Electronic Supplementary Information

2,7-Diazapyrenes: a brief review on synthetic strategies and application opportunities

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The calculations were carried out as reported earlier [1-4] in the Orca 4.0.1 software package using the DFT B3LYP, 6-311G * method. The calculations in a solvent were carried out by the CPCMC solvation method [5].

Table S1. HOMO-LUMO distributions of 2,7-diazapyrenes in a gas phase

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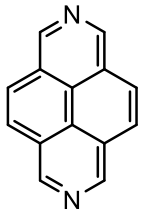
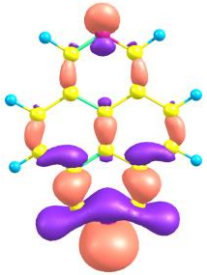
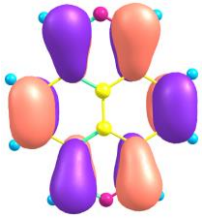
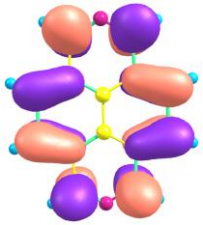
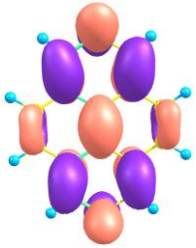
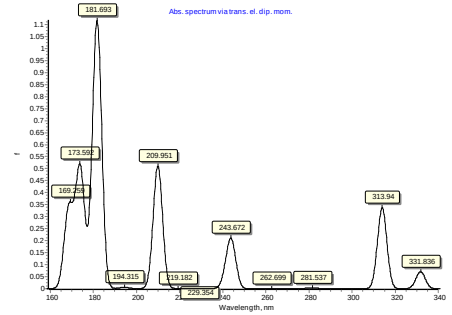
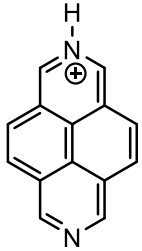
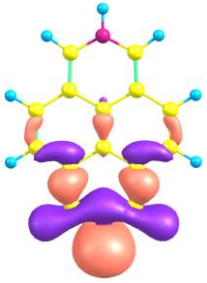
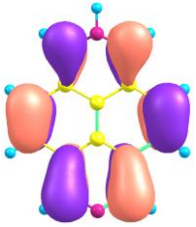
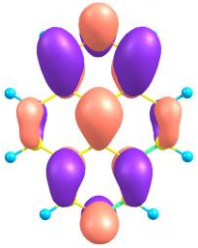
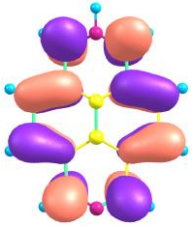
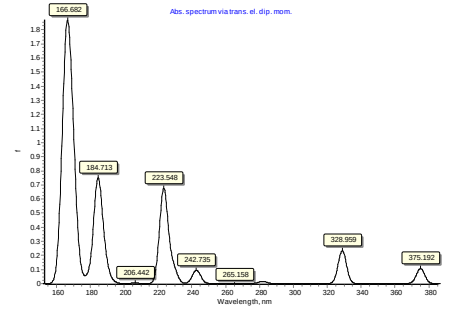
