

## Supporting Information

### **How Aromatic Are Molecular Nanorings? The Case of a Six-Porphyrin Nanoring\*\***

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## Supporting Information

### 1 Computational details

Following the computational work of Ref. 1, we have studied four different oxidation states of the six-porphyrin nanoring: neutral, +4, +6, and +12. The molecules have been studied considering not only the isolated belt structure (c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup>) but also taking into account the encapsulated template and the two phenyl substituents in each porphyrin (c-P6·T6, c-P6·T6<sup>4+</sup>, c-P6·T6<sup>6+</sup>, and c-P6·T6<sup>12+</sup>).

Geometry optimizations and frequency calculations have been performed with the Gaussian16 software package<sup>2</sup> using B3LYP,<sup>3-6</sup> CAM-B3LYP,<sup>7</sup> LC- $\omega$ HPBE ( $\omega=0.1$  and  $\omega=0.2$ ),<sup>8</sup> and M06-2X<sup>9</sup> density functional approximations (DFAs) including Grimme's D3 dispersion correction (for the first two DFAs)<sup>10</sup> and in combination with the 6-31G\* basis set.<sup>11</sup> The initial structures have been obtained from a previous work.<sup>1</sup> The geometry minima of all the oxidation states of c-P6 and the transition state of c-P6<sup>6+</sup> have been confirmed by analyzing the harmonic frequencies and the stability of the single-determinant wavefunction with respect to relaxing various constraints (spin and orbital symmetry, real orbitals) was confirmed. For c-P6<sup>4+</sup> and c-P6<sup>6+</sup>, single-point coupled-cluster calculations were performed with ORCA software package<sup>12</sup> using DLPNO-CCSD(T)<sup>13</sup> with resolution of identity<sup>14</sup> in combination with the Def-SVP/C basis set<sup>15</sup> and the corresponding auxiliary basis set in order to obtain accurate reference calculations to assess the accuracy of DFAs. Additional optimization and magnetic calculations have been performed with 6-31+G\* and 6-311+G\* basis sets. The results, which are collected in Tables S15 and S16, show that the conclusions drawn for these systems do not change with the basis set size.

The calculation of the electronic aromaticity indices (AV1245,<sup>16</sup> AV<sub>min</sub>,<sup>17</sup> BOA,<sup>18</sup> and FLU<sup>19,20</sup>) and the delocalization indices (DIs)<sup>21,22</sup> employs the quantum theory of atoms in molecules (QTAIM)<sup>23</sup> atomic partition performed by the AIMAll software.<sup>24</sup> The atomic overlap matrices resulting from this partition and the wavefunction files are the input of the in-house ESI-3D code,<sup>19,25,26</sup> which provides AV1245,<sup>16</sup> AV<sub>min</sub>,<sup>17</sup> BLA,<sup>18</sup> BOA,<sup>18</sup> DIs,<sup>22,26</sup> FLU,<sup>19,20</sup> the harmonic oscillator model of aromaticity (HOMA),<sup>27</sup> and MCI<sup>28</sup> values. The numerical integrations of the atoms in the QTAIM<sup>23</sup> as well as the corresponding oxidation states have errors below 0.004 and 0.03 electrons for c-P6 (in all its oxidation states) and c-P6·T6 (in all its oxidation states), respectively. The ESI-3D code is available upon request (ematito@gmail.com).<sup>19,25,26</sup> Anisotropy of the induced current density (ACID)<sup>29</sup> and nuclear-independent chemical shift (NICS)<sup>30-34</sup> calculations were conducted using the CSGT and GIAO methods, respectively, using Gaussian software packages (Gaussian09<sup>35</sup> and Gaussian16<sup>2</sup>). NICS grids were calculated with 1Å resolution (plots 20Å x 20Å grid) and the plots were generated with a Python script. The version 2.0.0 of the AICD program<sup>29</sup> was used to generate ACID results and they were visualized using POV-Ray.<sup>36</sup>

We also dissected AV1245 values and assigned a delocalization value to each atom in the corresponding pathway by splitting the MCI(1,2,4,5) of each five-atom fragment among the atoms in the fragment.<sup>16</sup> These profiles are called 1245-index distribution plots and help detect the fragments responsible for the loss of aromaticity.

The effective oxidation state (EOS) analysis<sup>37,38</sup> was performed with APOST-3D. The software provided in Ref. 39 was used to assess the similarity of two molecular geometries through the calculation of the root mean square deviation (RMSD) of the atomic distances.

NMR calculations were also performed using GIAO method in Gaussian16 software package<sup>2</sup> with B3LYP,<sup>3,4</sup> CAM-B3LYP,<sup>7</sup> and M06-2X<sup>9</sup> functionals including Grimme's D3 dispersion correction<sup>10</sup> and in combination with the 6-31G\* basis set.<sup>11</sup> Solvent effects of dichloromethane were taken into account using the Polarizable Continuum Model (PCM).<sup>40</sup>

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† Dedication: We dedicate this paper to the memory of our friend and colleague, Professor Istvan Mayer, whose works have been a continuous inspiration.

## 2 Geometry assessment

In order to quantify the structural differences among the several optimized geometries, the root mean square deviation (RMSD) of two molecules has been calculated. The RMSD of two structures was calculated using the software provided in Ref. 39. This program calculates the RMSD between two Cartesian geometries in either .xyz or .pdb format and uses the Kabsch algorithm (1976)<sup>41</sup> or Quaternion algorithm<sup>42</sup> if rotation is needed before the calculation of RMSD. All the RMSD values included in this work compare two structures ignoring all the hydrogen atoms.

From the data in Table S1, we conclude that the structures found by Anderson *et al.* at the B3LYP/6-31G\* level of theory were not absolute minima of the corresponding potential energies for c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup>. However, their geometries are very similar to the ones we have found in this work at the same level of theory.

**Table S1** Energy comparison and the RMSD of the minimum geometries calculated by Anderson *et al.*<sup>1</sup> and this work at the B3LYP/6-31G\* level of theory. Energy units are atomic units (au) while RMSD are in Ångstroms (Å).

Species	Energy (Ref. 1) <sup>a</sup>	Energy (this work)	RMSD
c-P6	-17512.513898	-17512.514222	0.001
c-P6 <sup>4+</sup>	-17511.456927	-17511.457194	0.040
c-P6 <sup>6+</sup>	-17510.640233	-17510.640427	0.033
c-P6 <sup>12+</sup>	-17507.033356	-17507.033566	0.015

<sup>a</sup> Geometries from Ref. 1.

**Table S2** Comparison between the geometries calculated at the B3LYP, CAM-B3LYP, and M06-2X methods. The columns 2-4 give the total energy of the molecules at the corresponding geometry. The third last columns correspond to the RMSD values obtained from these geometries. All the calculations employed the 6-31G\* basis set. Energy units are atomic units (au) while RMSD are in Ångstroms (Å).

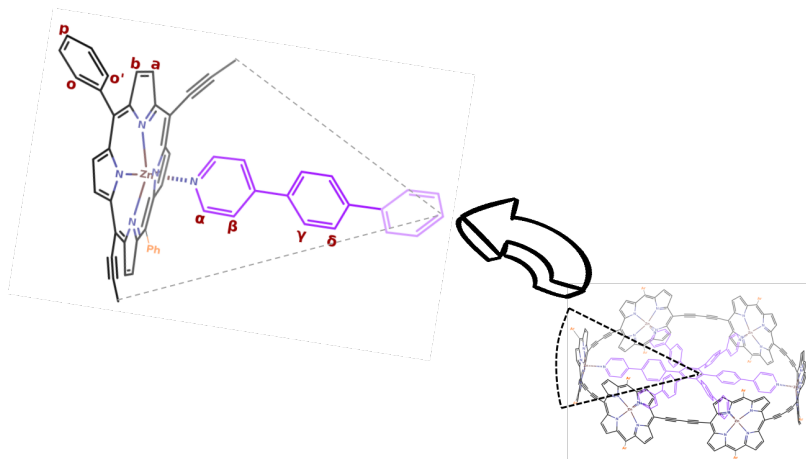
Species	G <sub>1</sub> (B3LYP)	G <sub>2</sub> (CAM-B3LYP)	G <sub>3</sub> (M06-2X)	RMSD(G <sub>1</sub> -G <sub>2</sub> )	RMSD(G <sub>2</sub> -G <sub>3</sub> )	RMSD (G <sub>1</sub> -G <sub>3</sub> )
c-P6	-17512.514222	-17509.042830	-17509.271928	0.049	0.021	0.041
c-P6 <sup>4+</sup>	-17511.457194	-17507.935387	-17508.138955	0.661	0.666	0.201
c-P6 <sup>6+</sup>	-17510.640427	-17507.119479	-17507.306773	0.224	0.031	0.206
c-P6 <sup>12+</sup>	-17507.033566	-17503.560977	-17503.701580	0.040	0.031	0.036

The results of Table S2 demonstrate that the B3LYP energy minima found for c-P6 and c-P6<sup>12+</sup> structures are well reproduced by the CAM-B3LYP and M06-2X methods. However, the geometries of the B3LYP energy minima of c-P6<sup>4+</sup> and c-P6<sup>6+</sup> are significantly different from those found at the M06-2X and CAM-B3LYP levels of theory. Since the latter functional approximations do not suffer from large electron delocalization errors, one is prompted to conclude that B3LYP overestimates the symmetry of c-P6<sup>6+</sup> (and, hence, its aromaticity, see below), whereas it overestimates the asymmetry of c-P6<sup>4+</sup> (RMSD=0.661) resulting in a spurious enhancement of the antiaromatic features of this molecule (see below). Similar results have been recently reported by our group<sup>18,43-46</sup> and others.<sup>47-50</sup>

We have also characterized the structure of c-P6<sup>6+</sup> using the LC- $\omega$ HPBE<sup>8,51</sup> method with  $\omega=0.1$  and  $\omega=0.2$  in combination with the 6-31G\* basis set. Using LC- $\omega$ HPBE with  $\omega=0.1$ , the optimized structure lies in between the B3LYP and CAM-B3LYP ones, as confirmed by the fact that the RMSD values between the LC- $\omega$ HPBE( $\omega=0.1$ ) geometry and these two geometries are quite similar (0.160 and 0.142, for B3LYP and CAM-B3LYP, respectively). On the contrary, LC- $\omega$ HPBE with  $\omega=0.2$  provides a geometry closer to the CAM-B3LYP one (RMSD=0.095). This further demonstrates the importance of including a large percentage (typically above 50%) of HF exchange in the functional in order to correctly characterize conjugated molecules (avoiding the delocalization error<sup>52</sup>).

### 3 $^1\text{H-NMR}$ calculations

We have calculated the  $^1\text{H-NMR}$  spectra for all species, including the template structure and the phenyl substituents. The most important protons for the study of aromaticity are highlighted in the following figure.



**Figure S1** Nanoring's structure where the most important protons of the  $^1\text{H-NMR}$  spectra are highlighted (see also Table S3).

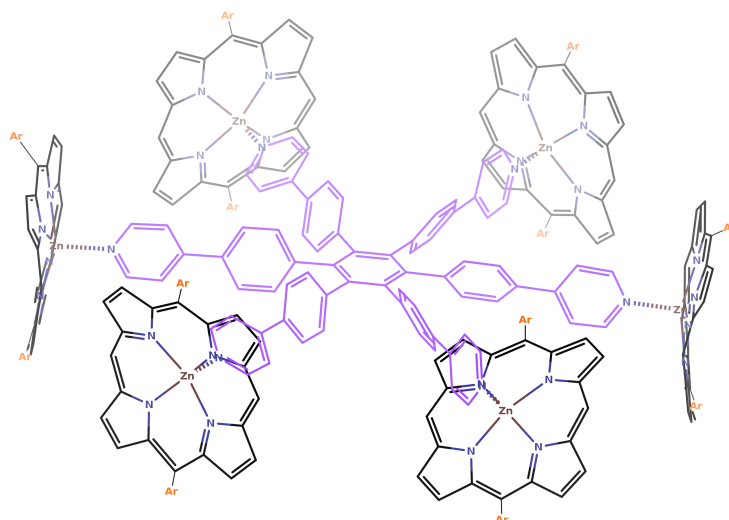
In Table S3, we have summarized the shielding of the most relevant protons for the study of aromaticity and compared them with the experimental values from the literature.<sup>1</sup>

**Table S3**  $^1\text{H-NMR}$  values (in ppm) calculated using CAM-B3LYP, M06-2X, and B3LYP methods in combination with 6-31G\* basis set and using  $\text{CH}_2\text{Cl}_2$  as a solvent (PCM model).<sup>40</sup> We have compared with the experimental data from the literature.<sup>1</sup> Maximum error (MAX), root mean square error (RMSE), and mean absolute error (MAE) of each method are also given.

Proton	c-P6·T6				c-P6·T6 <sup>4+</sup>				c-P6·T6 <sup>6+</sup>				c-P6·T6 <sup>12+</sup>			
	CAM-B3LYP	M06-2X	B3LYP	Experimental	CAM-B3LYP	M06-2X	B3LYP	Experimental	CAM-B3LYP	M06-2X	B3LYP	Experimental	CAM-B3LYP	M06-2X	B3LYP	Experimental
$\alpha$	2.28	2.72	3.18	2.41	6.69	9.02	68.95	22.7	7.65	8.08	-3.74	5.71	10.50	11.32	14.15	11.31
$\beta$	4.68	5.23	5.13	4.99	6.79	8.81	56.20	19.9	6.87	7.38	-2.75	5.27	8.35	9.10	9.78	8.83
$\gamma$	5.32	5.74	5.65	5.45	6.90	8.62	50.52	-	6.85	7.25	-1.65	5.17	7.96	8.55	8.93	7.94
$\delta$	5.55	5.94	5.83	5.56	6.91	8.49	49.97	-	6.82	7.18	-1.03	5.17	7.84	8.35	8.58	7.73
a	9.74	10.39	9.38	9.56	8.29	9.08	14.10	-	7.44	8.02	6.02	6.52	6.50	6.97	4.31	6.05
b	8.95	9.58	8.66	8.75	7.82	8.60	17.05	-	7.06	7.57	4.94	5.99	6.04	6.51	4.28	5.77
o	8.13	8.84	7.92	8.06	7.71	8.10	-0.63	-	7.69	8.39	9.36	7.78	7.90	8.56	8.49	7.31
o'	8.21	8.85	8.23	8.32	8.12	9.50	35.74	-	7.51	8.03	2.13	5.91	6.99	7.55	5.82	6.57
p	7.97	8.51	7.85	8.02	7.98	8.74	14.66	-	7.85	8.41	6.51	7.92	7.98	8.61	7.78	7.58
MAX	0.31	0.83	0.77	0.00	-	-	-	-	1.94	2.37	9.45	0.00	0.81	1.25	2.84	0.00
MAE	0.13	0.52	0.23	0.00	-	-	-	-	1.18	1.65	4.31	0.00	0.39	0.71	1.22	0.00
RMSE	0.16	0.57	0.30	0.00	-	-	-	-	1.35	1.77	5.36	0.00	0.45	0.80	1.41	0.00

All the errors presented in Table S3 (MAX, MAE, and RMSE) clearly indicate that the functional that better reproduces the experimental data is CAM-B3LYP. While errors are of similar magnitude for c-P6·T6, they are much larger for c-P6·T6<sup>6+</sup>, indicating that B3LYP geometry is quite different from the experimental one.

To assess to which extent we can rely on the  $^1\text{H-NMR}$  data to analyze the aromaticity of these systems, we have constructed a structure that has no current, therefore, is not aromatic. To construct it, we have taken the optimized structure of each species and replaced all the bridging butadiyne linkers by capping hydrogen atoms. Then, we made a single-point calculation to obtain the chemical shieldings of the disconnected structure (see Figure S2). In the following table, the chemical shielding of the protons that are used to analyze of the aromatic character are presented for both disconnected and connected structures of the nanoring's species. In addition, the  $^1\text{H-NMR}$  chemical shift of  $\alpha$  and  $\beta$  protons of the free template are presented in Table S5.



