Supporting Information

Computational Study of Phosphorus-Doped Graphdiynes and Several Corresponding Oxides by Simulated X-ray Spectroscopy

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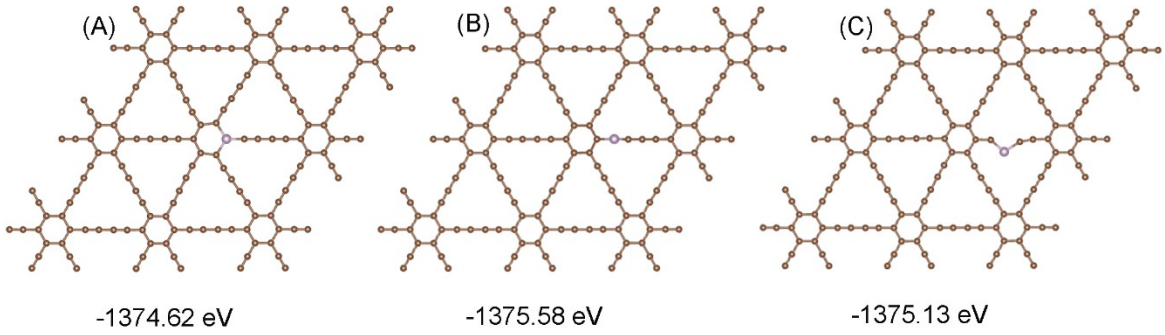

Fig. S1. Energy of single P-doped graphdiyne configurations (A-C) in the 3×3×1 supercell.

