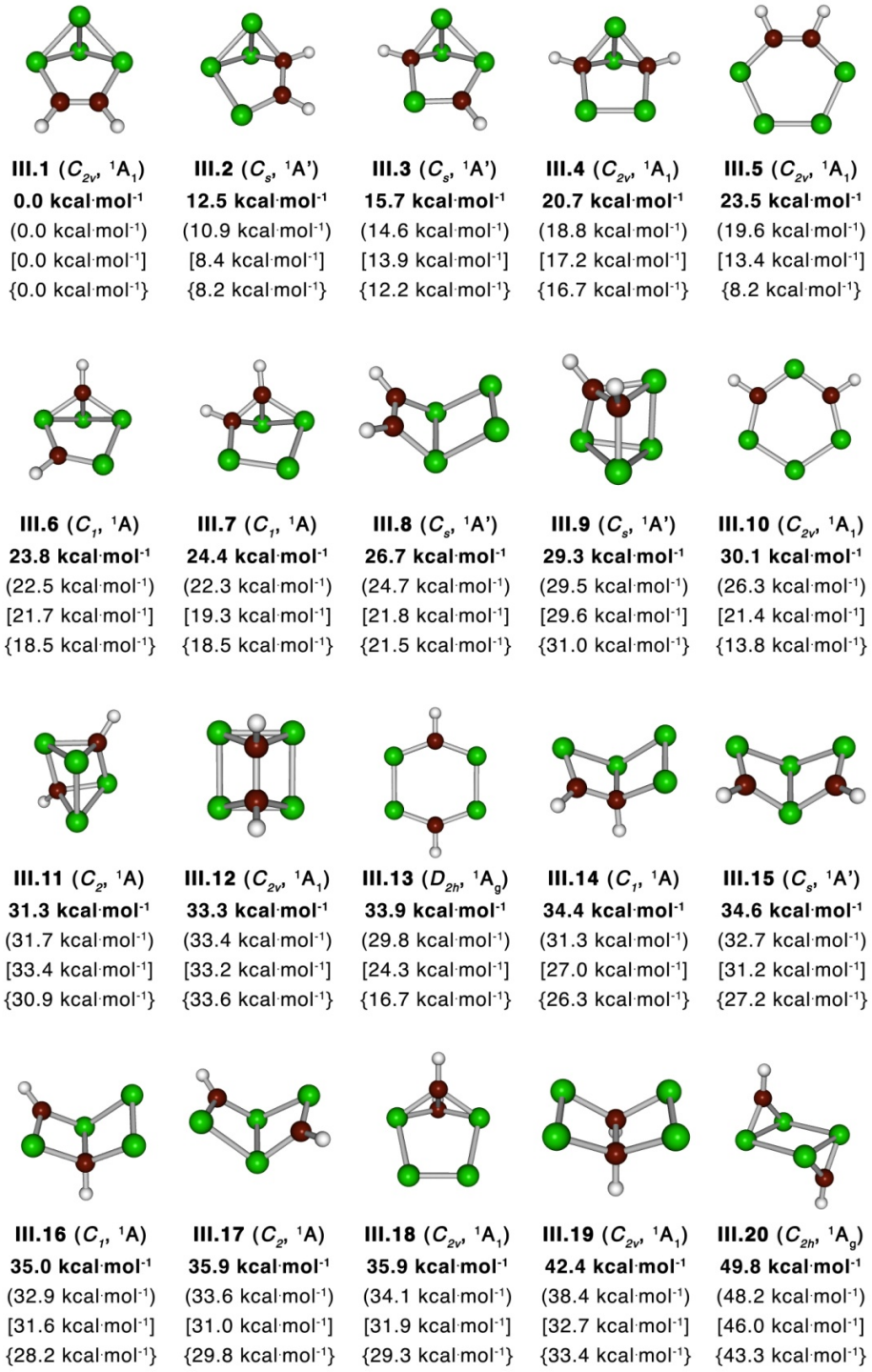

Fig. S3 Selected structures of $C_2H_2P_4$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G**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