**Figure S2** Nanoring's disconnected structure where the bridging butadiyne linkers have been removed.

**Table S4** Selected  $^1\text{H-NMR}$  chemical shift (in ppm) calculated using CAM-B3LYP and B3LYP methods in combination with 6-31G\* basis set and using  $\text{CH}_2\text{Cl}_2$  as a solvent (PCM model).<sup>40</sup> Experimental data is taken from Ref. 1 and Ref. 53. For each species we include the values of the nanoring's structure (connected) and an idealized model, where the bridging butadiyne linkers have been removed (disconnected) (See Figure S2)

Method	data	c-P6 · T6		c-P6 · T6 <sup>4+</sup>		c-P6 · T6 <sup>6+</sup>		c-P6 · T6 <sup>12+</sup>	
		Connected	Disconnected	Connected	Disconnected	Connected	Disconnected	Connected	Disconnected
CAM-B3LYP	$\alpha$	2.28	1.93	6.69	9.95	7.65	13.62	10.50	10.60
	$\beta$	4.68	4.47	6.79	7.77	6.87	9.32	8.35	8.35
	o	8.13	8.17	7.71	7.38	7.69	7.36	7.90	7.93
	o'	8.21	8.24	8.12	6.88	7.51	6.21	6.99	6.98
B3LYP	$\alpha$	3.18	2.09	68.95	9.03	-3.74	15.34	14.15	14.42
	$\beta$	5.13	4.46	56.20	6.66	-2.75	9.89	9.78	9.84
	o	7.92	8.02	-0.63	7.48	9.36	7.07	8.49	8.52
	o'	8.23	8.12	35.74	6.05	2.13	5.68	5.82	5.82
Experimental	$\alpha$	2.41	-	22.7	-	5.71	-	11.31	-
	$\beta$	4.99	-	19.9	-	5.27	-	8.83	-
	o	8.06	-	-	-	7.78	-	7.31	-
	o'	8.32	-	-	-	5.91	-	6.57	-

**Table S5**  $^1\text{H-NMR}$  chemical shift of  $\alpha$  and  $\beta$  protons of the free template (in ppm) calculated using CAM-B3LYP and B3LYP methods in combination with 6-31G\* basis set and using  $\text{CH}_2\text{Cl}_2$  as a solvent (PCM model).<sup>40</sup> Experimental data is taken from Ref. 1.

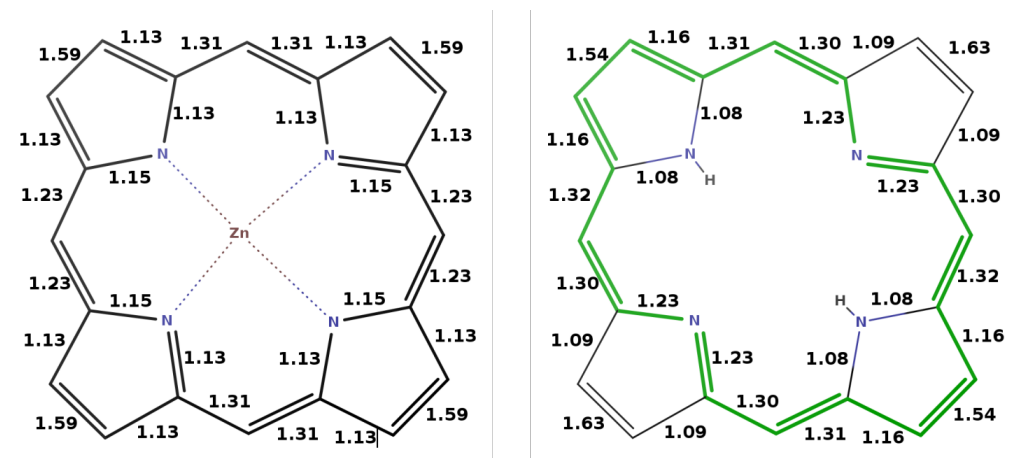
data	CAM-B3LYP	B3LYP	Experimental
$\alpha$	8.62	8.52	8.54
$\beta$	7.22	7.10	7.33

Comparing the  $^1\text{H-NMR}$  data of all the species' connected and disconnected structures, we can appreciate that the values are pretty similar. Even in some cases, the disconnected structure presents a slightly higher value. Therefore, these results show that, although the porphyrins are not connected, a ring current is present. For this reason, we can say that this is another piece of evidence that proves that none of the species studied is aromatic.

## 4 Aromaticity

### 4.1 Porphyrinoid reference systems

In order to assess the aromaticity of the molecules presented in the manuscript, we have collected in Table S6 the aromaticity indices for the different pathways of a simple aromatic porphyrin molecule, porphin (**18H**). All the values presented in this section regarding **18H** were calculated at the CAM-B3LYP/6-311G(d,p) level of theory.<sup>43</sup> A molecular graph of porphin, with delocalization indices values included, can be found in Figure S3. If the pathway goes either through C-N bonds of the pyrrole or the imine groups, this fragment is labeled as "i" (inner), otherwise "o" (outer) is used. As a result, all the pathways are characterized by four letters, the first of which corresponds to pyrrole group at the top-left corner of Figure S3. The "oioi" pathway corresponds to the annulene pathway.



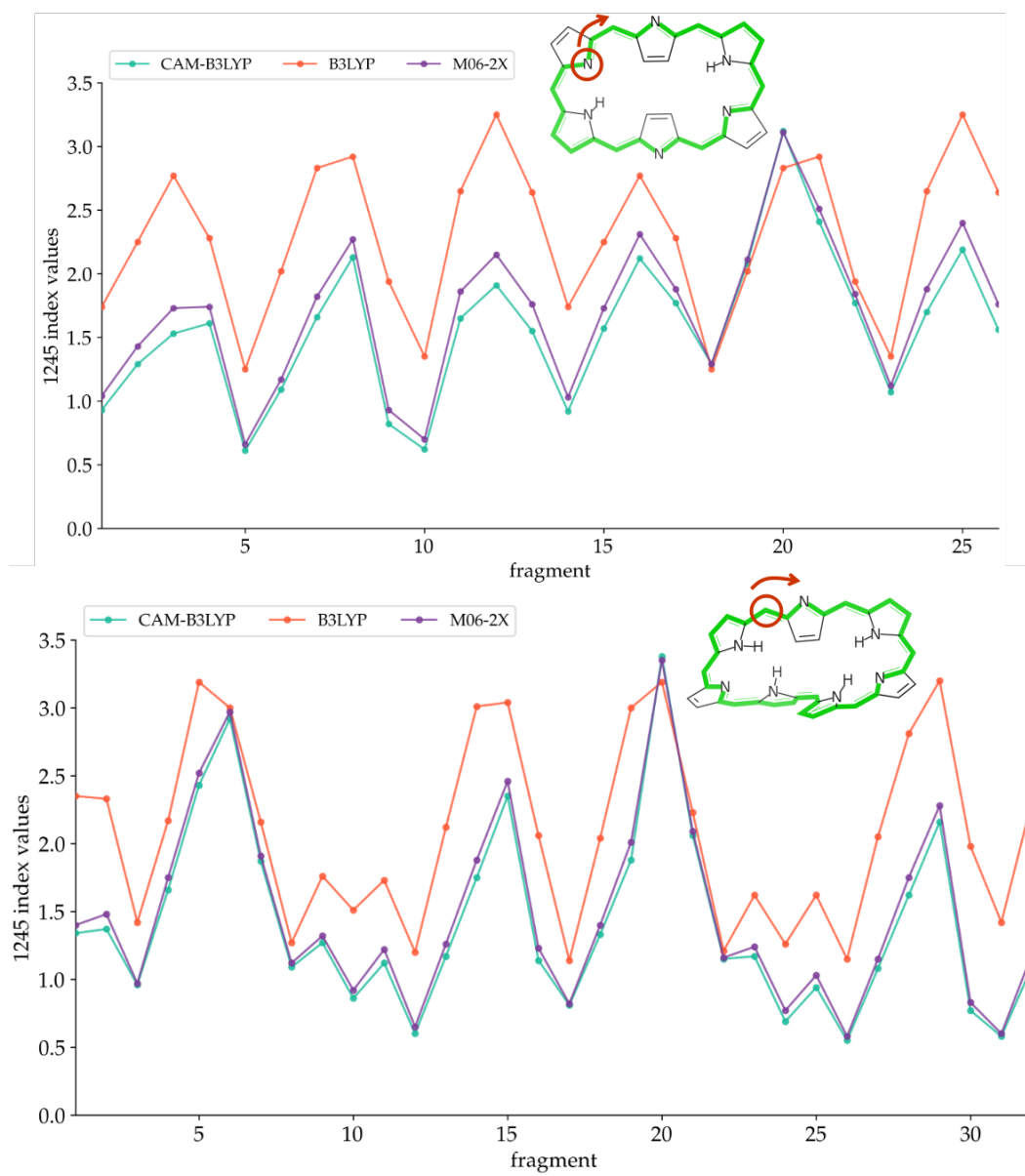
**Figure S3** Delocalization indices of (left) c-P6 porphyrins and (right) porphin. In green, we have highlighted the annulene pathway (the most aromatic one) of **18H**.<sup>43</sup> Calculations employed the CAM-B3LYP functional in combination with 6-31G\* and 6-311G\*\* basis set, respectively.

**Table S6** Aromaticity indices for the different pathways of porphin (**18H**). Geometries and some results extracted from Ref. 43. The number in parentheses indicates the number of pathways that are equivalent by symmetry.

pathway	FLU	BOA <sup>a</sup>	HOMA	BLA <sup>a</sup>	AV1245	AVmin
oioi	0.010	0.137	0.872	0.035	2.16	1.28
oooi (2)	0.016	0.202	0.734	0.047	1.91	0.49
oooo	0.022	0.260	0.610	0.058	1.70	0.49
ii oi (2)	0.008	0.111	0.917	0.026	1.57	0.13
ooii (4)	0.015	0.180	0.769	0.040	1.36	0.13
ooio (2)	0.021	0.243	0.637	0.052	1.17	0.13
iiii	0.006	0.081	0.968	0.016	0.91	0.13
iiio (2)	0.013	0.157	0.808	0.031	0.73	0.13
ioio	0.019	0.224	0.666	0.045	0.57	0.13

<sup>a</sup> BOA and BLA were recalculated according to the formulation of Ref. 44.

In order to compare 1245-index distribution graphs of the nanoring structure with different oxidation states, we have included the 1245-index distribution plots of the  $26\pi$ -electron porphyrin in Hückel conformation (**26H**) and the  $32\pi$ -electron porphyrin in Möbius conformation (**32M**) as examples of aromatic expanded porphyrins (see Figure S4). For a detailed analysis of the aromaticity of **26H** and **32M** see Ref 43.



**Figure S4** 1245-index distribution along the most aromatic path, the annulene path, of (top) **26H** and (bottom) **32M** for the three DFAs exposed in combination with the 6-311G(d,p) basis set.<sup>54</sup> We have highlighted the first atom of the starting fragment of the 1245-index distribution with an orange circle and used an arrow to indicate the direction of the x-axis.





**Table S9** Aromaticity indices values of the three asymmetric porphyrins of c-P6<sup>4+</sup>. We can group the six porphyrins of the structure into three groups of two porphyrins each, according to symmetry. The members of the same group exhibit very similar aromaticity values. Labels P<sub>1</sub>, P<sub>2</sub>, and P<sub>3</sub> match with the representation exposed in Figure 6 of the manuscript. These porphyrins host inside Zn<sub>33</sub>, Zn<sub>48</sub>, and Zn<sub>96</sub>, respectively, where the numeration of the Zn atoms follows the numeration of the Cartesian coordinates given in a separate file of this Supporting Information.

	pathway	B3LYP					CAM-B3LYP					M06-2X							
		FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>
P <sub>1</sub>	oooo	0.024	0.206	0.598	0.043	1.36	0.63	0.025	0.206	0.642	0.041	1.35	0.32	0.027	0.231	0.583	0.048	1.35	0.44
	iiii	0.011	0.075	0.823	0.026	1.24	0.29	0.016	0.112	0.784	0.039	1.29	0.09	0.013	0.099	0.845	0.034	1.17	0.13
	ioio (2)	0.018	0.148	0.698	0.036	1.31	0.29	0.021	0.164	0.705	0.040	1.33	0.09	0.021	0.173	0.699	0.042	1.27	0.13
	iiio (4)	0.014	0.116	0.761	0.031	1.25	0.29	0.018	0.141	0.754	0.039	1.25	0.09	0.016	0.140	0.781	0.037	1.20	0.13
	iiio (2)	0.018	0.148	0.698	0.036	1.31	0.29	0.021	0.164	0.705	0.040	1.33	0.09	0.021	0.173	0.699	0.042	1.27	0.13
	iooi (2)	0.018	0.143	0.691	0.036	1.36	0.64	0.022	0.160	0.683	0.041	1.45	0.32	0.021	0.170	0.673	0.043	1.32	0.44
	oooi (4)	0.021	0.176	0.642	0.040	1.36	0.63	0.023	0.184	0.662	0.041	1.40	0.32	0.024	0.202	0.626	0.046	1.34	0.44
	oooo	0.026	0.203	0.546	0.044	1.34	0.55	0.028	0.209	0.594	0.043	1.34	0.26	0.030	0.222	0.518	0.045	1.30	0.30
	iiii	0.012	0.060	0.801	0.032	1.14	0.27	0.018	0.108	0.759	0.044	1.18	0.08	0.017	0.107	0.757	0.044	1.12	0.08
	ioio (2)	0.020	0.139	0.661	0.038	1.26	0.28	0.023	0.164	0.669	0.043	1.28	0.09	0.024	0.171	0.626	0.045	1.23	0.09
	iiio (4)	0.016	0.098	0.724	0.035	1.23	0.28	0.021	0.134	0.701	0.044	1.29	0.09	0.021	0.139	0.675	0.045	1.22	0.09
	iiio (2)	0.020	0.140	0.659	0.039	1.25	0.28	0.023	0.164	0.667	0.043	1.26	0.09	0.024	0.171	0.624	0.045	1.22	0.09
	iooi (2)	0.020	0.148	0.665	0.038	1.20	0.27	0.022	0.171	0.686	0.042	1.16	0.08	0.023	0.176	0.649	0.043	1.15	0.08
	oooi (4)	0.023	0.177	0.601	0.041	1.27	0.27	0.025	0.191	0.637	0.042	1.25	0.08	0.027	0.200	0.579	0.044	1.23	0.08
P <sub>2</sub>	oooo	0.023	0.187	0.607	0.037	1.35	0.56	0.025	0.206	0.642	0.041	1.35	0.32	0.025	0.190	0.620	0.036	1.36	0.42
	iiii	0.012	0.072	0.789	0.027	1.37	0.49	0.016	0.112	0.784	0.039	1.29	0.09	0.016	0.083	0.789	0.034	1.39	0.41
	ioio (2)	0.018	0.135	0.688	0.033	1.36	0.49	0.021	0.164	0.705	0.040	1.33	0.09	0.021	0.143	0.695	0.035	1.38	0.41
	iiio (4)	0.016	0.105	0.735	0.030	1.36	0.49	0.019	0.137	0.731	0.040	1.38	0.09	0.019	0.115	0.739	0.035	1.38	0.41
	iiio (2)	0.018	0.135	0.688	0.033	1.36	0.49	0.021	0.164	0.705	0.040	1.33	0.09	0.021	0.143	0.695	0.035	1.38	0.41
	iooi (2)	0.018	0.135	0.688	0.033	1.36	0.49	0.020	0.168	0.727	0.040	1.20	0.09	0.021	0.143	0.695	0.035	1.38	0.41
	oooi (4)	0.021	0.162	0.645	0.035	1.36	0.49	0.023	0.188	0.682	0.188	1.28	0.09	0.023	0.168	0.656	0.036	1.37	0.41
	oooo	0.026	0.203	0.548	0.044	1.33	0.51	0.026	0.229	0.601	0.050	1.38	0.39	0.029	0.233	0.535	0.050	1.33	0.38
	iiii	0.012	0.060	0.803	0.031	1.13	0.24	0.010	0.051	0.911	0.027	1.00	0.37	0.013	0.073	0.853	0.035	1.02	0.17
	ioio (2)	0.020	0.141	0.656	0.039	1.21	0.24	0.019	0.152	0.733	0.040	1.17	0.37	0.022	0.164	0.670	0.044	1.15	0.17
	iiio (4)	0.016	0.108	0.728	0.035	1.14	0.24	0.015	0.105	0.818	0.034	1.09	0.37	0.017	0.123	0.766	0.039	1.08	0.17
	iiio (2)	0.020	0.140	0.662	0.038	1.24	0.28	0.019	0.150	0.738	0.040	1.21	0.39	0.022	0.163	0.676	0.043	1.18	0.22
	iooi (2)	0.020	0.131	0.656	0.038	1.29	0.59	0.019	0.150	0.735	0.040	1.20	0.44	0.022	0.159	0.657	0.045	1.19	0.46
	oooi (2)	0.023	0.168	0.602	0.041	1.33	0.52	0.023	0.190	0.668	0.045	1.32	0.41	0.025	0.197	0.596	0.047	1.29	0.40
P <sub>3</sub>	oooo	0.024	0.206	0.598	0.043	1.36	0.63	0.024	0.231	0.643	0.049	1.44	0.48	0.027	0.231	0.583	0.048	1.35	0.44
	iiii	0.011	0.075	0.823	0.026	1.24	0.29	0.008	0.068	0.917	0.021	1.07	0.50	0.013	0.099	0.845	0.034	1.17	0.13
	ioio (2)	0.018	0.148	0.698	0.036	1.31	0.29	0.017	0.159	0.765	0.037	1.27	0.50	0.021	0.173	0.699	0.042	1.27	0.13
	iiio (4)	0.015	0.111	0.753	0.031	1.31	0.29	0.013	0.116	0.837	0.029	1.18	0.50	0.017	0.137	0.754	0.039	1.25	0.13
	iiio (2)	0.018	0.148	0.698	0.036	1.31	0.29	0.017	0.159	0.765	0.037	1.28	0.48	0.021	0.173	0.699	0.042	1.27	0.13
	iooi (2)	0.018	0.153	0.706	0.036	1.25	0.29	0.017	0.159	0.765	0.037	1.27	0.50	0.020	0.176	0.725	0.040	1.22	0.13
	oooi (4)	0.021	0.181	0.649	0.040	1.31	0.29	0.021	0.197	0.701	0.043	1.36	0.48	0.023	0.205	0.650	0.044	1.29	0.13
	oooo	0.025	0.184	0.568	0.038	1.32	0.56	0.027	0.205	0.608	0.042	1.33	0.28	0.028	0.195	0.574	0.039	1.31	0.33
	iiii	0.014	0.060	0.774	0.033	1.24	0.47	0.017	0.102	0.771	0.042	1.19	0.10	0.018	0.080	0.761	0.041	1.23	0.24
	ioio (2)	0.021	0.128	0.652	0.036	1.25	0.47	0.023	0.161	0.671	0.042	1.23	0.10	0.024	0.141	0.645	0.041	1.25	0.24
	iiio (4)	0.017	0.096	0.710	0.035	1.25	0.47	0.020	0.138	0.730	0.042	1.15	0.10	0.021	0.114	0.706	0.040	1.20	0.24
	iiio (2)	0.020	0.129	0.659	0.036	1.29	0.47	0.023	0.161	0.684	0.042	1.26	0.10	0.023	0.142	0.661	0.039	1.27	0.24
	iooi (2)	0.020	0.129	0.659	0.036	1.29	0.47	0.023	0.153	0.662	0.044	1.39	0.28	0.024	0.138	0.649	0.041	1.34	0.33
	oooi (4)	0.023	0.158	0.614	0.037	1.33	0.51	0.025	0.179	0.635	0.042	1.39	0.28	0.026	0.169	0.613	0.040	1.34	0.33

