Supplementary Materials: *PP*-Rotation, *P*-Inversion and Metathesis in Diphosphines Studied by DFT Calculations: Comments on Some Literature Conflicts

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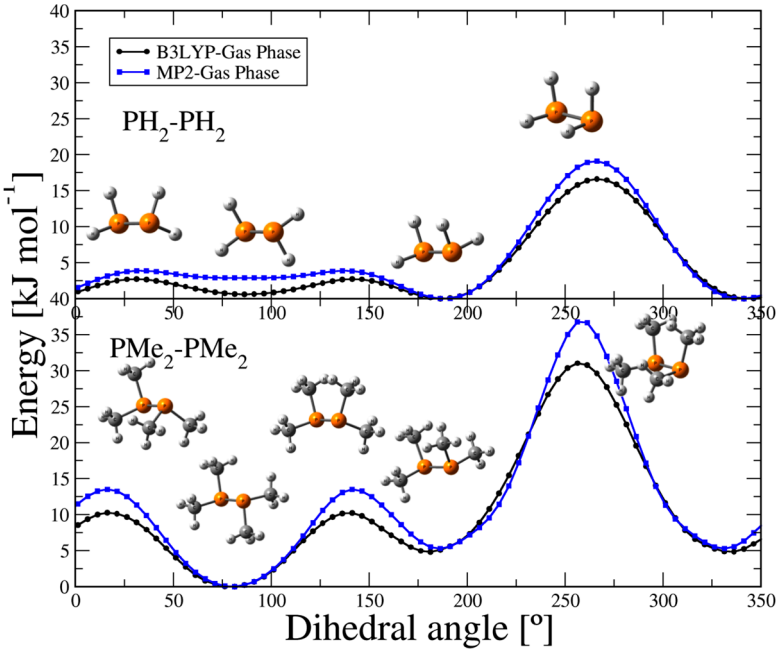

Figure S1. PES for H_4P_2 and Me_4P_2, corresponding to the rotation along the molecular axis, at MP2 and B3LYP/6-311++G(d,p) computational level in gas phase. Orange, grey and white atoms corresponds to P, C and H atoms respectively.

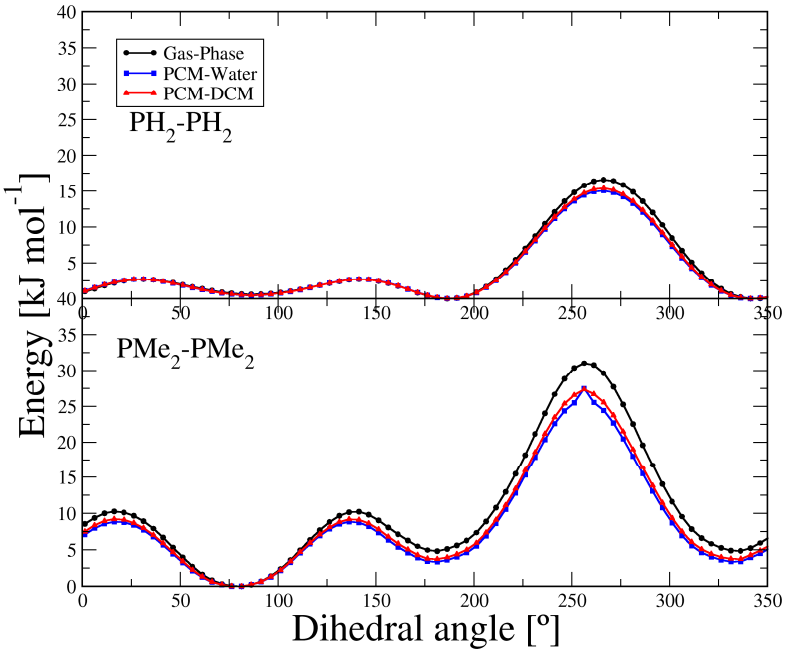

Figure S2. PES for H_4P_2 and Me_4P_2, corresponding to the rotation along the molecular axis and B3LYP/6-311+G(d,p), gas phase, PCM-Water and PCM-DCM.

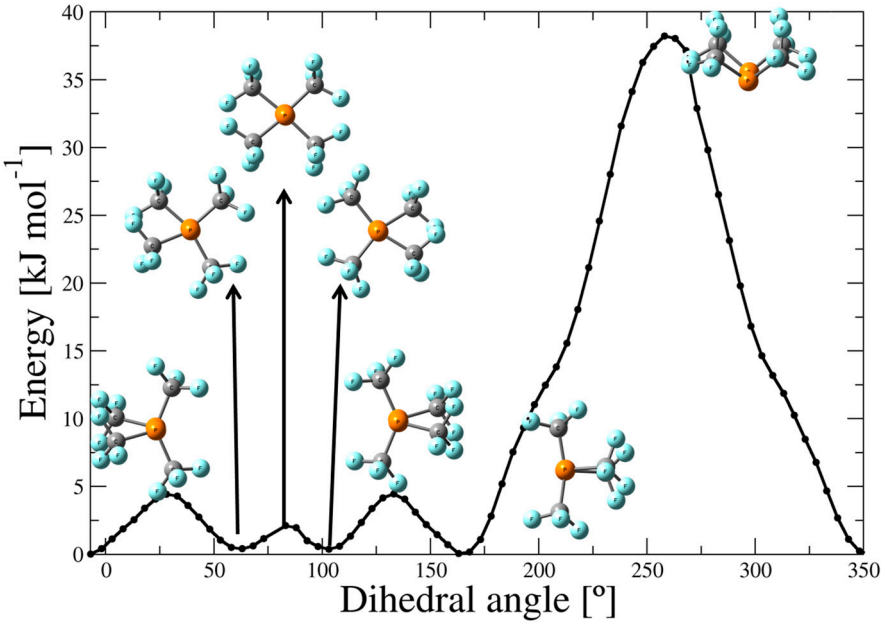

Figure S3. PES for $(CF_3)_4P_2$ corresponding to the rotation along the molecular axis and B3LYP/6-311++G(d,p)/PCM-DCM.

Table S1. Relative energies of *anti* and *gauche* conformers of H_4P_2, Me_4P_2, and $(CF_3)_2P_2$ systems at the B3LYP/6-311++G(d,p), M06-2X/6-311++G(d,p) and M06-2X/aug-cc-pVTZ computational level.

B3LYP/6-311++G(d,p)	M06-2X/6-311++G(d,p)	M06-2X/aug-cc-pVTZ
0.9	−1.1	−0.8
4.4	5.7	6.3
1.5	1.4	3.2