Captions to Figures S1 – S17

Figure S1   Selected internuclear distances (Å) in D_{2h} H_2P (upper panel) and H_2Pz (lower panel) molecules.

Figure S2   Selected internuclear distances (Å) in D_{2h} H_2TPP (upper panel) and H_2Pc (lower panel) molecules.

Figure S3   Selected internuclear distances (Å) in D_{4h} P^{2-} (upper panel) and Pz^{2-} (lower panel) molecular ions.

Figure S4   Selected internuclear distances (Å) in D_{4h} TPP^{2-} (upper panel) and Pc^{2-} (lower panel) molecular ions.

Figure S5   Energy position of the GS H_2P, H_2TPP, H_2Pc, and H_2Pz FMOs compared with the Py and i-Ind HOMO energies.

Figure S6   3D CPs of the Py $1a_2$ HOMO (left panel) and the i-Ind $2a_2$ HOMO (right panel). Displayed isosurfaces correspond to ± 0.02 $e^{1/2} \times$ Å$^{-3/2}$ values. Isolated Py and i-Ind have a C_{2v} symmetry.

Figure S7   3D CP of the i-IND $1a_2$ π MO. Displayed isosurfaces correspond to $\pm 0.02 e^{1/2} \times$ Å$^{-3/2}$ values.

Figure S8   3D CPs of the H_2P FMOs generated by the $1a_2$ Py HOMO. The 3D CP of the $5b_{1u}$ FMO has been also displayed to show the absence of any parenthood with the Py $1a_2$ HOMO. Displayed isosurfaces correspond to ± 0.02 $e^{1/2} \times$ Å$^{-3/2}$ values.

Figure S9   3D CPs of low-lying H_2P π MOs. Displayed isosurfaces correspond to $\pm 0.02 e^{1/2} \times$ Å$^{-3/2}$ values.

Figure S10   Qualitative representation of the parenthood between $^{pmc}\pi$ and $^{pmc}\pi^*$ FMOs upon the $D_{2h} \rightarrow D_{4h}$ switching. Energy differences are not in scale while the ordering of the energy levels is that of the H_2TPP (D_{2h}) and TPP^{2-} (D_{4h})

Figure S11   3D CPs of one partner of the unoccupied D_{4h} TPP^{2-} $12e_g$ and $9b_{1u}$ π^* MOs (upper panel). 3D CPs of one partner of the D_{4h} Pc^{2-} $6e_g$ and $3b_{1u}$ π^* MOs (lower panel). Displayed isosurfaces correspond to $\pm 0.02 e^{1/2} \times$ Å$^{-3/2}$ values. The 3D CP of the occupied TPP^{2-} and Pc^{2-} $2a_{1u}$ MO is also reported. The $2a_{1u}$ MO corresponds, both in TPP^{2-} and Pc^{2-}, to an occupied π orbital, highly localized on the pmc and characterized by four nodal planes passing through N^{Py} (σ_v) and X^m (σ_d), X = C in TPP^{2-} and X = N in Pc^{2-}. The $2a_{1u}$ MO absolute energy value is 0.924 eV and 0.883 eV in TPP^{2-} and Pc^{2-}, respectively. TPP^{2-} and Pc^{2-} optimized Cartesian coordinates are those reported in Table S7 and Table S8, respectively.

Figure S12   Licorice representation of superimposed optimized structures of (a) CoPc and CoPc$^+$, (b) NiPc and NiPc$^+$, (c) CuPc and CuPc$^+$, and (d) ZnPc and ZnPc$^+$. BP86 optimized Cartesian coordinates of $^2A_{1g}$ CoPc and $^3A_{1u}$ CoPc$^+$ are reported in Table S23 and Table S24, respectively; BP86 optimized Cartesian coordinates of $^1A_{1g}$ NiPc and $^2A_{1u}$ NiPc$^+$ are reported in Table S27 and Table S28, respectively; BP86 optimized Cartesian coordinates of $^2B_{1g}$ CuPc and $^3B_{1u}$ CuPc$^+$ are reported in Table S30 and Table S31, respectively; BP86 optimized Cartesian coordinates of $^1A_{1g}$ ZnPc and $^2A_{1u}$ ZnPc$^+$ are reported in Table S33 and Table S34, respectively.

Figure S13   Schematic representation of the $^S_TCM^{nnn}_{100}$ ns AOs SALC of symmetry a, b, and e. Large red and green spheres represent ^SCM ns AOs and corresponding different phases.

Figure S14   Schematic representation of the $^S_HCM^{nn}_{100}$ ns AOs SALC of symmetry a, b, and e. Large red and green spheres represent ^SCM ns AOs and corresponding different phases.

Figure S15   Schematic representation of the $^S_B CM^{nn}_{100}$ ns AOs SALC of symmetry a and b. Large red and green spheres represent ^{S}CM ns AOs and corresponding different phases.

Figure S16   Schematic representation of the $^S_T CM^{nnn}_{111}$ ns AOs SALC of symmetry a, b, and e (1e and 2e). Large red and green spheres represent ^{S}CM ns AOs and corresponding different phases.

Figure S17   Schematic representation of the $^S_H CM^{nnn}_{111}$ ns AOs SALC of symmetry a and e. Large red and green spheres represent ^{S}CM ns AOs and corresponding different phases.