Electronic Supplementary Information

Axially substituted phosphorous(V) corrole with polycyclic aromatic hydrocarbons: Synthesis, X-ray structure, and photoinduced energy and electron transfer studies

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Figure S14. Energies of the singlet and charge-transfer states of triads.
Table S1. Comparison of experimental optical properties with singlet excited state properties of dyads by B3LYP in DCM solvent.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\lambda_{\text{max}}^a$</th>
<th>$\lambda_{\text{max}}^b$</th>
<th>$f^c$</th>
<th>$E^d$</th>
<th>% of molecular orbital composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triad 1</td>
<td>580</td>
<td>535</td>
<td>0.1202</td>
<td>2.31</td>
<td>H-1-&gt;L+1 (22%), HOMO-&gt;LUMO (76%)</td>
</tr>
<tr>
<td>Triad 2</td>
<td>584</td>
<td>624</td>
<td>0.0145</td>
<td>1.98</td>
<td>HOMO-&gt;LUMO (98%)</td>
</tr>
</tbody>
</table>

$^a$Recorded absorbance in nm, $^b$Theoretical absorbance in nm, $^c$Oscillation strength, and $^d$Excited state energy in eV.