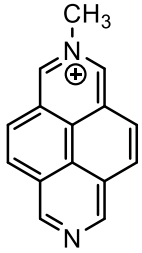
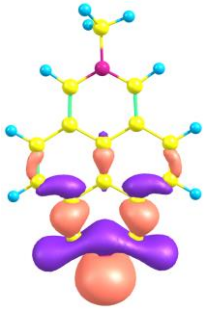
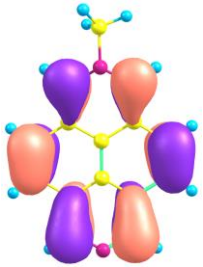
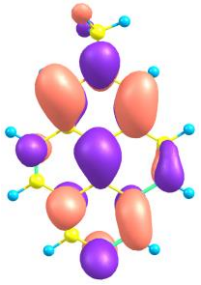
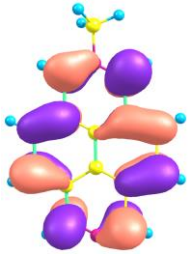
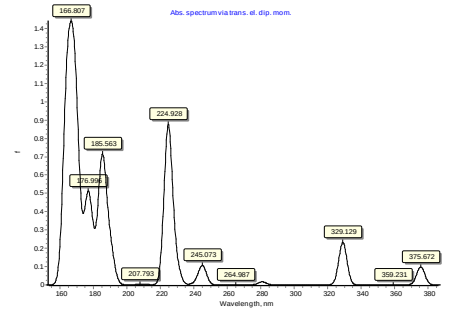
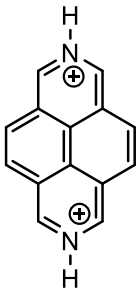
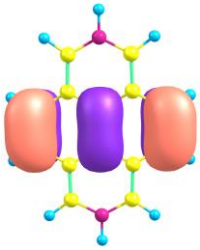
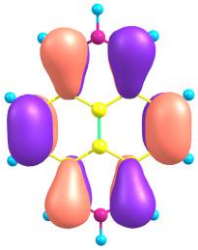
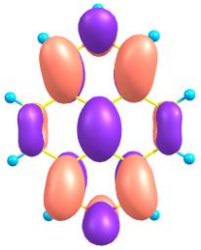
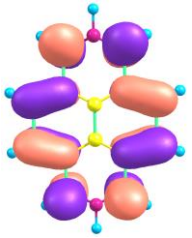
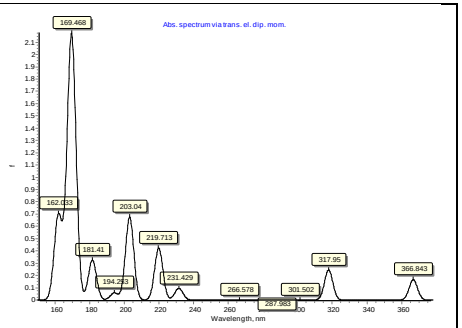
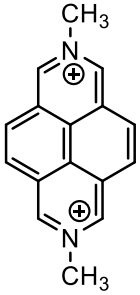
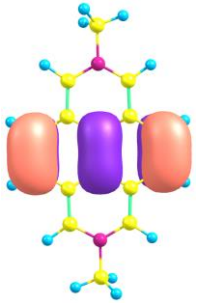
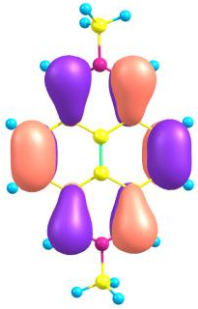
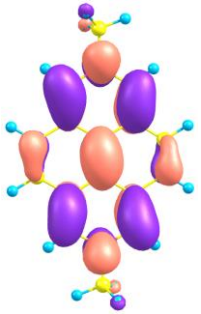
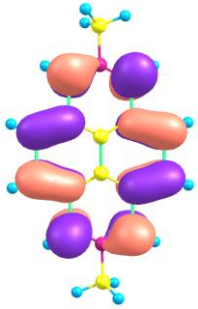
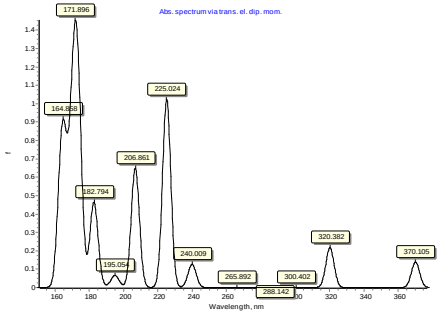
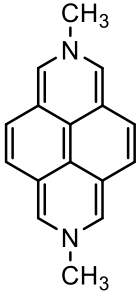
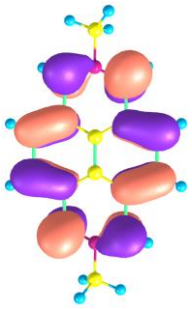
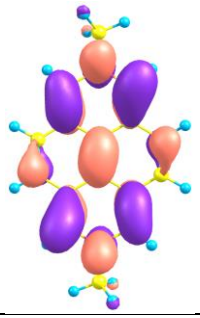
1.		-7.1346 	-5.9814 	-2.1156 	-1.6774 	3.8658	
2.		-10.5139 	-9.9152 	-6.3504 	-6.1311 	3.5648	
3.		-10.3920 	-9.7740 	-6.1724 	-5.9879 	3.6016	