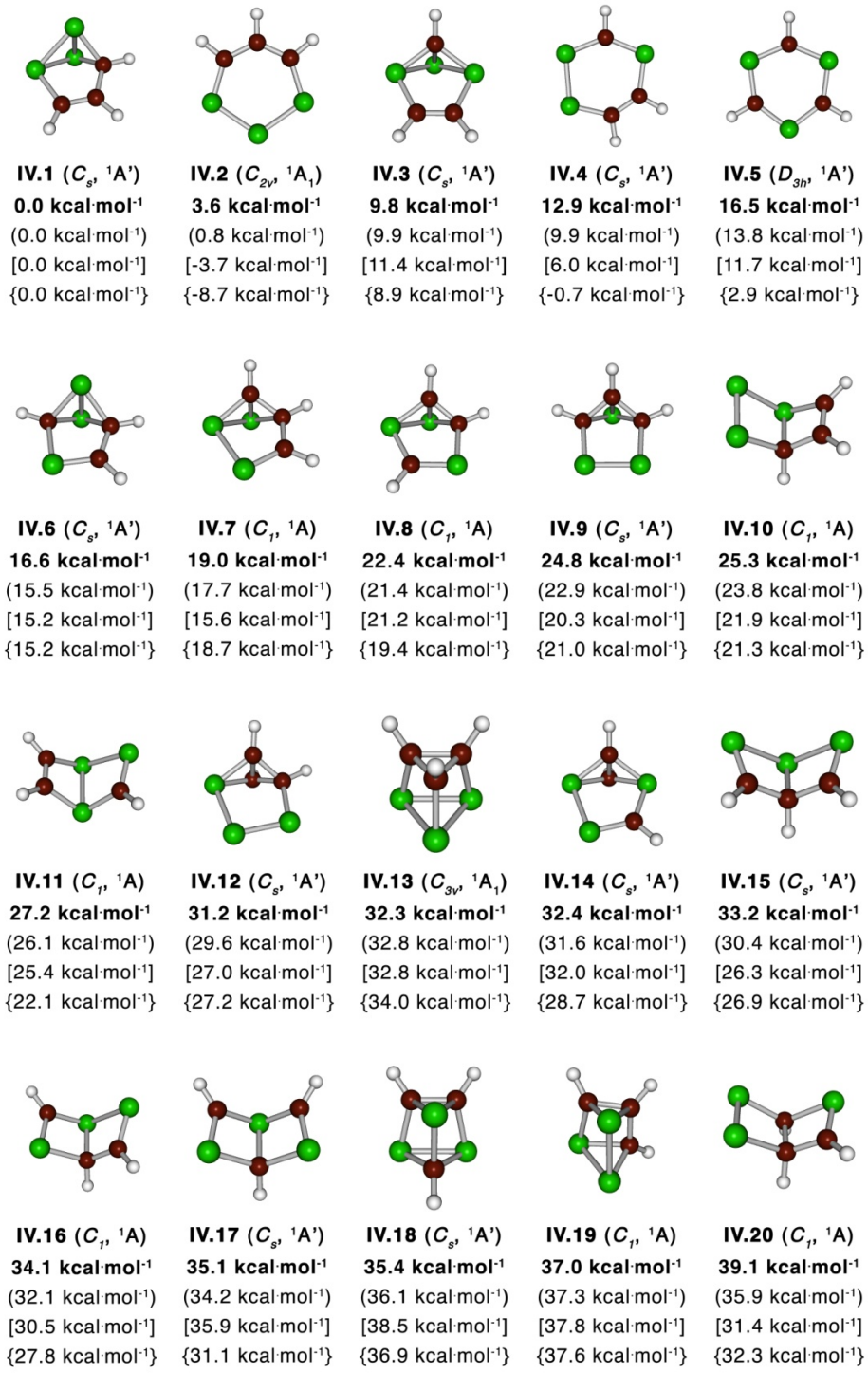

Fig. S4 Selected isomers of $C_3H_3P_3$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G**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