### 4.3 Global Aromaticity indices values

In this section, we have gathered different tables with aromaticity indices and images related to the global aromaticity of the nanoring structure. In Tables S10 and S11, the MCI values of the linkers bridging the porphyrins are analyzed, while in Tables S12 and S13, the aromatic pathways consisting of large conjugated chains along the whole belt structure of the nanoring are given. Afterward, we present the 1245-index distribution plots, ACID plots, and NICS values.

**Table S10** MCI ( $\times 1000$ ) values for the six carbon atoms that form the linker bridging two porphyrins for c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup> calculated at the B3LYP, CAM-B3LYP, and M06-2X/6-31G\* levels of theory.

Species/Linker	B3LYP						CAM-B3LYP						M06-2X					
	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>
c-P6	2	2	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1
c-P6 <sup>4+</sup>	7	7	2	7	7	2	20	4	4	20	4	4	14	14	2	14	14	2
c-P6 <sup>6+</sup>	6	6	6	6	6	6	1	21	1	21	1	21	2	21	2	21	2	21
c-P6 <sup>12+</sup>	2	2	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1

**Table S11** MCI ( $\times 1000$ ) values for the six carbon atoms that form the linker bridging two porphyrins for c-P6·T6, c-P6·T6<sup>4+</sup>, c-P6·T6<sup>6+</sup>, and c-P6·T6<sup>12+</sup> calculated at the B3LYP, CAM-B3LYP, and M06-2X/6-31G\* levels of theory.

Species/Linker	B3LYP						CAM-B3LYP						M06-2X					
	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>4</sub>	L <sub>5</sub>	L <sub>6</sub>
c-P6·T6	3	3	3	3	3	3	1	1	1	1	1	2	2	2	2	2	2	2
c-P6·T6 <sup>4+</sup>	3	11	11	4	11	12	4	5	4	21	4	21	2	10	18	2	9	19
c-P6·T6 <sup>6+</sup>	5	14	5	14	5	14	1	22	1	22	1	22	1	22	1	22	1	22
c-P6·T6 <sup>12+</sup>	3	3	3	3	3	3	1	1	1	1	1	1	1	1	1	1	1	1

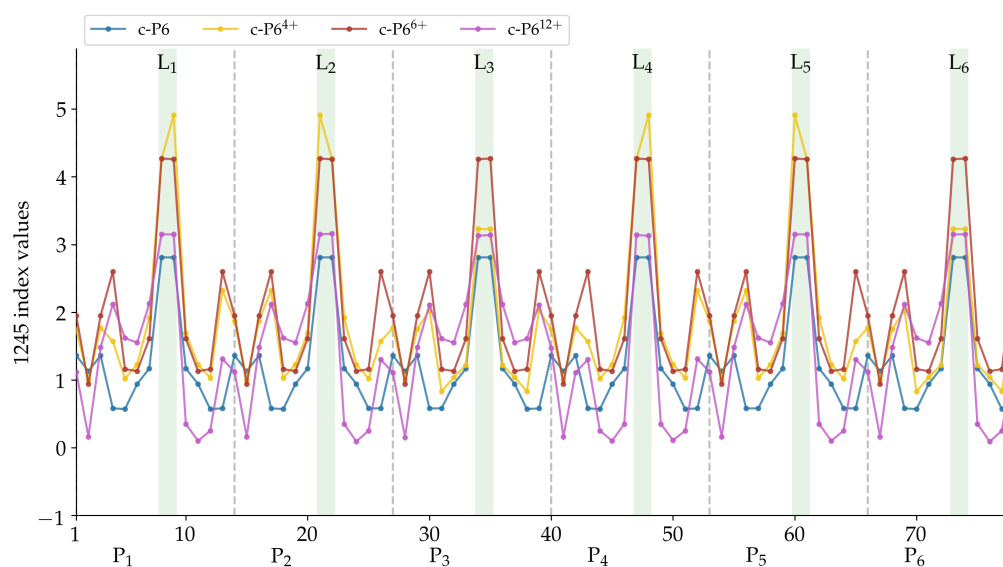
**Table S12** Aromaticity indices for several pathways of c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup> calculated at the B3LYP, CAM-B3LYP, and M06-2X/6-31G\* levels of theory.

pathway	B3LYP						CAM-B3LYP						M06-2X						
	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	
c-P6	ii ii ii ii ii ii	0.082	0.375	-0.116	0.061	1.23	0.57	0.097	0.431	-0.182	0.068	0.99	0.50	0.097	0.427	-0.172	0.069	1.01	0.52
	oo oo oo oo oo oo	0.082	0.435	-0.190	0.073	1.48	0.19	0.096	0.493	-0.272	0.083	1.25	0.03	0.096	0.491	-0.286	0.082	1.26	0.04
	oo ii oo ii oo ii	0.082	0.407	-0.161	0.067	1.37	0.19	0.097	0.464	-0.235	0.076	1.13	0.03	0.096	0.461	-0.240	0.076	1.14	0.04
	oo oo ii oo oo ii	0.082	0.417	-0.172	0.069	1.41	0.19	0.096	0.474	-0.249	0.078	1.17	0.03	0.096	0.427	-0.257	0.078	1.18	0.04
	oo oo oo ii oo oo	0.082	0.426	-0.182	0.071	1.45	0.19	0.096	0.484	-0.261	0.081	1.21	0.03	0.096	0.482	-0.273	0.080	1.22	0.04
	oi oi oi oi oi oi	0.082	0.407	-0.161	0.067	1.37	0.19	0.097	0.464	-0.235	0.076	1.13	0.03	0.096	0.461	-0.240	0.076	1.14	0.04
	oi io oi io oi io	0.082	0.407	-0.161	0.067	1.37	0.19	0.097	0.464	-0.235	0.076	1.13	0.03	0.096	0.461	-0.240	0.076	1.14	0.04
	oi ii io ii io ii	0.082	0.387	-0.133	0.063	1.28	0.19	0.097	0.443	-0.202	0.071	1.04	0.03	0.097	0.439	-0.197	0.072	1.06	0.04
c-P6 <sup>4+</sup>	ii ii ii ii ii ii	0.067	0.337	-0.033	0.062	1.87	0.83	0.073	0.361	-0.047	0.067	1.70	0.81	0.072	0.367	-0.035	0.069	1.79	0.68
	oo oo oo oo oo oo	0.067	0.386	-0.111	0.067	1.55	0.08	0.072	0.404	-0.121	0.070	1.51	0.07	0.073	0.413	-0.140	0.071	1.53	0.01
	oo ii oo ii oo ii	0.067	0.364	-0.081	0.065	1.70	0.08	0.072	0.384	-0.091	0.069	1.60	0.07	0.073	0.392	-0.098	0.070	1.65	0.01
	oo oo ii oo oo ii	0.067	0.370	-0.089	0.065	1.65	0.08	0.072	0.382	-0.083	0.066	1.58	0.12	0.072	0.397	-0.107	0.070	1.61	0.01
	oo oo oo ii oo oo	0.067	0.378	-0.101	0.066	1.60	0.08	0.073	0.400	-0.117	0.070	1.54	0.07	0.073	0.405	-0.124	0.070	1.57	0.01
	oi oi oi oi oi oi	0.067	0.364	-0.081	0.065	1.70	0.08	0.072	0.384	-0.091	0.069	1.60	0.07	0.073	0.392	-0.098	0.070	1.65	0.01
	oi io oi io oi io	0.067	0.364	-0.081	0.065	1.70	0.08	0.072	0.384	-0.091	0.069	1.60	0.07	0.073	0.392	-0.098	0.070	1.65	0.01
	oi ii io ii io ii	0.067	0.347	-0.053	0.063	1.81	0.08	0.072	0.367	-0.058	0.067	1.67	0.12	0.073	0.377	-0.063	0.070	1.74	0.01
c-P6 <sup>6+</sup>	ii ii ii ii ii ii	0.063	0.326	-0.017	0.062	2.03	0.94	0.073	0.379	-0.102	0.075	1.54	0.69	0.073	0.376	-0.092	0.075	1.61	0.74
	oo oo oo oo oo oo	0.064	0.373	-0.098	0.066	1.41	0.10	0.072	0.408	-0.157	0.071	1.25	0.01	0.073	0.411	-0.177	0.072	1.26	0.00
	oo ii oo ii oo ii	0.064	0.351	-0.066	0.064	1.70	0.10	0.073	0.394	-0.136	0.073	1.38	0.01	0.073	0.395	-0.145	0.073	1.42	0.00
	oo oo ii oo oo ii	0.064	0.359	-0.079	0.065	1.60	0.10	0.073	0.399	-0.144	0.072	1.34	0.01	0.073	0.400	-0.157	0.073	1.36	0.00
	oo oo oo ii oo oo	0.064	0.366	-0.089	0.065	1.50	0.10	0.072	0.404	-0.151	0.072	1.29	0.01	0.073	0.406	-0.168	0.072	1.31	0.00
	oi oi oi oi oi oi	0.064	0.351	-0.066	0.064	1.70	0.10	0.073	0.394	-0.136	0.073	1.38	0.01	0.073	0.395	-0.145	0.073	1.42	0.00
	oi io oi io oi io	0.064	0.351	-0.066	0.064	1.70	0.10	0.073	0.391	-0.158	0.073	1.45	0.01	0.073	0.391	-0.164	0.073	1.48	0.00
	oi ii io ii io ii	0.063	0.335	-0.036	0.063	1.91	0.10	0.073	0.383	-0.123	0.074	1.51	0.01	0.073	0.381	-0.119	0.074	1.56	0.00
c-P6 <sup>12+</sup>	ii ii ii ii ii ii	0.081	0.465	-0.285	0.090	1.42	0.09	0.107	0.579	-0.521	0.113	0.93	0.02	0.106	0.575	-0.518	0.113	0.97	0.03
	oo oo oo oo oo oo	0.083	0.493	-0.403	0.089	0.71	0.03	0.106	0.587	-0.639	0.105	0.50	0.01	0.106	0.587	-0.662	0.105	0.51	0.01
	oo ii oo ii oo ii	0.082	0.480	-0.355	0.089	1.04	0.03	0.106	0.583	-0.594	0.109	0.70	0.01	0.106	0.581	-0.603	0.109	0.73	0.02
	oo oo ii oo oo ii	0.082	0.485	-0.372	0.089	0.93	0.03	0.106	0.585	-0.611	0.107	0.63	0.01	0.106	0.583	-0.624	0.108	0.65	0.02
	oo oo oo ii oo oo	0.083	0.489	-0.388	0.089	0.82	0.03	0.106	0.586	-0.626	0.106	0.56	0.01	0.106	0.585	-0.643	0.106	0.58	0.01
	oi oi oi oi oi oi	0.082	0.475	-0.351	0.088	1.09	0.02	0.106	0.581	-0.590	0.108	0.71	0.01	0.106	0.578	-0.600	0.108	0.74	0.01
	oi io oi io oi io	0.082	0.477	-0.353	0.089	1.06	0.02	0.106	0.582	-0.592	0.108	0.70	0.01	0.106	0.580	-0.601	0.109	0.73	0.02
	oi ii io ii io ii	0.081	0.468	-0.310	0.089	1.31	0.03	0.106	0.579	-0.547	0.111	0.86	0.01	0.106	0.576	-0.549	0.111	0.90	0.02

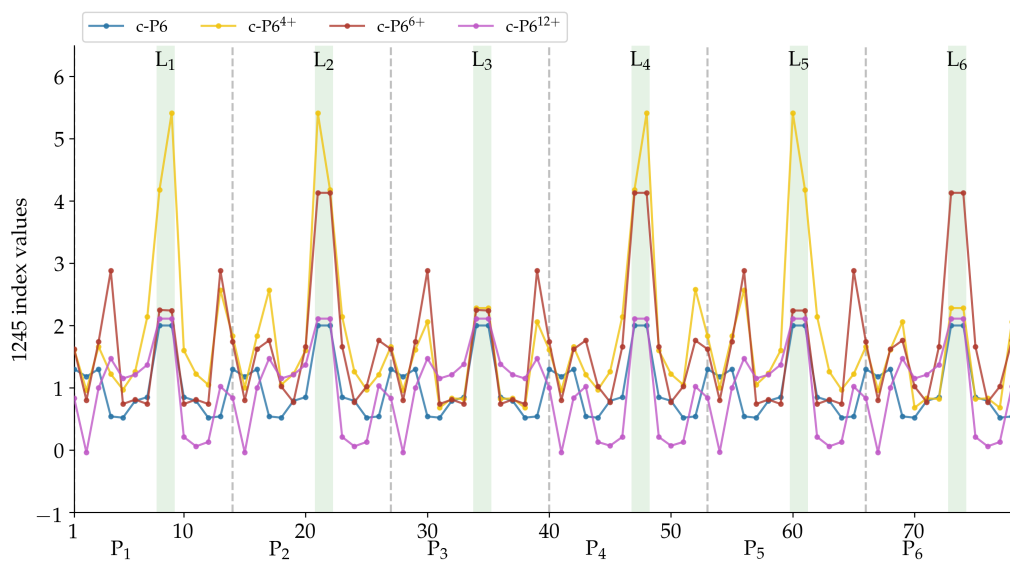
**Table S13** Aromaticity indices for several pathways of c-P6·T6, c-P6·T6<sup>4+</sup>, c-P6·T6<sup>6+</sup>, and c-P6·T6<sup>12+</sup> calculated at the B3LYP, CAM-B3LYP, and M06-2X/6-31G\* levels of theory.