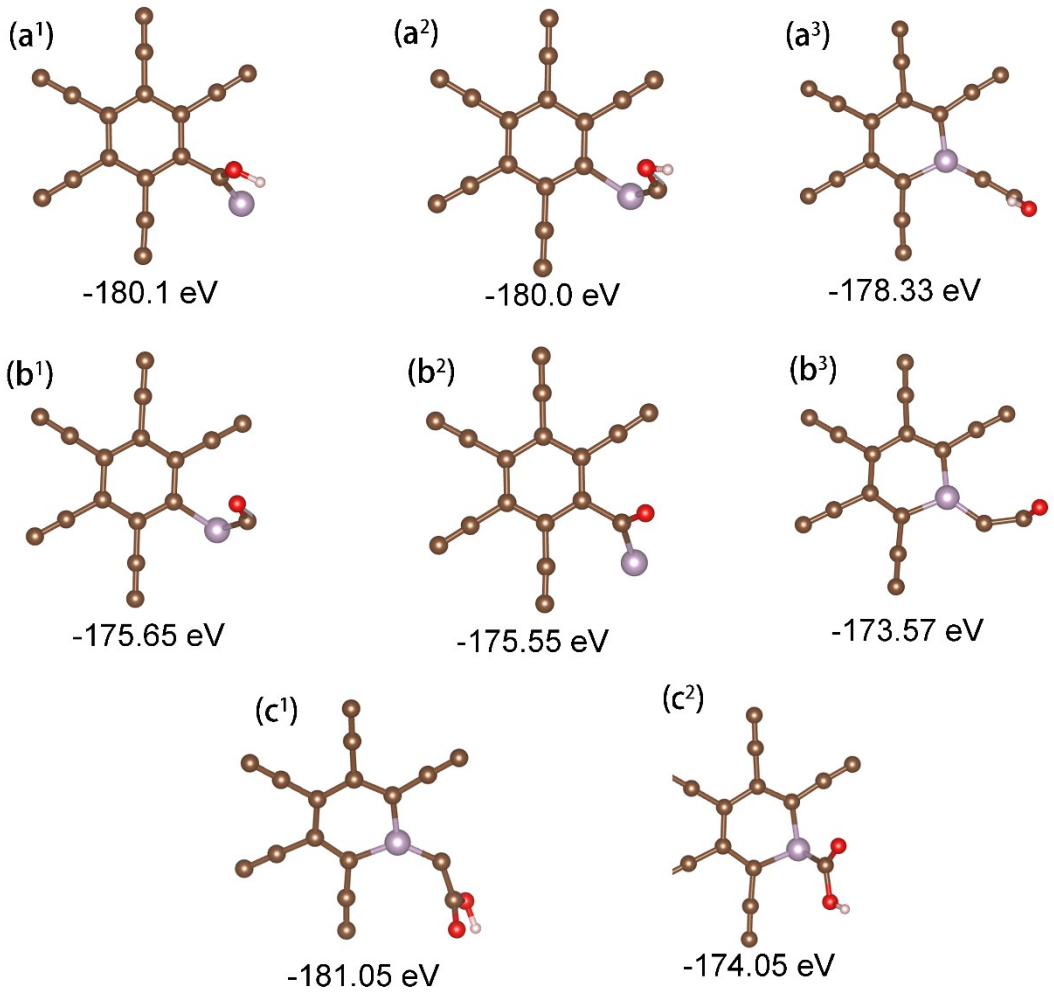

Fig. S2. The eight probable configurations for P-doped graphdiyne molecules in the 1×1×1 supercell

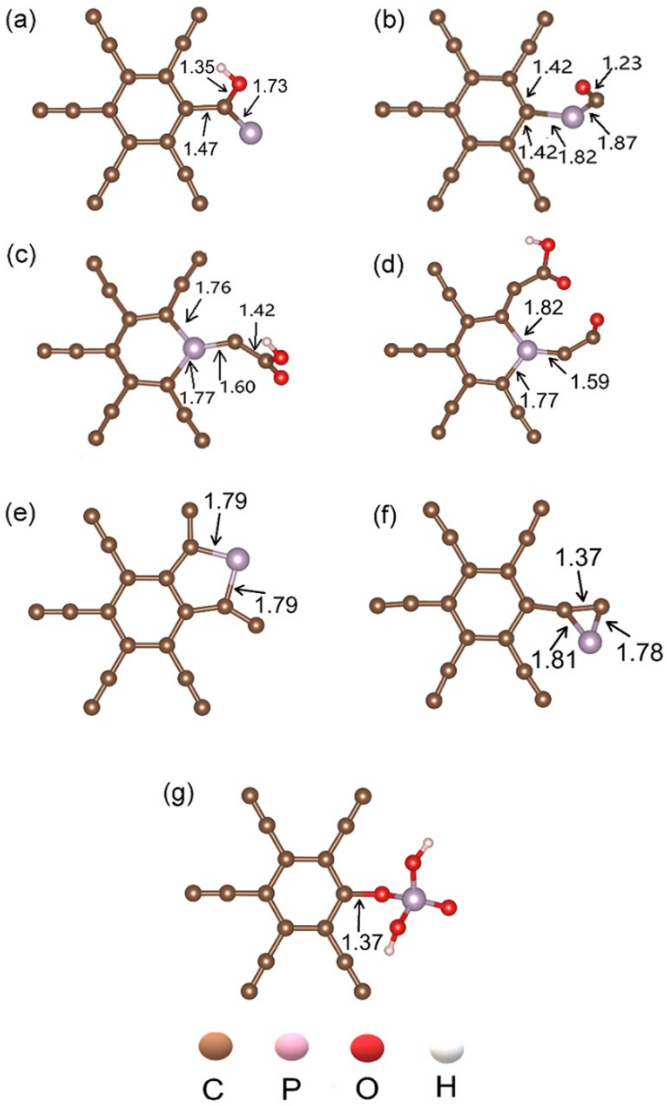

Fig. S3. The bond lengths (in Å) for the 7 P-doped graphdiyne molecules of the 3×3×1 supercell surrounding the P-doped core.

Table S1 Theoretically simulated C 1s ionization energy of different bonding types in pure graphdiyne and 7 P-doped graphdiyne molecules.

structures		C 1s edge				
		C-C(sp^2)	C-C(sp)	C-P(sp)	C-O	C=O
pure		284.8	284.0			
P-GDY	a	285.0	284.3		286.3	
	b	285.3	284.5	284.7	286.3	
	c	285.7	284.5	285.4		287.6
	d	285.9	284.7	285.0	286.3	288.2
	e	285.0	284.1	284.8		
	f	285.0	284.3	284.5		
	g	285.7	284.9		286.6	
Fitted[(a-g)]		285.3	284.5	286.4	285.0	287.7