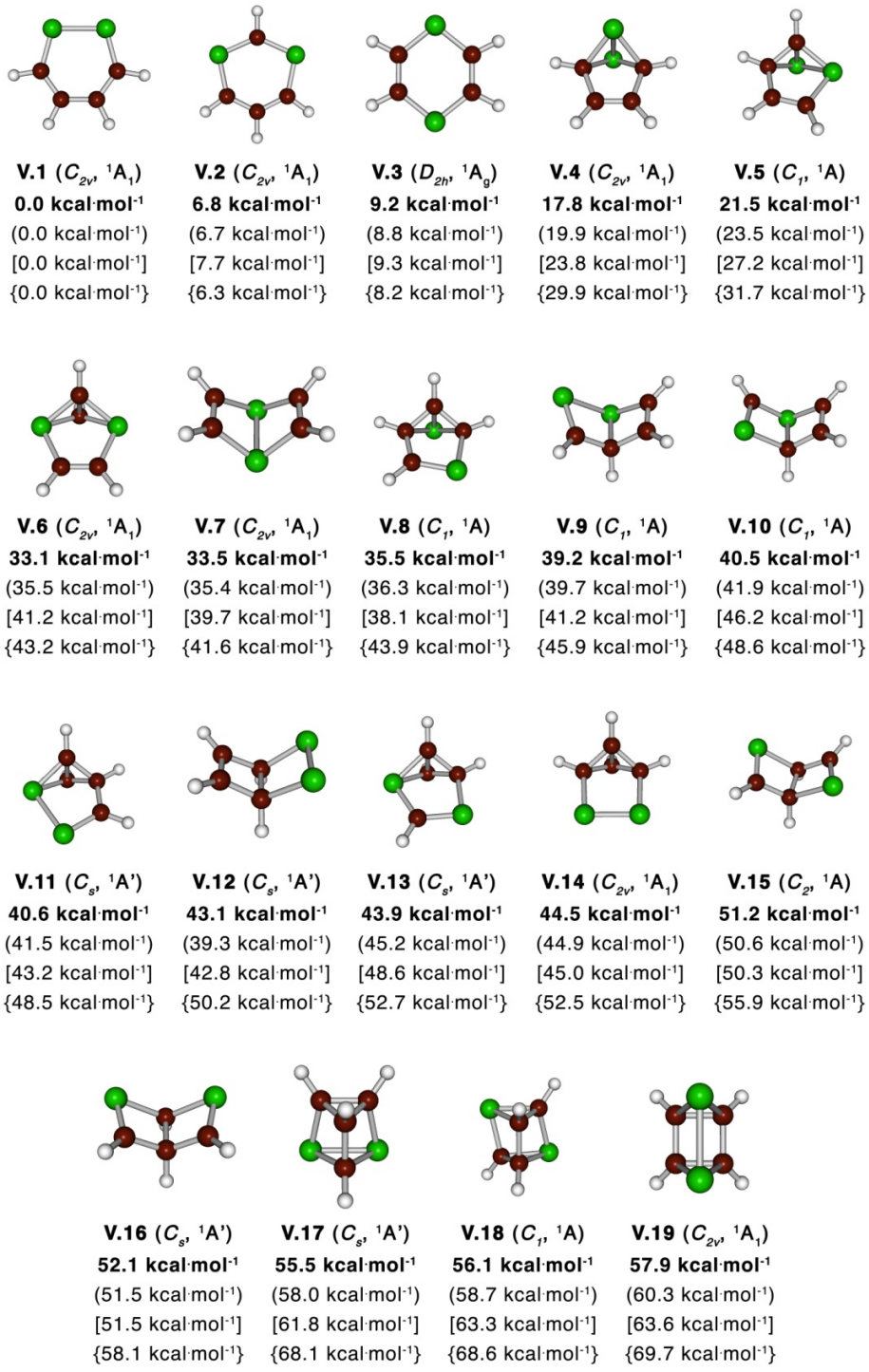

Fig. S5 Selected isomers of $C_4H_4P_2$, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G**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

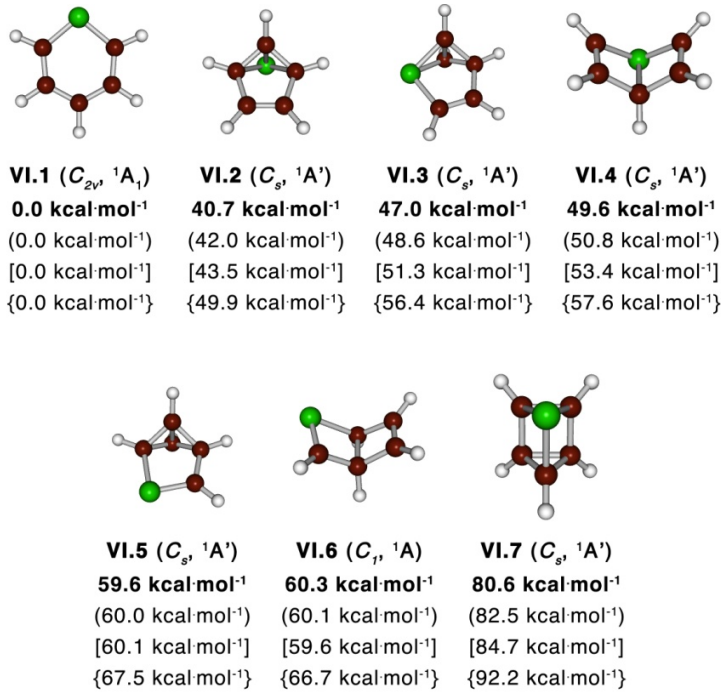

Fig. S6 Selected isomers of C_5H_5P, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G**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

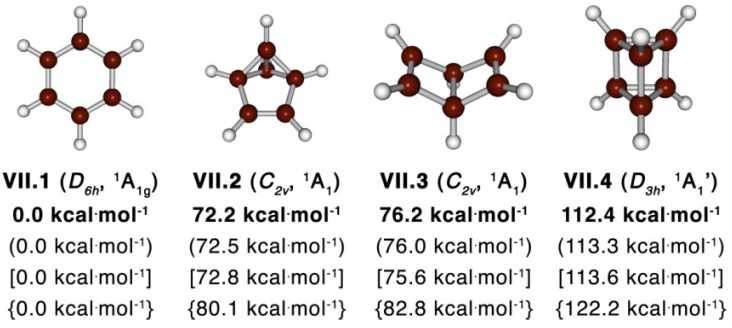

Fig. S7 Selected isomers of C_6H_6, their point group symmetries, spectroscopic states and ZPE corrected relative energies. The energies are given at: CCSD(T)/CBS (bold), CCSD(T)/cc-pVTZ (in brackets), CCSD(T)/cc-pVDZ (square brackets), and B3LYP/6-311++G** (curly brackets), all at B3LYP/6-311++G** optimized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

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

Distance (Å)	P_6	CHP_5	$C_2H_2P_4$			$C_3H_3P_3$			$C_4H_4P_2$			C_5H_5P	C_6H_6
	I.11	II.16	III.5	III.10	III.13	IV.2	IV.4	IV.5	V.I	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	$C_2H_2P_4$			$C_3H_3P_3$			$C_4H_4P_2$			C_5H_5P	C_6H_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