pathway	B3LYP						CAM-B3LYP						M06-2X						
	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	FLU	BOA	HOMA	BLA	AV1245	AV <sub>min</sub>	
c-P6·T6	ii ii ii ii ii ii	0.081	0.354	-0.138	0.064	1.25	0.42	0.096	0.412	-0.196	0.070	1.01	0.35	0.096	0.407	-0.189	0.071	1.03	0.37
	oo oo oo oo oo oo	0.082	0.425	-0.235	0.073	1.44	0.16	0.096	0.484	-0.315	0.082	1.21	0.00	0.096	0.481	-0.324	0.081	1.22	0.01
	oo ii oo ii oo ii	0.082	0.392	-0.197	0.069	1.35	0.16	0.096	0.451	-0.266	0.076	1.12	0.00	0.096	0.447	-0.270	0.076	1.13	0.01
	oo oo ii oo oo ii	0.082	0.403	-0.212	0.070	1.38	0.16	0.096	0.462	-0.285	0.078	1.15	0.00	0.096	0.459	-0.291	0.078	1.16	0.01
	oo oo oo ii oo oo	0.082	0.414	-0.224	0.071	1.41	0.16	0.096	0.473	-0.301	0.080	1.18	0.00	0.096	0.470	-0.308	0.079	1.19	0.01
	oi oi oi oi oi oi	0.082	0.392	-0.196	0.069	1.36	0.16	0.096	0.450	-0.265	0.076	1.12	0.00	0.096	0.446	-0.269	0.076	1.14	0.01
	oi io oi io oi io	0.082	0.392	-0.196	0.069	1.35	0.17	0.096	0.451	-0.266	0.076	1.11	0.01	0.096	0.447	-0.271	0.076	1.12	0.02
	oi ii ii io ii ii	0.081	0.368	-0.161	0.066	1.28	0.18	0.096	0.426	-0.223	0.072	1.04	0.01	0.096	0.421	-0.221	0.073	1.06	0.03
c-P6·T6 <sup>4+</sup>	ii ii ii ii ii ii	0.068	0.328	-0.078	0.065	1.85	0.87	0.073	0.352	-0.094	0.070	1.67	0.75	0.073	0.006	-0.087	0.072	1.73	0.75
	oo oo oo oo oo oo	0.069	0.383	-0.169	0.067	1.55	0.08	0.074	0.402	-0.184	0.070	1.49	0.06	0.074	0.409	-0.200	0.071	1.51	0.00
	oo ii oo ii oo ii	0.068	0.357	-0.134	0.066	1.69	0.08	0.074	0.379	-0.149	0.070	1.57	0.08	0.074	0.385	-0.156	0.071	1.62	0.01
	oo oo ii oo oo ii	0.069	0.369	-0.155	0.068	1.64	0.08	0.074	0.392	-0.172	0.072	1.53	0.06	0.074	0.397	-0.187	0.073	1.57	0.00
	oo oo oo ii oo oo	0.069	0.374	-0.158	0.067	1.60	0.08	0.074	0.397	-0.179	0.071	1.51	0.06	0.074	0.402	-0.187	0.071	1.54	0.00
	oo oo oo ii oo oo	0.068	0.357	-0.132	0.066	1.70	0.09	0.074	0.379	-0.146	0.070	1.58	0.06	0.074	0.385	-0.152	0.071	1.63	0.01
	oi io oi oi oi oi	0.068	0.357	-0.133	0.066	1.69	0.09	0.074	0.379	-0.148	0.070	1.57	0.08	0.074	0.385	-0.156	0.071	1.61	0.00
	oi ii ii io ii ii	0.068	0.339	-0.102	0.066	1.79	0.09	0.073	0.359	-0.109	0.069	1.64	0.13	0.073	0.366	-0.113	0.071	1.69	0.08
c-P6·T6 <sup>6+</sup>	ii ii ii ii ii ii	0.066	0.322	-0.088	0.066	1.92	0.81	0.075	0.379	-0.164	0.077	1.48	0.64	0.075	0.375	-0.157	0.077	1.54	0.65
	oo oo oo oo oo oo	0.068	0.377	-0.173	0.066	1.43	0.04	0.074	0.409	-0.225	0.071	1.27	0.06	0.075	0.410	-0.240	0.071	1.28	0.05
	oo ii oo ii oo ii	0.067	0.352	-0.140	0.066	1.66	0.04	0.075	0.395	-0.202	0.074	1.37	0.07	0.075	0.394	-0.209	0.074	1.40	0.07
	oo oo ii oo oo ii	0.067	0.361	-0.153	0.066	1.58	0.05	0.074	0.399	-0.211	0.073	1.34	0.06	0.075	0.399	-0.221	0.073	1.36	0.05
	oo oo oo ii oo oo	0.068	0.369	-0.163	0.066	1.50	0.04	0.074	0.404	-0.218	0.072	1.30	0.06	0.075	0.405	-0.232	0.072	1.32	0.05
	oi oi oi oi oi oi	0.067	0.352	-0.138	0.066	1.66	0.05	0.074	0.395	-0.200	0.074	1.38	0.08	0.075	0.393	-0.207	0.074	1.41	0.05
	oi io oi io oi io	0.067	0.347	-0.141	0.066	1.67	0.14	0.075	0.391	-0.216	0.074	1.43	0.07	0.075	0.390	-0.222	0.075	1.46	0.08
	oi ii ii io ii ii	0.067	0.331	-0.109	0.066	1.83	0.14	0.075	0.384	-0.185	0.076	1.46	0.07	0.075	0.380	-0.183	0.076	1.51	0.08
c-P6·T6 <sup>12+</sup>	ii ii ii ii ii ii	0.082	0.425	-0.300	0.080	1.45	0.24	0.105	0.552	-0.523	0.106	0.95	0.01	0.104	0.544	-0.514	0.105	0.99	0.02
	oo oo oo oo oo oo	0.082	0.449	-0.365	0.078	0.94	0.02	0.103	0.553	-0.609	0.098	0.70	0.01	0.103	0.550	-0.610	0.098	0.71	0.01
	oo ii oo ii oo ii	0.082	0.438	-0.341	0.079	1.18	0.02	0.104	0.552	-0.577	0.102	0.82	0.01	0.104	0.547	-0.574	0.101	0.84	0.01
	oo oo ii oo oo ii	0.082	0.443	-0.355	0.079	1.09	0.03	0.104	0.553	-0.594	0.101	0.77	0.02	0.104	0.549	-0.592	0.100	0.79	0.02
	oo oo oo ii oo oo	0.082	0.446	-0.359	0.078	1.02	0.02	0.103	0.553	-0.600	0.099	0.74	0.01	0.103	0.549	-0.599	0.099	0.75	0.01
	oi oi oi oi oi oi	0.082	0.439	-0.348	0.079	1.16	0.03	0.105	0.556	-0.601	0.102	0.78	0.01	0.105	0.550	-0.597	0.102	0.80	0.00
	oi io oi io oi io	0.083	0.440	-0.354	0.079	1.14	0.02	0.104	0.554	-0.587	0.102	0.79	0.01	0.104	0.549	-0.584	0.101	0.82	0.00
	oi ii ii io ii ii	0.083	0.431	-0.325	0.080	1.33	0.06	0.105	0.552	-0.544	0.105	0.90	0.01	0.104	0.545	-0.537	0.104	0.94	0.00

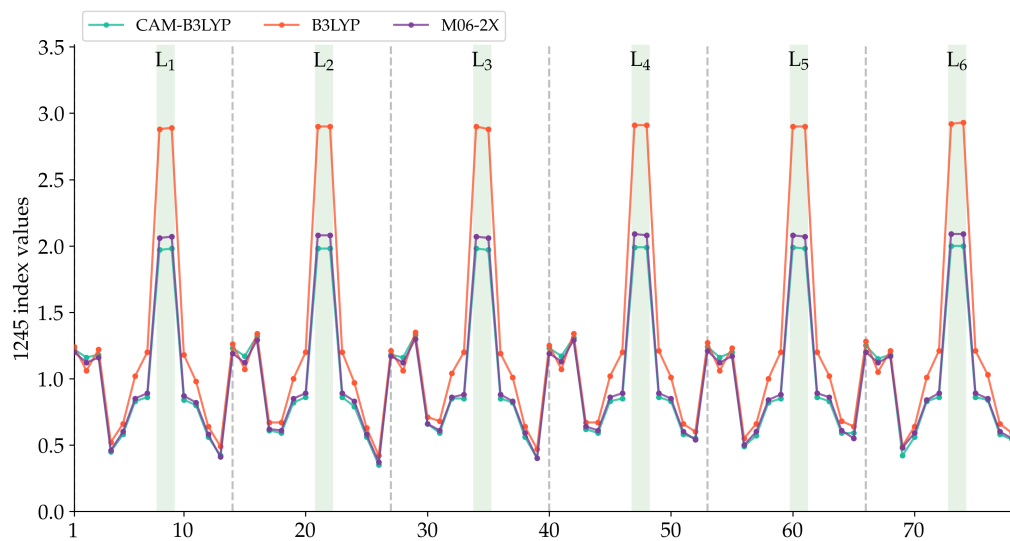
### 4.3.1 1245-index distribution plots



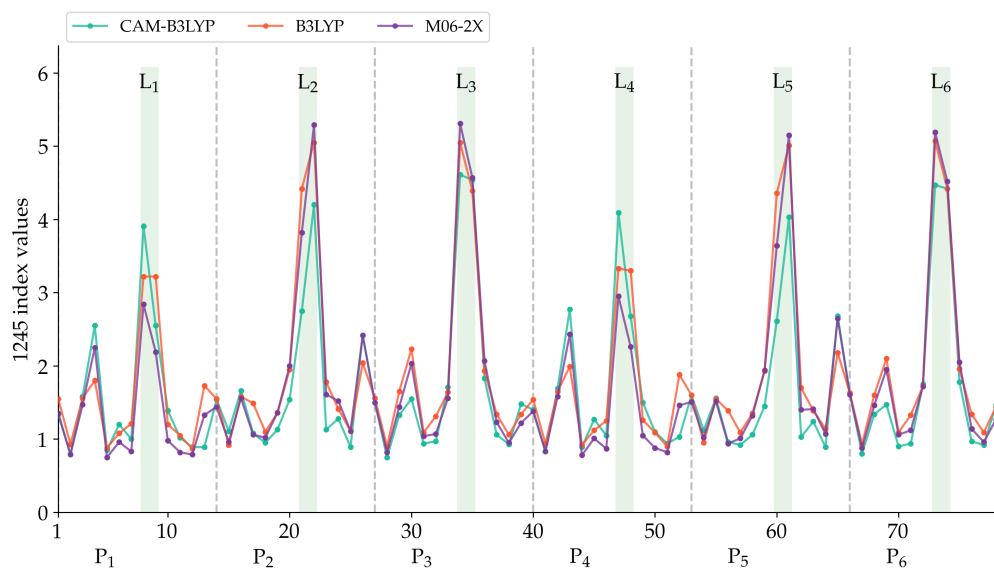
**Figure S5** 1245-index distribution including the individual MCI(1,2,4,5) values along the most aromatic path of c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup> calculated at the B3LYP/6-31G\* level of theory.



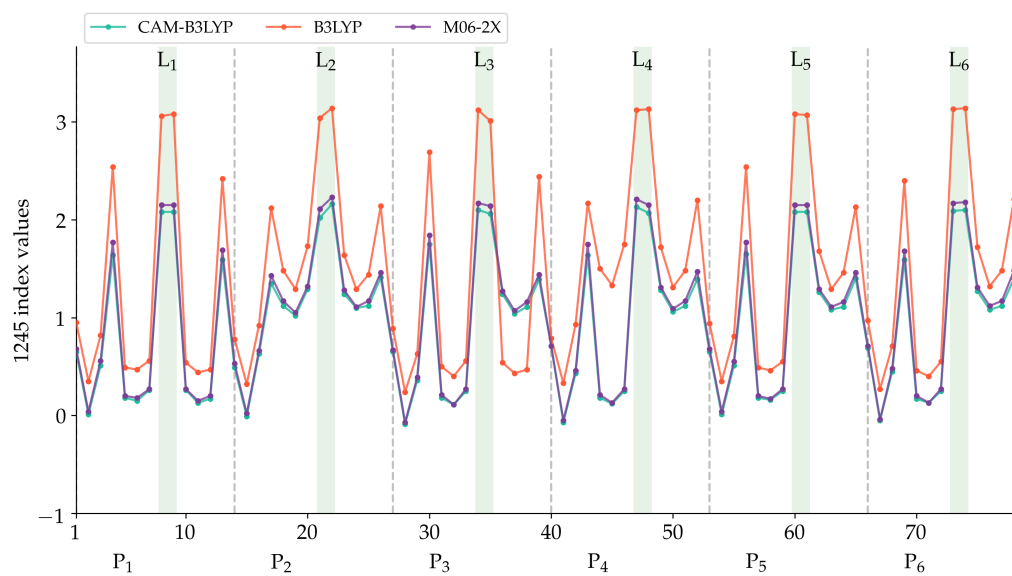
**Figure S6** 1245-index distribution including the individual MCI(1,2,4,5) values along the most aromatic path of c-P6, c-P6<sup>4+</sup>, c-P6<sup>6+</sup>, and c-P6<sup>12+</sup> calculated at the M06-2X/6-31G\* level of theory.



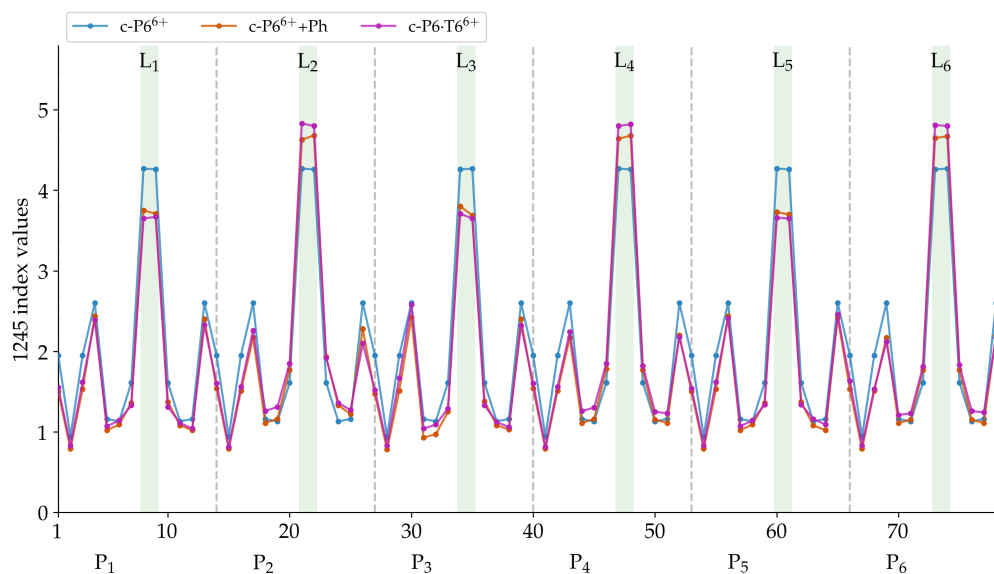
**Figure S7** Comparison of the 1245-index distributions including the individual MCI(1,2,4,5) values along the most aromatic path of c-P6·T6 calculated at different levels of theory.



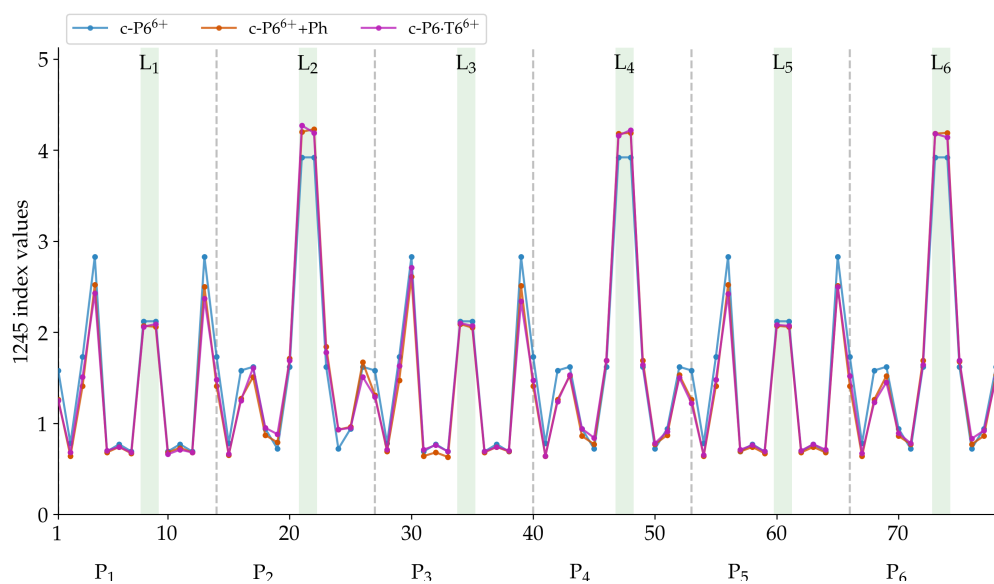
**Figure S8** Comparison of the 1245-index distributions including the individual MCI(1,2,4,5) values along the most aromatic path of  $c\text{-P6}\cdot\text{T6}^{4+}$  calculated at different levels of theory.