4.		-15.0642 	-13.9682 	-10.4358 	-10.0694 	3.5324	
5.		-14.6932 	-13.5723 	-9.9681 	-9.6769 	3.6042	
6.			-2.5108 	-1.4594 		1.0514	

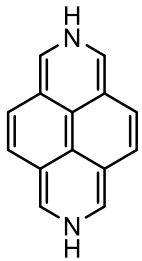
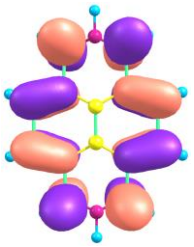
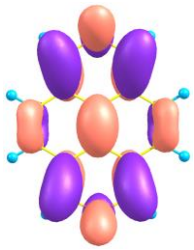
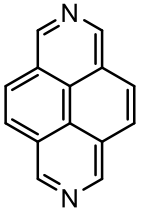
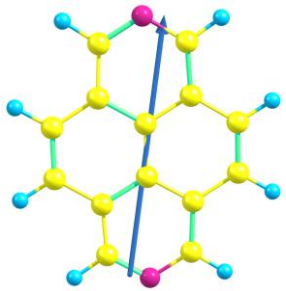
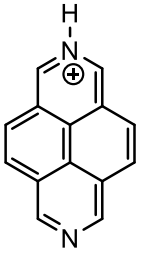
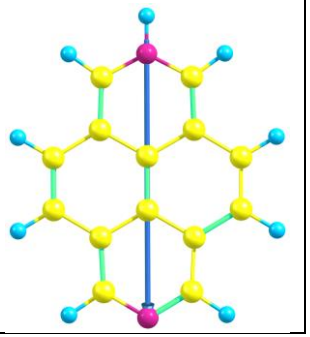
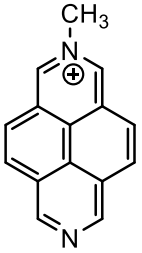
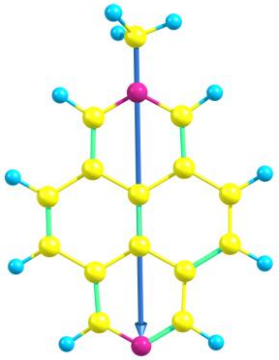
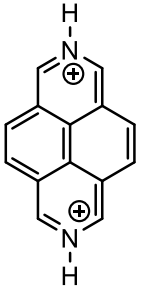
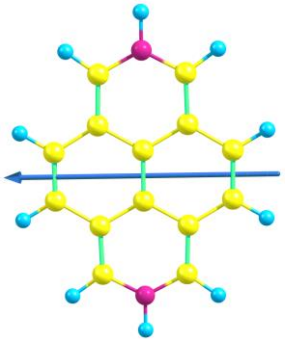
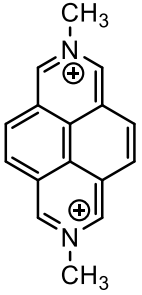
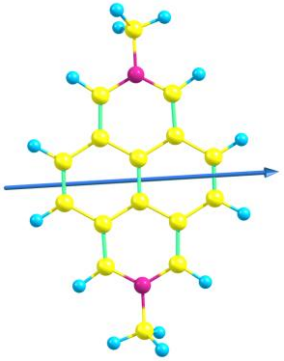
7.			-2.6134 	-1.4975 		1.1159	

