

Supporting Information

Table S1: Total energies, E , in a.u., of the planar and butterfly structures and relative energies, ΔE , in kcal/mol, with the aug-cc-pVTZ basis set.

		$E(\text{CASSCF})$	ΔE	$E(\text{MCQDPT})$	ΔE
$[\text{P}(\mu\text{-NH})]_2$	planar	-791.6258543167	0.0	-792.3244086628	0.0
	butterfly	-791.5818591473	27.6	-792.2900883300	21.5
$[\text{P}(\mu\text{-PH})]_2$	planar	-1364.1246368859	0.0	-1364.7283170654	0.0
	butterfly	-1364.2089191167	-52.9	-1364.8036314186	-47.3
$[\text{P}(\mu\text{-AsH})]_2$	planar	-5151.1376314112	0.0	-5151.6989709794	0.0
	butterfly	-5151.1975694157	-37.6	-5151.7728376173	-46.4
$[\text{As}(\mu\text{-NH})]_2$	planar	-4578.5870774368	0.0	-4579.2700045286	0.0
	butterfly	-4578.5504031071	23.0	-4579.2425912021	17.2
$[\text{As}(\mu\text{-PH})]_2$	planar	-5151.1651792766	0.0	-5151.7384822577	0.0
	butterfly	-5151.2098052964	-28.0	-5151.782614662	-27.7
$[\text{As}(\mu\text{-AsH})]_2$	planar	-8938.1579075249	0.0	-8938.6745275000	0.0
	butterfly	-8938.2065856835	-30.5	-8938.7447733220	-44.1