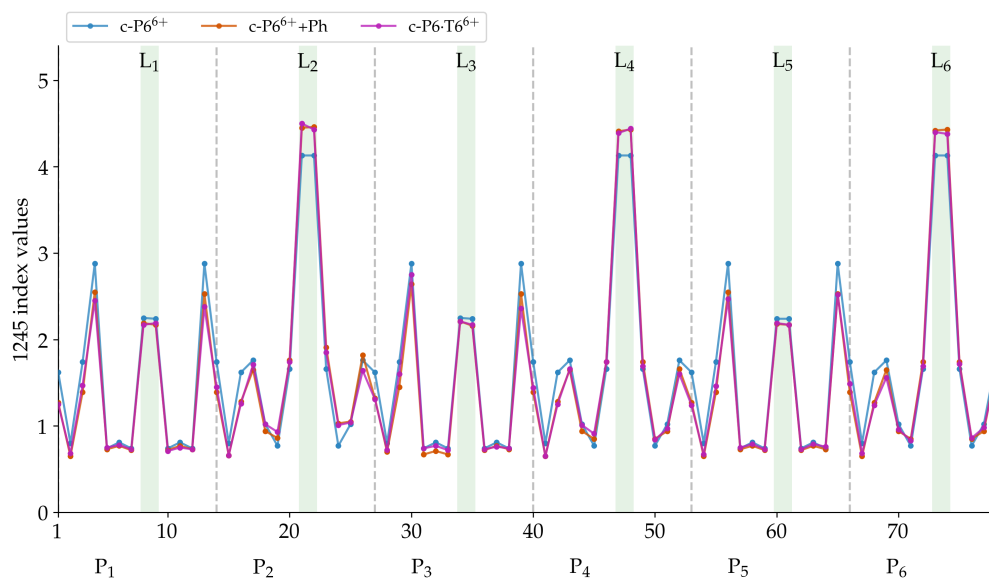
**Figure S9** Comparison of the 1245-index distributions including the individual MCI(1,2,4,5) values along the most aromatic path of  $c\text{-P6}\cdot\text{T6}^{12+}$  calculated at different levels of theory.



**Figure S10** 1245-index distribution including the individual MCI(1,2,4,5) values along the most aromatic path of c-P6<sup>6+</sup>, c-P6<sup>6+</sup> with Ph substituents, and c-P6·T6<sup>6+</sup> calculated at the B3LYP/6-31G\* level of theory.



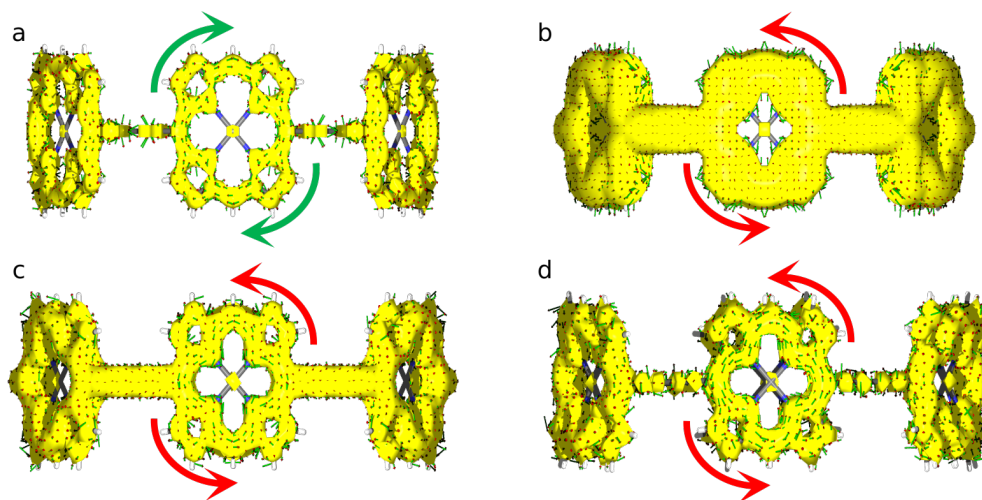
**Figure S11** 1245-index distribution including the individual MCI(1,2,4,5) values along the most aromatic path of c-P6<sup>6+</sup>, c-P6<sup>6+</sup> with Ph substituents, and c-P6·T6<sup>6+</sup> calculated at the CAM-B3LYP/6-31G\* level of theory.



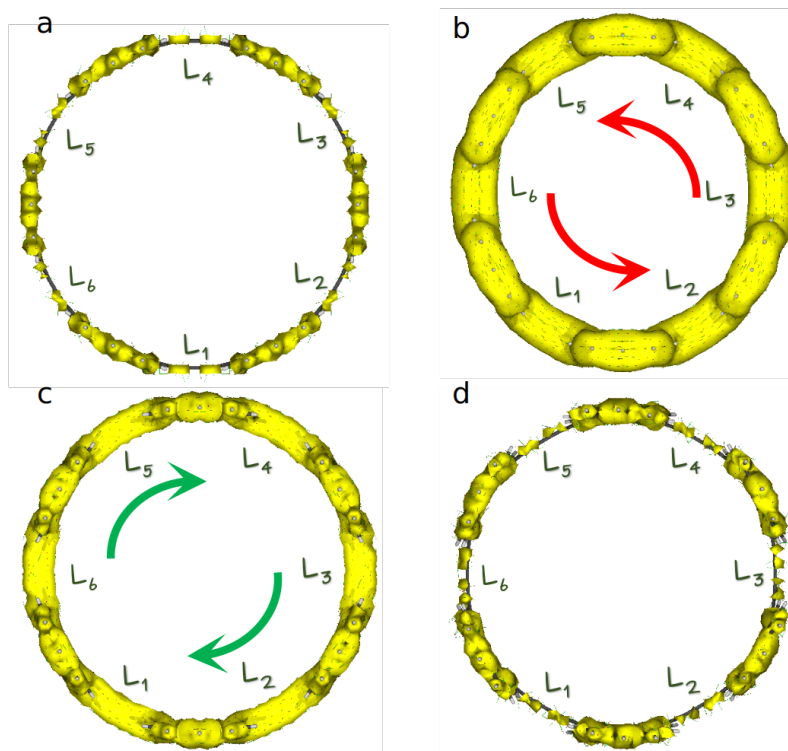
**Figure S12** 1245-index distribution along the most aromatic path of  $c\text{-P6}^{6+}$ ,  $c\text{-P6}^{6+}$  with Ph substituents, and  $c\text{-P6-T6}^{6+}$  calculated at the M06-2X/6-31G\* level of theory.

### 4.3.2 ACID plots

ACID calculations were performed using the CSGT method with B3LYP and CAM-B3LYP density functional approximations in combination with the 6-31G\* basis set, including Grimme's dispersion (no solvent model was employed). In Figures S13 and S14, we present two perspectives of the ACID plots for the four oxidation states of the nanoring at the B3LYP/6-31G\* computational level. The former picture can be used to assess the local aromaticity of the porphyrin, whereas the latter is useful in analyzing the global aromaticity of nanoring. Similar pictures of the CAM-B3LYP geometries can be found in the manuscript.



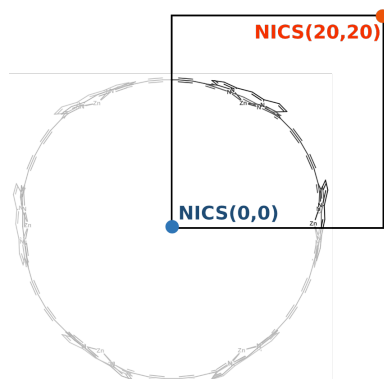
**Figure S13** ACID isosurface plots (isocontour value 0.06) for a)  $c\text{-P6}$ , b)  $c\text{-P6}^{4+}$ , c)  $c\text{-P6}^{6+}$ , and d)  $c\text{-P6}^{12+}$  at the B3LYP/6-31G\* level of theory (employed for both geometry optimization and ACID calculation).



**Figure S14** ACID isosurface plots (isocontour value 0.06) for a) c-P6, b) c-P6<sup>4+</sup>, c) c-P6<sup>6+</sup>, and d) c-P6<sup>12+</sup> using B3LYP/6-31G\* level of theory (employed for both geometry optimization and ACID calculation).

### 4.3.3 NICS

NICS values calculated with CAM-B3LYP and B3LYP density functional approximations in combination with the 6-31G\* basis set. NICS(0,0) refers to the NICS value computed at the center of the nanoring (blue circle), whereas NICS(20,20) corresponds to the NICS value calculated at point (20,20) (orange circle) of a frame centered at the center of the nanoring with x- and y-axis pointing towards one linker and the center of a porphyrin, respectively (see Figure S15). Therefore, (20,20) corresponds to a point outside the nanoring at a fairly large distance. The distance unit is Ångstroms (Å).



Species	CAM-B3LYP		B3LYP	
	NICS(0,0)	NICS(20,20)	NICS(0,0)	NICS(20,20)
c-P6	-1.68	-0.08	-1.42	-0.09
c-P6 <sup>4+</sup>	0.88	-0.12	102.24	-6.46
c-P6 <sup>6+</sup>	-0.42	-0.01	-13.36	0.86
c-P6 <sup>12+</sup>	0.47	0.02	1.37	0.08

**Figure S15 & Table S14** NICS(0,0) and NICS(20,20) values.

We have checked the dependency of the NICS with the basis set and included these results in Tables S15 and S16. Since there is a good agreement between the experimental and computational data for c-P6 and c-P6<sup>12+</sup> (regardless of the density functional approximation employed in the calculation), we have only included the results for c-P6<sup>4+</sup> and c-P6<sup>6+</sup>. In particular, we have performed optimization and NMR calculations using various combinations of 6-31G\*, 6-31+G\*, and 6-311+G\* basis sets. As we can see in Tables S15, the results barely change with the basis set size for c-P6<sup>6+</sup> and only small changes occur in the case of c-P6<sup>4+</sup> (see Table S16). All in all, the conclusions drawn in the manuscript are not affected by the use of the 6-31G\* basis set.



**Table S15** NICS(0,0) and NICS(20,20) values for c-P6<sup>6+</sup> using B3LYP and CAM-B3LYP with different basis set for the optimization and the calculation of the NICS (NMR).

Optimization	NMR	NICS(0,0)	NICS(20,20)
B3LYP/6-31G*	B3LYP/6-31G*	-13.36	0.86
B3LYP/6-31G*	B3LYP/6-31+G*	-13.51	0.85
B3LYP/6-31G*	B3LYP/6-311+G*	-13.51	0.85
B3LYP/6-31+G*	B3LYP/6-31+G*	-13.61	0.87
B3LYP/6-311+G*	B3LYP/6-311+G*	-13.62	0.86
CAM-B3LYP/6-31G*	CAM-B3LYP/6-31G*	-0.42	-0.01
CAM-B3LYP/6-31G*	CAM-B3LYP/6-31+G*	-0.52	-0.01
CAM-B3LYP/6-31G*	CAM-B3LYP/6-311+G*	-0.48	-0.01
CAM-B3LYP/6-31+G*	CAM-B3LYP/6-31+G*	-0.53	-0.01
CAM-B3LYP/6-311+G*	CAM-B3LYP/6-311+G*	-0.49	-0.02
CAM-B3LYP/6-31G*	B3LYP/6-31G*	-1.61	0.10

**Table S16** NICS(0,0) and NICS(20,20) values for c-P6<sup>4+</sup> using B3LYP and CAM-B3LYP with different basis set for the optimization and the calculation of the NICS (NMR).

Optimization	NMR	NICS(0,0)	NICS(20,20)
B3LYP/6-31G*	B3LYP/6-31G*	102.24	-6.46
B3LYP/6-31G*	B3LYP/6-31+G*	96.13	-6.10
B3LYP/6-31G*	B3LYP/6-311+G*	96.44	-6.12
B3LYP/6-31+G*	B3LYP/6-31+G*	90.44	-5.63
B3LYP/6-311+G*	B3LYP/6-311+G*	86.03	-5.31
CAM-B3LYP/6-31G*	CAM-B3LYP/6-31G*	0.88	-0.12
CAM-B3LYP/6-31G*	CAM-B3LYP/6-31+G*	0.71	-0.12
CAM-B3LYP/6-31G*	CAM-B3LYP/6-311+G*	0.71	-0.12
CAM-B3LYP/6-31+G*	CAM-B3LYP/6-31+G*	0.61	-0.12
CAM-B3LYP/6-311+G*	CAM-B3LYP/6-311+G*	0.56	-0.11
CAM-B3LYP/6-31G*	B3LYP/6-31G*	28.18	-1.75

## 5 Aromaticity indices

In the present section, the aromaticity indices used in the manuscript will be briefly reviewed. Henceforth, we will use the short-hand notation  $\mathbf{1} \equiv (\vec{r}_1, \sigma_1)$  to denote the coordinates of an electron and  $d\mathbf{1} \equiv d\vec{r}_1, d\sigma_1$  for the electron positions and their derivatives. To provide a general expression, we will consider a molecule including at least one ring structure consisting of  $n$  atoms, represented by the string  $\mathcal{A} = \{A_1, A_2, \dots, A_n\}$  and whose elements are ordered according to the connectivity of the atoms in the ring.

First of all, we will define the delocalization index (DI)<sup>21,22,26</sup> using the exchange-correlation density (XCD)<sup>55</sup> between points belonging to two different atoms  $A_1$  and  $A_2$ ,

$$\delta(A_1, A_2) = 2 \int_{A_1} \int_{A_2} d\mathbf{1} d\mathbf{2} \rho_{xc}(\mathbf{1}, \mathbf{2}) = -2 \text{cov}(N_{A_1}, N_{A_2}), \quad (1)$$

where  $N_{A_1}$  and  $N_{A_2}$  are the atomic populations of atoms  $A_1$  and  $A_2$ . The delocalization index is related to the covariance of these populations and, for this reason, the DI is a measure of the number of electrons fluctuating between these atoms concurrently. On the other hand, the localization index (LI) is defined as

$$\lambda(A) = \int_A \int_A d\mathbf{1} d\mathbf{2} \rho_{xc}(\mathbf{1}, \mathbf{2}), \quad (2)$$

where we integrate the two points of the XCD over the same atom  $A_1$ .

Secondly, we define the geometric aromaticity indices: the so-called harmonic oscillator model of aromaticity (HOMA)<sup>56</sup> and the bond-length alternation (BLA). Kruszewski and Krygowski defined the former, and they used bond-length references,  $R_{opt}$ , to compare with the actual bond length of the ring structure:

$$HOMA(\mathcal{A}) = 1 - \frac{1}{n} \sum_i^n \alpha_i (r_{opt} - r_{A_i A_{i+1}})^2, \quad (3)$$

where  $r_{A,B}$  is the distance between atoms  $A$  and  $B$ , and  $\alpha_i$  is an empirical constant fixed to give values close to one for aromatic species and small or negative values for non-aromatic and antiaromatic species. The geometrical data of reference ( $R_{opt}$ ) is such that the compression energy of the double bond and the expansion energy of the single bond are minimal in accordance with the harmonic potential model. The bond-length alternation indicator compares the bond-length among the consecutive bonds along the perimeter of the ring,

$$BLA(\mathcal{A}) = \frac{1}{2n} \sum_{i=1}^n |r_{A_i A_{i+1}} - r_{A_{i+1} A_{i+2}}|, \quad (4)$$

where  $n_1 = \lfloor (n+1)/2 \rfloor$  and  $n_2 = \lfloor n/2 \rfloor$ ,  $\lfloor n \rfloor$  being floor function of  $x$ , which returns the largest integer less than or equal to  $x$ .

We now consider the electronic aromaticity indices. The bond-order alternation (BOA) is one of the most popular aromatic indicators, and it corresponds to the electronic structure analogous to BLA. BOA uses bond orders or electron-sharing indices<sup>26</sup> rather than the bond length,

$$BOA(\mathcal{A}) = \frac{1}{2n} \sum_{i=1}^n |\delta(A_i, A_{i+1}) - \delta(A_{i+1}, A_{i+2})|. \quad (5)$$

Aromaticity indicators based on bond orders, such as BLA or FLU (see below), do not have a strong dependency on the computational method used.<sup>57</sup>

Just as we had the electronic counterpart of BLA, we have the counterpart of HOMA, the aromatic fluctuation index (FLU), which goes beyond the bond length information employed in HOMA.<sup>19,20</sup> The FLU index also employs references to measure the electron delocalization:

$$FLU(\mathcal{A}) = \frac{1}{n} \sum_{i=1}^n \left[ \left( \frac{\delta(A_i)}{\delta(A_{i-1})} \right)^\alpha \left( \frac{\delta(A_i, A_{i-1}) - \delta_{ref}(A_i, A_{i-1})}{\delta_{ref}(A_i, A_{i-1})} \right) \right]^2 \quad (6)$$

where  $\alpha$  is a simple function to ensure the first term in Eq. 6 is always greater or equal to 1,

$$\alpha \begin{cases} 1 & \delta(A_{i-1}) \leq \delta(A_i) \\ -1 & \delta(A_i) < \delta(A_{i-1}) \end{cases} \quad (7)$$

and  $\delta_{ref}(A,B)$  is the DI of an aromatic molecule of reference. For C-C bonds, benzene is used as a reference while the C-N value is taken from pyridine.<sup>19</sup> When the molecule is aromatic, the FLU index will be close to zero, whereas for non-aromatic or antiaromatic species it will be greater than zero.