Table S2. Dipole moments of 2,7-diazapyrenes in a gas phase

#	Structure	Dipole moment, Debye
1		0.00000 
2		12.21599 

3		11.76324 
4		0.00000 
5		0.00000 

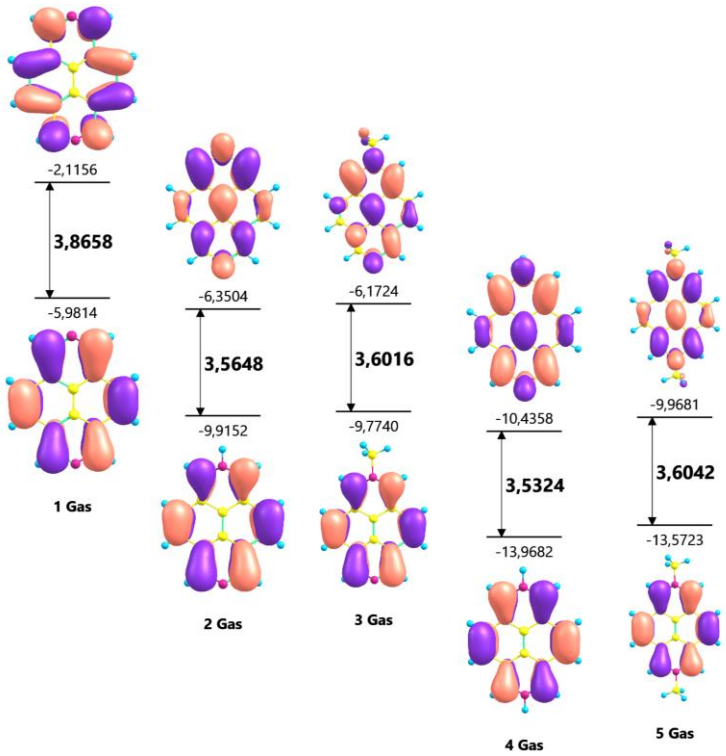
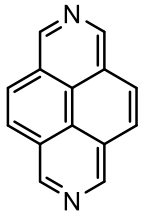
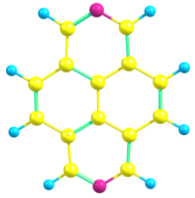
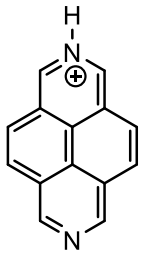
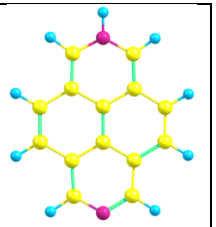
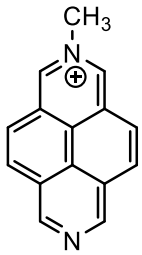
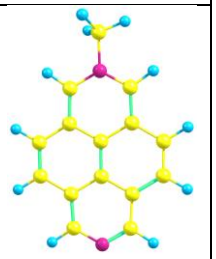
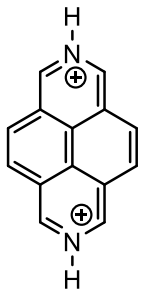
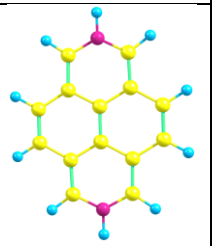
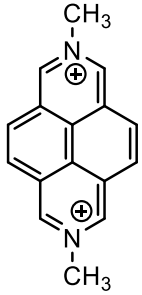
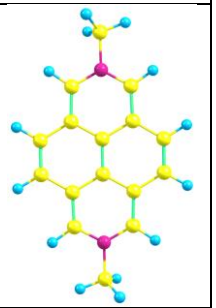
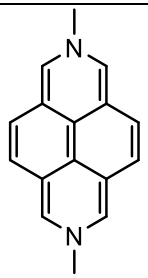
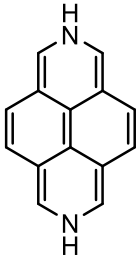
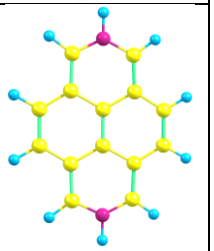
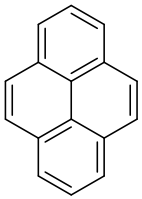
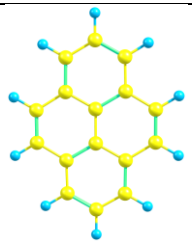


Figure S1. HOMO-LUMO distributions of 2,7-diazapyrenes **1-5**

Table S3. Structure optimization of 2,7-diazapyrenes in a gas phase

#	Structure	Optimization
1		

2		
3		
4		
5		

6		
7		
8		

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