Giambiagi employed one of the most reliable electronic multicenter indices as an aromaticity index. This many-center electron delocalization index ( $I_{ring}$ ) measures the delocalization along the ring:<sup>58</sup>

$$I_{ring}(\mathcal{A}) = \sum_{i_1 i_2 \dots i_n}^{occ} S_{i_1 i_2}(A_1) S_{i_2 i_3}(A_2) \dots S_{i_n, i_1}(A_n) \quad (8)$$

and if one takes into account all the permutations of the atoms in the ring, thus including delocalization patterns across the ring, we obtain the expression of the multicenter index (MCI):<sup>28</sup>

$$MCI(\mathcal{A}) = \frac{1}{2n} \sum_{\mathcal{P}(\mathcal{A})} I_{ring}(\mathcal{A}) = \frac{1}{2n} \sum_{\mathcal{P}(\mathcal{A})} \sum_{i_1 i_2 \dots i_n}^{occ} S_{i_1 i_2}(A_1) S_{i_2 i_3}(A_2) \dots S_{i_n, i_1}(A_n) \quad (9)$$

where  $\mathcal{P}(\mathcal{A})$  stands for the  $n!$  permutations of the elements in the string  $\mathcal{A}$ . Like  $I_{ring}$ , MCI gives large numbers for aromatic species and the authors claim negative values for antiaromatic molecules.<sup>59</sup> However, these two electronic indices are not suitable for large (anti)aromatic molecules because they scale exponentially with the number of atoms in the ring and present large numerical errors derived from the numerical integration of the atomic overlap matrices.

In order to solve the drawbacks of  $I_{ring}$  and MCI, one of us defined the AV1245 index<sup>16</sup> as the average value of the four-atom MCI index between relative positions 1-2 and 4-5 constructed from every five consecutive atoms along the perimeter of the ring. Lately, it has been seen that the average value could hinder some important values and that the minimal value of the index,  $AV_{min}$ ,<sup>17,43</sup> could be more useful. The  $AV_{min}$  value corresponds to the least delocalized fragment of the ring. Aromatic molecules present large values of  $AV_{min}$  while non-aromatic molecules exhibit low values. Antiaromatic molecules are more difficult to identify because they usually present intermediate values of  $AV_{min}$ . To identify the antiaromatic molecules, we could help ourselves using BOA values (if the species are smaller) or the 1245-index distributions plots (from which the average value, AV1245, is obtained) along the ring (see *e.g.*, Figure S12).

Finally, we have the magnetic aromaticity indices. When an (anti)aromatic species is exposed to an external field, this field induces a  $\pi$ -electron ring current that can be measured to characterize the molecule either as an aromatic or antiaromatic molecule. Aromatic molecules will show diatropic ring currents. On the contrary, the antiaromatic species will present paratropic ring currents. The most important and popular magnetic index of aromaticity is the nucleus independent chemical shift (NICS) due to Paul Schleyer and co-workers.<sup>30</sup> NICS is defined as the negative value of the absolute shielding computed at a certain point of the space. It is usually calculated at the center of the ring, NICS(0). However, it could also be calculated in other important points (see *e.g.*, Table S14), or one could calculate a NICS scan along some region of the space to obtain a NICS grid plot (see manuscript).<sup>60</sup> Negative values are a signature of aromaticity, whereas positive values indicate antiaromaticity. Another well-known magnetic index is the Anisotropy of the Induced Current Density (ACID)<sup>29</sup>. Using the ACID software,<sup>29</sup> one can visualize ACID scalar field isosurfaces and the current density vectors (see *e.g.* Figure S14).

## Notes and references

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## Electronic Supplementary Information

Complete optimized geometries (in Å) of the studied six-porphyrin nanoring in four different oxidation states using B3LYP, CAM-B3LYP, and M06-2X density functional approximations in combination with 6-31G\* basis set and Grimme's D3 dispersion correction. First the naked belt geometries (c-P6) for all the species are given and then the structure including the phenyl substituents and the encapsulated template (c-P6·T6) are provided.

c-P6 optimized with B3LYP.....	2
c-P6 optimized with CAM-B3LYP.....	6
c-P6 optimized with M06-2X.....	10
c-P6 <sup>+4</sup> optimized with B3LYP.....	14
c-P6 <sup>+4</sup> optimized with CAM-B3LYP.....	18
c-P6 <sup>+4</sup> optimized with M06-2X.....	22
c-P6 <sup>+6</sup> optimized with B3LYP.....	26
c-P6 <sup>+6</sup> optimized with CAM-B3LYP.....	30
c-P6 <sup>+6</sup> optimized with M06-2X.....	34
c-P6 <sup>+12</sup> optimized with B3LYP.....	38
c-P6 <sup>+12</sup> optimized with CAM-B3LYP.....	42
c-P6 <sup>+12</sup> optimized with M06-2X.....	46
c-P6·T6 optimized with B3LYP.....	50
c-P6·T6 optimized with CAM-B3LYP.....	58
c-P6·T6 optimized with M06-2X.....	66
c-P6·T6 <sup>+4</sup> optimized with B3LYP.....	75
c-P6·T6 <sup>+4</sup> optimized with CAM-B3LYP.....	83
c-P6·T6 <sup>+4</sup> optimized with M06-2X.....	91
c-P6·T6 <sup>+6</sup> optimized with B3LYP.....	99
c-P6·T6 <sup>+6</sup> optimized with CAM-B3LYP.....	107
c-P6·T6 <sup>+6</sup> optimized with M06-2X.....	116
c-P6·T6 <sup>+12</sup> optimized with B3LYP.....	124
c-P6·T6 <sup>+12</sup> optimized with CAM-B3LYP.....	132
c-P6·T6 <sup>+12</sup> optimized with M06-2X.....	140

**c-P6** optimized with **B3LYP** - E=-17512.514222au

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6	1.247039000	12.876952000	2.792695000
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6	11.77528700	-5.35850800	-2.79269500
6	12.33689400	-4.22530200	3.48416800

6	12.674327000	-3.307521000	2.532637000
6	12.549048000	-3.266373000	0.000000000
6	12.674327000	-3.307521000	-2.532637000
6	12.336894000	-4.225302000	-3.484168000
1	12.439388000	-4.142671000	4.558805000
1	13.111427000	-2.327880000	2.667097000
6	12.895545000	-1.896136000	0.000000000
1	13.111427000	-2.327880000	-2.667097000
1	12.439388000	-4.142671000	-4.558805000
6	13.019063000	-0.676702000	0.000000000
6	13.019063000	0.676702000	0.000000000
6	12.895545000	1.896136000	0.000000000
6	12.549048000	3.266373000	0.000000000
6	12.345130000	3.893044000	1.255794000
6	12.345130000	3.893044000	-1.255794000
6	12.674327000	3.307521000	2.532637000
7	11.806688000	5.138537000	1.432644000
7	11.806688000	5.138537000	-1.432644000
6	12.674327000	3.307521000	-2.532637000
6	12.336894000	4.225302000	3.484168000
1	13.111427000	2.327880000	2.667097000
6	11.775287000	5.358508000	2.792695000
30	11.090462000	6.403081000	0.000000000
6	11.775287000	5.358508000	-2.792695000
6	12.336894000	4.225302000	-3.484168000
1	13.111427000	2.327880000	-2.667097000
1	12.439388000	4.142671000	4.558805000
6	11.210300000	6.472269000	3.411291000
7	10.353448000	7.655623000	1.432644000
7	10.353448000	7.655623000	-1.432644000
6	11.210300000	6.472269000	-3.411291000
1	12.439388000	4.142671000	-4.558805000
6	10.528248000	7.518443000	2.792695000
6	9.544040000	8.744675000	1.255794000
6	9.544040000	8.744675000	-1.255794000
6	10.528248000	7.518443000	-2.792695000
6	9.827666000	8.571412000	3.484168000
6	9.201561000	9.322529000	2.532637000
6	9.103285000	9.234608000	0.000000000
6	9.201561000	9.322529000	-2.532637000
6	9.827666000	8.571412000	-3.484168000
1	9.807353000	8.701490000	4.558805000
1	8.571717000	10.190889000	2.667097000
6	8.089875000	10.219801000	0.000000000
1	8.571717000	10.190889000	-2.667097000
1	9.807353000	8.701490000	-4.558805000
6	7.095573000	10.936488000	0.000000000
1	-11.254926000	6.498034000	-4.496488000
1	-11.254926000	-6.498034000	-4.496488000
1	0.000000000	-12.996069000	-4.496488000
1	11.254926000	-6.498034000	-4.496488000
1	11.254926000	6.498034000	-4.496488000
1	0.000000000	12.996069000	-4.496488000
1	11.254926000	-6.498034000	4.496488000
1	0.000000000	-12.996069000	4.496488000
1	-11.254926000	-6.498034000	4.496488000
1	-11.254926000	6.498034000	4.496488000
1	0.000000000	12.996069000	4.496488000
1	11.254926000	6.498034000	4.496488000

**c-P6** optimized with **CAM-B3LYP** - E=-17509.042830au

6	2.784061000	12.591836000	1.246438000
6	3.455843000	12.576991000	2.520012000
6	2.499013000	12.743582000	3.466808000
6	1.239430000	12.829653000	2.777056000
7	1.442860000	12.751104000	1.424728000
1	4.521799000	12.460698000	2.651712000
1	2.620756000	12.787125000	4.540864000
6	0.000000000	12.896316000	3.397172000
6	-1.239430000	12.829653000	2.777056000
6	-2.499013000	12.743582000	3.466808000
7	-1.442860000	12.751104000	1.424728000
6	-3.455843000	12.576991000	2.520012000
1	-2.620756000	12.787125000	4.540864000
6	-2.784061000	12.591836000	1.246438000
1	-4.521799000	12.460698000	2.651712000
6	-3.423966000	12.462500000	0.000000000
6	-2.784061000	12.591836000	-1.246438000
6	-3.455843000	12.576991000	-2.520012000
7	-1.442860000	12.751104000	-1.424728000
6	-2.499013000	12.743582000	-3.466808000
1	-4.521799000	12.460698000	-2.651712000
6	-1.239430000	12.829653000	-2.777056000
1	-2.620756000	12.787125000	-4.540864000
6	0.000000000	12.896316000	-3.397172000
6	1.239430000	12.829653000	-2.777056000
6	2.499013000	12.743582000	-3.466808000
7	1.442860000	12.751104000	-1.424728000
6	3.455843000	12.576991000	-2.520012000
1	2.620756000	12.787125000	-4.540864000
6	2.784061000	12.591836000	-1.246438000
1	4.521799000	12.460698000	-2.651712000
6	3.423966000	12.462500000	0.000000000
30	0.000000000	12.769438000	0.000000000
6	4.792629000	12.080850000	0.000000000
6	5.903982000	11.590924000	0.000000000
6	-4.792629000	12.080850000	0.000000000
6	-5.903982000	11.590924000	0.000000000
6	-11.168537000	6.448158000	-3.397172000
6	-11.730520000	5.341449000	-2.777056000
6	-10.491090000	7.488204000	-2.777056000
6	-12.285772000	4.207583000	-3.466808000
7	-11.764210000	5.125999000	-1.424728000
6	-9.786760000	8.536000000	-3.466808000
7	-10.321350000	7.625105000	-1.424728000
6	-12.619915000	3.295648000	-2.520012000
1	-12.384353000	4.123922000	-4.540864000
6	-12.296881000	3.884850000	-1.246438000
30	-11.058658000	6.384719000	0.000000000
6	-9.164072000	9.281343000	-2.520012000
1	-9.763597000	8.663203000	-4.540864000
6	-9.512820000	8.706986000	-1.246438000
1	-13.052181000	2.314356000	-2.651712000
6	-12.504824000	3.266009000	0.000000000
7	-10.321350000	7.625105000	1.424728000
7	-11.764210000	5.125999000	1.424728000

1	-8.530382000	10.146342000	-2.651712000
6	-9.080858000	9.196491000	0.000000000
6	-12.296881000	3.884850000	1.246438000
6	-12.858638000	1.889887000	0.000000000
6	-9.512820000	8.706986000	1.246438000
6	-10.491090000	7.488204000	2.777056000
6	-11.730520000	5.341449000	2.777056000
6	-8.066009000	10.190964000	0.000000000
6	-12.619915000	3.295648000	2.520012000
6	-12.990025000	0.682464000	0.000000000
6	-9.164072000	9.281343000	2.520012000
6	-9.786760000	8.536000000	3.466808000
6	-11.168537000	6.448158000	3.397172000
6	-12.285772000	4.207583000	3.466808000
6	-7.086043000	10.908460000	0.000000000
1	-13.052181000	2.314356000	2.651712000
1	-8.530382000	10.146342000	2.651712000
1	-9.763597000	8.663203000	4.540864000
1	-12.384533000	4.123922000	4.540864000
6	-7.086043000	-10.908460000	0.000000000
6	-5.903982000	-11.590924000	0.000000000
6	-8.066009000	-10.190964000	0.000000000
6	-4.792629000	-12.080850000	0.000000000
6	-9.080858000	-9.196491000	0.000000000
6	-3.423966000	-12.462500000	0.000000000
6	-9.512820000	-8.706986000	-1.246438000
6	-9.512820000	-8.706986000	1.246438000
6	-2.784061000	-12.591836000	-1.246438000
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7	-1.442860000	-12.751104000	1.424728000
6	-3.455843000	-12.576991000	2.520012000
6	-9.786760000	-8.536000000	-3.466808000
1	-8.530382000	-10.146342000	-2.651712000
6	-10.491090000	-7.488204000	-2.777056000
30	-11.058658000	-6.384719000	0.000000000
6	-9.786760000	-8.536000000	3.466808000
1	-8.530382000	-10.146342000	2.651712000
6	-10.491090000	-7.488204000	2.777056000
6	-1.239430000	-12.829653000	-2.777056000
30	0.000000000	-12.769438000	0.000000000
6	-2.499013000	-12.743582000	-3.466808000
1	-4.521799000	-12.460698000	-2.651712000
6	-1.239430000	-12.829653000	2.777056000
6	-2.499013000	-12.743582000	3.466808000
1	-4.521799000	-12.460698000	2.651712000
1	-9.763597000	-8.663203000	-4.540864000
6	-11.168537000	-6.448158000	-3.397172000
7	-11.764210000	-5.125999000	-1.424728000
7	-11.764210000	-5.125999000	1.424728000
1	-9.763597000	-8.663203000	4.540864000
6	-11.168537000	-6.448158000	3.397172000
6	0.000000000	-12.896316000	-3.397172000
7	1.442860000	-12.751104000	-1.424728000

7	1.442860000	-12.751104000	1.424728000
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6	0.000000000	-12.896316000	3.397172000
1	-2.620756000	-12.787125000	4.540864000
6	-11.730520000	-5.341449000	-2.777056000
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6	-12.296881000	-3.884850000	1.246438000
6	1.239430000	-12.829653000	-2.777056000
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6	2.784061000	-12.591836000	1.246438000
6	1.239430000	-12.829653000	2.777056000
6	-12.285772000	-4.207583000	-3.466808000
6	-12.619915000	-3.295648000	-2.520012000
6	-12.504824000	-3.266009000	0.000000000
6	-12.285772000	-4.207583000	3.466808000
6	-12.619915000	-3.295648000	2.520012000
6	2.499013000	-12.743582000	-3.466808000
6	3.455843000	-12.576991000	-2.520012000
6	3.423966000	-12.462500000	0.000000000
6	3.455843000	-12.576991000	2.520012000
6	2.499013000	-12.743582000	3.466808000
1	-12.384353000	-4.123922000	-4.540864000
1	-13.052181000	-2.314356000	-2.651712000
6	-12.858638000	-1.889887000	0.000000000
1	-12.384353000	-4.123922000	4.540864000
1	-13.052181000	-2.314356000	2.651712000
1	2.620756000	-12.787125000	-4.540864000
1	4.521799000	-12.460698000	-2.651712000
6	4.792629000	-12.080850000	0.000000000
1	4.521799000	-12.460698000	2.651712000
1	2.620756000	-12.787125000	4.540864000
6	-12.990025000	-0.682464000	0.000000000
6	5.903982000	-11.590924000	0.000000000
6	7.086043000	-10.908460000	0.000000000
6	8.066009000	-10.190964000	0.000000000
6	9.080858000	-9.196491000	0.000000000
6	9.512820000	-8.706986000	1.246438000
6	9.512820000	-8.706986000	-1.246438000
6	9.164072000	-9.281343000	2.520012000
7	10.321350000	-7.625105000	1.424728000
7	10.321350000	-7.625105000	-1.424728000
6	9.164072000	-9.281343000	-2.520012000
6	9.786760000	-8.536000000	3.466808000
1	8.530382000	-10.146342000	2.651712000
6	10.491090000	-7.488204000	2.777056000
30	11.058658000	-6.384719000	0.000000000
6	10.491090000	-7.488204000	-2.777056000
6	9.786760000	-8.536000000	-3.466808000
1	8.530382000	-10.146342000	-2.651712000
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7	11.764210000	-5.125999000	-1.424728000
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6	11.730520000	-5.341449000	2.777056000
6	12.296881000	-3.884850000	1.246438000
6	12.296881000	-3.884850000	-1.246438000

6	11.730520000	-5.341449000	-2.777056000
6	12.285772000	-4.207583000	3.466808000
6	12.619915000	-3.295648000	2.520012000
6	12.504824000	-3.266009000	0.000000000
6	12.619915000	-3.295648000	-2.520012000
6	12.285772000	-4.207583000	-3.466808000
1	12.384353000	-4.123922000	4.540864000
1	13.052181000	-2.314356000	2.651712000
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1	13.052181000	-2.314356000	-2.651712000
1	12.384353000	-4.123922000	-4.540864000
6	12.990025000	-0.682464000	0.000000000
6	12.990025000	0.682464000	0.000000000
6	12.858638000	1.889887000	0.000000000
6	12.504824000	3.266009000	0.000000000
6	12.296881000	3.884850000	1.246438000
6	12.296881000	3.884850000	-1.246438000
6	12.619915000	3.295648000	2.520012000
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7	11.764210000	5.125999000	-1.424728000
6	12.619915000	3.295648000	-2.520012000
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1	13.052181000	2.314356000	2.651712000
6	11.730520000	5.341449000	2.777056000
30	11.058658000	6.384719000	0.000000000
6	11.730520000	5.341449000	-2.777056000
6	12.285772000	4.207583000	-3.466808000
1	13.052181000	2.314356000	-2.651712000
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6	11.168537000	6.448158000	3.397172000
7	10.321350000	7.625105000	1.424728000
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6	11.168537000	6.448158000	-3.397172000
1	12.384353000	4.123922000	-4.540864000
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6	9.512820000	8.706986000	1.246438000
6	9.512820000	8.706986000	-1.246438000
6	10.491090000	7.488204000	-2.777056000
6	9.786760000	8.536000000	3.466808000
6	9.164072000	9.281343000	2.520012000
6	9.080858000	9.196491000	0.000000000
6	9.164072000	9.281343000	-2.520012000
6	9.786760000	8.536000000	-3.466808000
1	9.763597000	8.663203000	4.540864000
1	8.530382000	10.146342000	2.651712000
6	8.066009000	10.190964000	0.000000000
1	8.530382000	10.146342000	-2.651712000
1	9.763597000	8.663203000	-4.540864000
6	7.086043000	10.908460000	0.000000000
1	-11.209852000	6.472011000	-4.481464000
1	-11.209852000	-6.472011000	-4.481464000
1	0.000000000	-12.944022000	-4.481464000
1	11.209852000	-6.472011000	-4.481464000
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1	0.000000000	12.944022000	-4.481464000
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1	0.000000000	-12.944022000	4.481464000
1	-11.209852000	-6.472011000	4.481464000
1	-11.209852000	6.472011000	4.481464000

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1	11.209852000	6.472011000	4.481464000

**c-P6** optimized with **M06-2X** E=-17509.271928au

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6	2.507434000	12.735727000	3.478217000
6	1.245158000	12.826452000	2.785518000
7	1.452439000	12.765253000	1.434327000
1	4.534419000	12.471187000	2.657808000
1	2.627106000	12.766469000	4.553180000
6	0.000000000	12.883438000	3.405925000
6	-1.245158000	12.826452000	2.785518000
6	-2.507434000	12.735727000	3.478217000
7	-1.452439000	12.765253000	1.434327000
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1	-2.627106000	12.766469000	4.553180000
6	-2.791976000	12.612039000	1.252824000
1	-4.534419000	12.471187000	2.657808000
6	-3.431206000	12.489763000	0.000000000
6	-2.791976000	12.612039000	-1.252824000
6	-3.467224000	12.584989000	-2.528636000
7	-1.452439000	12.765253000	-1.434327000
6	-2.507434000	12.735727000	-3.478217000
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6	-1.245158000	12.826452000	-2.785518000
1	-2.627106000	12.766469000	-4.553180000
6	0.000000000	12.883438000	-3.405925000
6	1.245158000	12.826452000	-2.785518000
6	2.507434000	12.735727000	-3.478217000
7	1.452439000	12.765253000	-1.434327000
6	3.467224000	12.584989000	-2.528636000
1	2.627106000	12.766469000	-4.553180000
6	2.791976000	12.612039000	-1.252824000
1	4.534419000	12.471187000	-2.657808000
6	3.431206000	12.489763000	0.000000000
30	0.000000000	12.792194000	0.000000000
6	4.802150000	12.108343000	0.000000000
6	5.917653000	11.618512000	0.000000000
6	-4.802150000	12.108343000	0.000000000
6	-5.917653000	11.618512000	0.000000000
6	-11.157385000	6.441719000	-3.405925000
6	-11.730613000	5.334888000	-2.785518000
6	-10.485454000	7.491565000	-2.785518000
6	-12.283180000	4.196362000	-3.478217000
7	-11.781253000	5.124778000	-1.434327000
6	-9.775747000	8.539365000	-3.478217000
7	-10.328814000	7.640475000	-1.434327000
6	-12.632532000	3.289791000	-2.528636000
1	-12.369639000	4.108094000	-4.553180000
6	-12.318334000	3.888097000	-1.252824000
30	-11.078365000	6.396097000	0.000000000
6	-9.165308000	9.295198000	-2.528636000
1	-9.742534000	8.658375000	-4.553180000
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6	13.297824000	1.250754000	-2.792466000
30	13.195585000	-0.000855000	0.000077000
6	13.297769000	1.250767000	2.792616000
6	13.242291000	2.508719000	3.486424000
1	12.934940000	4.539268000	2.678997000
1	13.340436000	2.636115000	-4.556424000
6	13.390801000	-0.000870000	-3.402496000
7	13.158424000	-1.456529000	-1.434362000
7	13.158395000	-1.456522000	1.434522000
6	13.390734000	-0.000854000	3.402654000

1	13.340345000	2.636137000	4.556568000
6	13.297746000	-1.252485000	-2.792460000
6	12.993763000	-2.796632000	-1.270125000
6	12.993738000	-2.796626000	1.270288000
6	13.297690000	-1.252471000	2.792622000
6	13.242207000	-2.510434000	-3.486268000
6	13.032403000	-3.473726000	-2.538223000
6	12.808337000	-3.437426000	0.000082000
6	13.032352000	-3.473713000	2.538391000
6	13.242138000	-2.510417000	3.486436000
1	13.340275000	-2.637858000	-4.556410000
1	12.934708000	-4.540963000	-2.678847000
6	12.362861000	-4.750349000	0.000081000
1	12.934654000	-4.540950000	2.679019000
1	13.340184000	-2.637836000	4.556580000
6	11.793395000	-5.849403000	0.000075000
6	11.087009000	-6.978469000	0.000060000
6	10.329825000	-7.957647000	0.000045000
6	9.353010000	-8.943846000	0.000032000
6	8.584320000	-9.386970000	-1.269365000
6	8.858398000	-9.386970000	1.269416000
6	9.470016000	-9.092884000	-2.542545000
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6	9.469949000	-9.092884000	2.542612000
6	8.705367000	-9.706444000	-3.491306000
1	10.371867000	-8.513365000	-2.681053000
6	7.614293000	-10.345178000	-2.798459000
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6	7.614219000	-10.345178000	2.798477000
6	8.705275000	-9.706444000	3.491353000
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6	6.548641000	-10.993549000	-3.408156000
7	5.171312000	-11.503306000	-1.434004000
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6	6.548551000	-10.993549000	3.408145000
1	8.854613000	-9.720457000	4.563112000
6	5.400178000	-11.505601000	-2.788988000
6	3.907646000	-11.997028000	-1.261396000
6	3.907613000	-11.997029000	1.261316000
6	5.400104000	-11.505602000	2.788947000
6	4.257684000	-12.035815000	-3.484606000
6	3.319193000	-12.325063000	-2.534647000
6	3.273338000	-12.166689000	-0.000049000
6	3.319126000	-12.325063000	2.534551000
6	4.257592000	-12.035816000	3.484535000
1	4.182789000	-12.159527000	-4.557036000
1	2.330223000	-12.738127000	-2.674457000
6	1.896925000	-12.464629000	-0.000067000
1	2.330152000	-12.738128000	2.674335000
1	4.182668000	-12.159528000	4.556963000
6	0.673469000	-12.564217000	-0.000082000
1	-13.497777000	0.000668000	4.483838000
1	-6.584592000	11.070358000	4.491083000
1	6.586017000	11.069740000	4.491061000
1	13.497714000	-0.000854000	4.483885000
1	6.584755000	-11.070377000	4.491079000
1	-6.586130000	-11.069558000	4.491014000

1	13.497804000	-0.000876000	-4.483725000
1	6.586087000	11.069740000	-4.491106000
1	-6.584673000	11.070353000	-4.491084000
1	-13.497854000	0.000744000	-4.483772000
1	-6.586185000	-11.069552000	-4.491155000
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**c-P6<sup>+4</sup>** optimized with **CAM-B3LYP** - E=-17507.935387au

6	-9.857571000	-8.400201000	-1.257711000
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6	-10.999187000	-7.329665000	-2.769379000
7	-10.777802000	-7.408436000	-1.427559000
1	-8.784528000	-9.767328000	-2.658965000
1	-10.223396000	-8.458116000	-4.534023000
6	-11.818458000	-6.366042000	-3.388070000
6	-12.461839000	-5.311268000	-2.790225000
6	-13.162941000	-4.262109000	-3.476791000
7	-12.447884000	-5.043560000	-1.428059000
6	-13.533540000	-3.354863000	-2.535323000
1	-13.336504000	-4.225352000	-4.543726000
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7	-12.447877000	-5.043563000	1.428138000
6	-13.162919000	-4.262116000	3.476877000
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6	-12.461821000	-5.311274000	2.790304000
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6	-7.173474000	-10.262734000	0.000005000
6	-13.576233000	-1.902183000	0.000046000
6	-13.693550000	-0.660001000	0.000036000
6	-11.824632000	6.357733000	3.387992000
6	-11.006155000	7.322014000	2.769318000
6	-12.467048000	5.302336000	2.790163000
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6	-9.865325000	8.393404000	1.257667000
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6	-13.085373000	3.865998000	1.276329000
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7	-12.452640000	5.034463000	-1.428171000
7	-10.784605000	7.400784000	-1.427683000
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6	-8.255100000	9.675125000	-0.000078000
6	-13.085277000	3.865910000	-1.276441000
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6	-13.536770000	3.344779000	-2.535407000
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6	9.490840000	8.962484000	2.517599000
7	10.777651000	7.408352000	-1.427506000
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6	1.235005000	11.882344000	-2.779326000
6	10.999386000	7.329856000	2.769483000
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6	10.222233000	8.302391000	3.464110000
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1	8.784304000	9.767194000	-2.658889000
1	2.616100000	11.888412000	4.544437000
6	-0.005217000	11.947499000	3.398077000



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6	11.818698000	6.366266000	3.388173000
7	12.447952000	5.043647000	1.428198000
7	12.447706000	5.043456000	-1.427999000
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6	11.818119000	6.365815000	-3.388042000
1	10.222983000	8.457835000	-4.533989000
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6	-2.790354000	11.663102000	1.253060000
6	-1.245173000	11.881543000	-2.779386000
6	-2.790317000	11.662924000	-1.253128000
6	12.462021000	5.311447000	2.790346000
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6	13.081401000	3.875486000	-1.276259000
6	12.461543000	5.311075000	-2.790184000
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6	13.533690000	3.355019000	2.535487000
6	13.271252000	3.222260000	0.000151000
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6	-4.800963000	11.219270000	-0.000034000
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1	-4.533196000	11.588455000	-2.662377000
1	13.336828000	4.225646000	4.543847000
1	14.079113000	2.432467000	2.670498000
6	13.576170000	1.902168000	0.000210000
1	14.078652000	2.432109000	-2.670229000
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6	-5.954439000	10.822621000	-0.000043000
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6	13.578098000	-1.892087000	0.000153000
6	13.274431000	-3.212462000	0.000109000
6	13.085313000	-3.865920000	-1.276299000
6	13.085360000	-3.866022000	1.276471000
6	13.536827000	-3.344779000	-2.535253000
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7	12.452733000	-5.034589000	1.428148000
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6	12.466905000	-5.302144000	-2.790207000
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6	9.498865000	-8.955746000	-2.517567000
6	9.360621000	-8.813617000	-0.000047000
6	9.498942000	-8.955941000	2.517457000
6	10.229763000	-8.295246000	3.463996000
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1	10.231397000	-8.451308000	4.533998000
6	7.182586000	-10.257894000	-0.000089000
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6	4.800984000	-11.219283000	-0.000149000
6	3.430374000	-11.547214000	-0.000131000
6	2.790337000	-11.663013000	-1.253217000
6	2.790369000	-11.663018000	1.252971000
6	3.464874000	-11.671435000	-2.526122000
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6	1.245196000	-11.881736000	-2.779463000
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6	-3.454779000	-11.673631000	-2.526013000
6	-3.420291000	-11.549450000	-0.000042000
6	-3.454714000	-11.673636000	2.525929000
6	-2.494855000	-11.826267000	3.471439000
1	-2.616209000	-11.888046000	-4.544458000
1	-4.523180000	-11.591525000	-2.662338000
6	-4.791181000	-11.222469000	-0.000026000
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1	-2.616092000	-11.888059000	4.544352000
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1	11.908961000	6.440782000	-4.467523000
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1	-11.915390000	6.432457000	-4.467650000
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**c-P6<sup>+4</sup>** optimized with **M06-2X** - E=-17508.138955au

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6	6.557743000	-10.764802000	3.404365000
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7	7.781042000	-9.967164000	1.436407000
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1	10.444196000	-8.407140000	2.677248000
6	9.415651000	-8.828794000	0.000070000
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6	9.525942000	-8.961506000	-2.544692000
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**c-P6<sup>+</sup>** optimized with **B3LYP** - E=-17510.640427au

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**c-P6<sup>+</sup>** optimized with **M06-2X** - E=-17507.306773au

6	-10.537792000	-7.826432000	-1.285367000
6	-10.358856000	-8.496954000	-2.549563000
6	-10.884589000	-7.670789000	-3.491874000
6	-11.350092000	-6.491972000	-2.800467000
7	-11.129459000	-6.640408000	-1.436849000
1	-9.917643000	-9.474476000	-2.683435000
1	-10.950878000	-7.831281000	-4.559874000
6	-11.853125000	-5.360460000	-3.397172000
6	-12.197462000	-4.133789000	-2.773974000
6	-12.566545000	-2.940665000	-3.475553000
7	-12.156233000	-3.911375000	-1.436407000
6	-12.721404000	-1.968958000	-2.527918000
1	-12.686442000	-2.854731000	-4.547048000
6	-12.472950000	-2.594599000	-1.260541000
1	-13.001226000	-0.934685000	-2.670009000
6	-12.559232000	-1.956091000	0.000077000
6	-12.473186000	-2.594628000	1.260700000
6	-12.721876000	-1.969020000	2.528046000
7	-12.156496000	-3.911406000	1.436593000
6	-12.567181000	-2.940750000	3.475687000
1	-13.001734000	-0.934752000	2.670109000
6	-12.197961000	-4.133857000	2.774147000
1	-12.687273000	-2.854840000	4.547163000
6	-11.853709000	-5.360539000	3.397375000
6	-11.350557000	-6.492035000	2.800731000
6	-10.885160000	-7.670864000	3.492189000
7	-11.129694000	-6.640439000	1.437149000
6	-10.359266000	-8.497006000	2.549946000
1	-10.951625000	-7.831381000	4.560174000
6	-10.538000000	-7.826458000	1.285733000
1	-9.918068000	-9.474528000	2.683869000
6	-10.115780000	-8.357148000	0.000212000
30	-11.714693000	-5.288963000	0.000118000
6	-9.207237000	-9.365006000	0.000286000
6	-8.261247000	-10.187983000	0.000393000
6	-12.687236000	-0.540028000	0.000073000
6	-12.645173000	0.678018000	0.000093000
6	-10.435348000	7.767262000	3.396681000
6	-9.701866000	8.764946000	2.800004000
6	-11.034004000	6.642540000	2.773527000
6	-8.995441000	9.817182000	3.491454000

7	-9.454406000	8.862698000	1.436421000
6	-11.649749000	5.556034000	3.475217000
7	-11.041110000	6.416236000	1.436005000
6	-8.305109000	10.511812000	2.549204000
1	-9.026097000	9.988258000	4.559427000
6	-8.622973000	9.894874000	1.285004000
30	-10.314947000	7.667347000	-0.000497000
6	-12.008553000	4.639691000	2.527705000
1	-11.785408000	5.497888000	4.546702000
6	-11.631931000	5.197526000	1.260274000
1	-7.665325000	11.372560000	2.683096000
6	-8.097019000	10.322981000	-0.000518000
7	-11.040470000	6.415680000	-1.436835000
7	-9.453725000	8.862116000	-1.437500000
1	-12.502944000	3.689144000	2.670002000
6	-11.852205000	4.591869000	-0.000244000
6	-8.622357000	9.894345000	-1.286113000
6	-6.994173000	11.113372000	-0.000415000
6	-11.631379000	5.197043000	-1.260891000
6	-11.032756000	6.641456000	-2.774441000
6	-9.700561000	8.763824000	-2.801159000
6	-12.279779000	3.235848000	-0.000084000
6	-8.303894000	10.510771000	-2.550413000
6	-5.894458000	11.715709000	-0.000314000
6	-12.007434000	4.638714000	-2.528274000
6	-11.648194000	5.554680000	-3.475983000
6	-10.433793000	7.765919000	-3.397772000
6	-8.993798000	9.815773000	-3.492704000
6	-12.498795000	2.036885000	0.000037000
1	-7.664037000	11.371457000	-2.684354000
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6	8.011278000	9.799277000	0.000438000
6	5.874287000	11.251638000	0.000545000
6	8.940012000	9.010052000	0.000313000
6	4.583982000	11.848872000	0.000372000
6	9.901444000	7.962483000	0.000159000
6	3.987782000	12.093661000	1.260877000
6	3.987901000	12.093175000	-1.260275000
6	10.316140000	7.469156000	1.260686000
6	10.315634000	7.469056000	-1.260493000
6	4.653717000	11.996155000	2.528322000
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6	4.653951000	11.995177000	-2.527620000
7	2.689237000	12.477498000	-1.436257000
7	11.077630000	6.349161000	1.436411000
6	10.020602000	8.073874000	2.528109000
7	11.077052000	6.349042000	-1.436431000
6	10.019584000	8.073667000	-2.527851000
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1	5.689285000	11.721285000	2.670604000
6	2.517029000	12.625077000	2.774135000
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6	3.734952000	12.346451000	-3.475360000
1	5.689532000	11.720248000	-2.669698000
6	2.517289000	12.624014000	-2.773870000
6	11.270334000	6.230136000	2.773924000



30	11.799813000	5.095696000	-0.000103000
6	10.635787000	7.305779000	3.475625000
1	9.443342000	8.976491000	2.670446000
6	11.269198000	6.229893000	-2.774012000
6	10.634357000	7.305469000	-3.475551000
1	9.442272000	8.976274000	-2.670031000
1	3.868857000	12.408603000	4.547361000
6	1.282622000	12.940839000	3.397265000
7	-0.187614000	12.954733000	1.436806000
7	-0.187485000	12.954183000	-1.436933000
1	3.869286000	12.406875000	-4.546887000
6	1.282941000	12.939529000	-3.397244000
6	11.946755000	5.150376000	3.397013000
7	12.407023000	3.753842000	1.436724000
7	12.406408000	3.753699000	-1.437057000
1	10.653056000	7.452387000	4.547106000
6	11.945338000	5.150063000	-3.397285000
1	10.651185000	7.451975000	-4.547051000
6	0.051314000	13.071630000	2.800473000
6	-1.510536000	13.035776000	1.285388000
6	0.051576000	13.070549000	-2.800624000
6	-1.510420000	13.035304000	-1.285674000
6	12.445841000	4.017145000	2.800309000
6	12.887000000	2.518392000	1.285307000
6	12.886440000	2.518257000	-1.285729000
6	12.444652000	4.016876000	-2.800682000
6	-1.202292000	13.258508000	3.491849000
6	-2.180633000	13.216570000	2.549554000
6	-2.181222000	12.935669000	-0.000156000
6	-1.201965000	13.257175000	-3.492190000
6	-2.180394000	13.215619000	-2.549975000
6	13.005609000	2.880065000	3.491740000
6	13.263573000	1.935329000	2.549485000
6	12.995465000	1.848964000	-0.000200000
6	13.262480000	1.935076000	-2.550010000
6	13.004117000	2.879724000	-3.492245000
1	-1.308060000	13.396357000	4.559827000
1	-3.247741000	13.323753000	2.683418000
6	-3.508288000	12.652783000	-0.000165000
1	-1.307630000	13.394610000	-4.560232000
1	-3.247487000	13.322769000	-2.683985000
1	13.169368000	2.821491000	4.559694000
1	13.691032000	0.951721000	2.683370000
6	13.129749000	0.498781000	-0.000151000
1	13.689882000	0.951455000	-2.683986000
1	13.167424000	2.821050000	-4.560263000
6	-4.694171000	12.245570000	-0.000220000
6	13.101630000	-0.754751000	-0.000101000
6	12.960564000	-2.059160000	-0.000029000
6	12.719743000	-3.289642000	-0.000013000
6	12.299680000	-4.579943000	-0.000038000
6	12.050159000	-5.210401000	-1.285586000
6	12.050142000	-5.210430000	1.285490000
6	12.542318000	-4.721087000	-2.549814000
7	11.317115000	-6.314672000	-1.437006000
7	11.317097000	-6.314706000	1.436875000
6	12.542291000	-4.721146000	2.549733000
6	12.088183000	-5.588716000	-3.492081000
1	13.170087000	-3.851538000	-2.683680000

6	11.298500000	-6.579982000	-2.800599000
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6	11.298481000	-6.580053000	2.800460000
6	12.088146000	-5.588797000	3.491976000
1	13.170058000	-3.851600000	2.683624000
1	12.260556000	-5.566429000	-4.560052000
6	10.569088000	-7.580612000	-3.397309000
7	9.464848000	-8.566836000	-1.436581000
7	9.464862000	-8.566888000	1.436380000
6	10.569082000	-7.580710000	3.397141000
1	12.260509000	-5.566532000	4.559949000
6	9.678154000	-8.491423000	-2.774134000
6	8.482317000	-9.498966000	-1.260726000
6	8.482339000	-9.499017000	1.260500000
6	9.678168000	-8.491516000	2.773937000
6	8.828709000	-9.406968000	-3.475765000
6	8.064411000	-10.026672000	-2.528107000
6	7.972167000	-9.892559000	-0.000116000
6	8.064445000	-10.026778000	2.527862000
6	8.828742000	-9.407102000	3.475539000
1	8.814159000	-9.553802000	-4.547254000
1	7.308144000	-10.785649000	-2.670348000
6	6.809549000	-10.711097000	-0.000110000
1	7.308183000	-10.785765000	2.670079000
1	8.814198000	-9.553976000	4.547023000
6	5.733527000	-11.283332000	-0.000023000
6	4.483217000	-11.835396000	0.000232000
6	3.335364000	-12.245023000	0.000413000
6	1.947300000	-12.553403000	0.000409000
6	1.312810000	-12.665502000	-1.260189000
6	1.312803000	-12.665448000	1.261007000
6	1.984423000	-12.712001000	-2.527517000
7	-0.037947000	-12.764119000	-1.436105000
7	-0.037952000	-12.764057000	1.436913000
6	1.984406000	-12.711907000	2.528338000
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6	-0.237214000	-12.870966000	-2.773693000
30	-1.484552000	-12.762131000	0.000401000
6	-0.237232000	-12.870856000	2.774504000
6	1.011641000	-12.859570000	3.476027000
1	3.054780000	-12.663825000	2.670504000
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7	-2.949885000	-12.615366000	-1.436586000
7	-2.949891000	-12.615323000	1.437370000
6	-1.510522000	-12.915639000	3.397780000
1	1.129951000	-12.947523000	4.547538000
6	-2.741344000	-12.780466000	-2.800232000
6	-4.259665000	-12.412398000	-1.285169000
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6	-4.952877000	-12.446025000	-2.549376000
6	-4.893533000	-12.171604000	0.000376000
6	-4.952891000	-12.445958000	2.550138000
6	-4.005956000	-12.695508000	3.492446000
1	-4.138620000	-12.807907000	-4.559633000
1	-6.018324000	-12.323452000	-2.683226000

6	-6.129726000	-11.612164000	0.000376000
1	-6.018341000	-12.323392000	2.683978000
1	-4.138648000	-12.807757000	4.560414000
6	-7.201583000	-10.961624000	0.000384000
1	-10.534722000	7.819021000	4.477846000
1	1.311376000	13.049065000	4.478431000
1	12.041258000	5.210721000	4.478170000
1	10.648343000	-7.659718000	4.478318000
1	-1.505515000	-13.027282000	4.478964000
1	-11.961924000	-5.389869000	4.478532000
1	10.648348000	-7.659592000	-4.478489000
1	12.039391000	5.210309000	-4.478487000
1	1.311804000	13.047338000	-4.478449000
1	-10.532674000	7.817245000	-4.479002000
1	-11.961150000	-5.389760000	-4.478348000
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**c-P6<sup>+12</sup>** optimized with **B3LYP** - E=-17507.033566au

6	3.862411000	-12.548154000	1.230231000
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6	4.322023000	-12.943469000	3.400510000
6	5.385935000	-12.180125000	2.761569000
7	5.043008000	-11.951512000	1.412230000
1	2.447016000	-13.712482000	2.549296000
1	4.327224000	-13.275187000	4.431593000
6	6.535207000	-11.743554000	3.360078000
6	7.572082000	-10.940487000	2.760751000
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7	7.695022000	-10.710166000	1.440617000
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1	8.715794000	-10.273494000	4.591972000
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6	8.738941000	-9.816822000	-1.213298000
6	9.522181000	-9.724895000	-2.433970000
7	7.616267000	-10.516568000	-1.394857000
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1	9.129449000	-10.611253000	-4.408569000
6	6.669482000	-11.694799000	-3.338849000
6	5.442264000	-12.159154000	-2.740894000
6	4.301411000	-12.643656000	-3.501167000
7	5.176890000	-12.136197000	-1.421806000
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1	4.284348000	-12.800819000	-4.572234000
6	3.844962000	-12.539749000	-1.289000000
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6	3.169047000	-12.627263000	-0.072301000
30	6.391742000	-11.344577000	0.009023000
6	1.769776000	-12.809436000	-0.050007000
6	0.538432000	-12.849916000	-0.009674000
6	10.044661000	-8.156631000	0.061888000
6	10.719042000	-7.125647000	0.019822000
6	13.455177000	-0.079145000	-3.361914000
6	13.284966000	1.139433000	-2.765428000

6	13.247203000	-1.373403000	-2.761220000
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7	12.916547000	1.332182000	-1.417221000
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7	13.101684000	-1.589899000	-1.441076000
6	13.178102000	3.377394000	-2.459942000
1	13.740817000	2.591987000	-4.436162000
6	12.872005000	2.654460000	-1.237017000
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6	12.777863000	-3.572242000	-2.618427000
1	13.214102000	-2.699633000	-4.590512000
6	12.786967000	-2.945113000	-1.304451000
1	13.216632000	4.453481000	-2.557597000
6	12.605684000	3.302055000	0.064308000
7	12.892779000	-1.609928000	1.394400000
7	13.140252000	1.307704000	1.417090000
1	12.596392000	-4.621690000	-2.805201000
6	12.532261000	-3.572646000	-0.085348000
6	12.853562000	2.669329000	1.282099000
6	12.091969000	4.616215000	0.039898000
6	12.818951000	-2.930970000	1.214556000
6	13.271809000	-1.425092000	2.740751000
6	13.287635000	1.088025000	2.736496000
6	11.990678000	-4.875535000	-0.058493000
6	12.864483000	3.296387000	2.596096000
6	11.534984000	5.715132000	-0.000867000
6	13.115289000	-3.660246000	2.436127000
6	13.406879000	-2.727211000	3.380340000
6	13.470948000	-0.210400000	3.336247000
6	13.162907000	2.322339000	3.494960000
6	11.409739000	-5.961909000	-0.016239000
1	12.706243000	4.349433000	2.783782000
1	13.130973000	-4.736902000	2.533819000
1	13.704364000	-2.887040000	4.409482000
1	13.291915000	2.414488000	4.565958000
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6	2.044913000	12.768724000	0.100378000
6	-1.771165000	12.813882000	0.110867000
6	3.439848000	12.553498000	0.103232000
6	-3.170341000	12.628995000	0.121481000
6	4.110691000	12.441981000	-1.208587000
6	4.133286000	12.468403000	1.310240000
6	-3.855384000	12.559789000	-1.186059000
6	-3.854531000	12.532917000	1.332946000
6	3.613945000	13.048707000	-2.432132000
7	5.276113000	11.819247000	-1.400539000
6	3.618170000	12.807620000	2.629128000
7	5.459527000	12.041361000	1.427655000
7	-5.035501000	11.966096000	-1.379936000
6	-3.357776000	13.183523000	-2.400577000
7	-5.187943000	12.129799000	1.454160000
6	-3.320242000	12.832404000	2.653773000
6	4.543845000	12.798286000	-3.391045000
1	2.697807000	13.615753000	-2.521718000
6	5.602268000	12.022534000	-2.758047000
30	6.634837000	11.204608000	-0.010181000
6	4.626913000	12.592936000	3.513451000
1	2.629443000	13.196944000	2.829125000

6	5.745950000	12.076104000	2.742004000
6	-5.370839000	12.207566000	-2.729053000
30	-6.393156000	11.348572000	0.009887000
6	-4.302292000	12.974927000	-3.355259000
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1	-13.332846000	-1.517542000	4.556485000
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6	-12.845037000	3.426137000	-3.505682000
6	-12.456819000	4.362894000	-2.616871000
6	-12.237880000	4.352496000	-0.098518000

6	-12.840151000	4.493253000	2.408432000
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6	-11.599729000	5.624841000	-0.067514000
1	-12.782982000	5.568986000	2.493858000
1	-13.507251000	3.784213000	4.371594000
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1	13.652564000	-1.142137000	4.388234000
1	6.074435000	-12.372368000	4.370986000
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1	-13.742162000	1.121612000	4.358463000
1	-5.899238000	12.455937000	4.370175000
1	-7.644192000	-11.368727000	-4.387194000
1	5.857233000	-12.476559000	-4.368135000
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**c-P6<sup>+12</sup>** optimized with **M06-2X** - E=-17503.701580au

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6	-6.525997000	-11.640213000	-2.743879000
7	-6.153663000	-11.436619000	-1.397735000
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6	-13.206117000	-1.341049000	3.526404000
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7	8.592053000	9.740091000	-1.380715000
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6	9.984355000	8.363490000	0.133081000
6	10.429972000	8.778868000	-2.387558000
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6	10.157153000	-7.898603000	0.002627000
6	9.415702000	-8.868509000	0.046448000
6	8.445990000	-9.914172000	0.078775000
6	7.988521000	-10.446403000	-1.227111000
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**c-P6-T6** optimized with **B3LYP** - E=-23379.854115au

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6	-12.259077000	-5.064216000	-2.701646000
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6	2.535274000	-12.727667000	2.073541000
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**c-P6-T6** optimized with **M06-2X** - E=-23380.884725au

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**c-P6-T6<sup>+</sup>** optimized with **B3LYP** - E=-23385.818909au

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**c-P6-T6<sup>+4</sup>** optimized with **CAM-B3LYP** - E=-23378.852940au

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**c-P6-T6<sup>6</sup>** optimized with **B3LYP** - E=-23385.062850au

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**c-P6-T6<sup>+6</sup>** optimized with **CAM-B3LYP** - E=-23378.097541au

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