Supporting information

Photoelectron angular distribution of heteroaromatic molecules studied by a continuum multiple scattering Xα method: comparison with benzene

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Table 1: Constant potential($V_{\rm II}$) and Muffin-tin radius in atomic unit.

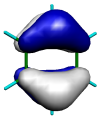
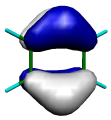
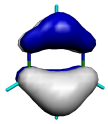
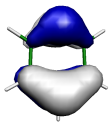
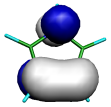
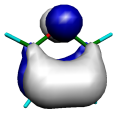
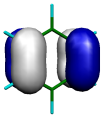
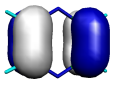
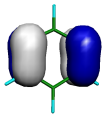
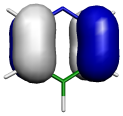
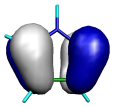
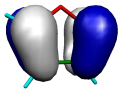
benzene	$V_{\rm II}$	R	C	H					
	-0.38	5.42	1.32	0.73					
pyrazine	$V_{\rm II}$	R	N	C	H				
	-0.42	5.33	1.20	1.32	0.75				
pyridine	$V_{\rm II}$	R	N	o-C	m-C	p-C	o-H	m-H	p-H
	-0.39	5.50	1.26	1.26	1.37	1.26	0.79	0.68	0.78
pyrimidine	$V_{\rm II}$	R	N	C^a_{NN}	C^a_{NC}	C^a_{CC}	H^a_{NN}	H^a_{NC}	H^a_{CC}
	-0.41	5.37	1.25	1.25	1.30	1.34	0.79	0.74	0.72
pyrrole	$V_{\rm II}$	R	N	C_α	C_β	H_N	H_α	H_β	
	-0.42	5.06	1.28	1.31	1.31	0.60	0.73	0.73	
furan	$V_{\rm II}$	R	O	C_α	C_β	H_α	H_β		
	-0.40	5.09	1.29	1.29	1.29	0.75	0.75		

[a]Subscript indicates neighboring atoms.

Table 2: Experimental ionization potentials, truncated to one decimal places.

benzene	9.2($1e_{1g}$)	11.5($3e_{2g}$)	13.9($3e_{1u}$)			
pyrazine	9.3($6a_g$)	10.2($1b_{1g}$)	11.4($5b_{1u}$)	11.8($1b_{2g}$)	13.3($3b_{3g}$)	15.0($4b_{2u}$)
pyridine	9.7($1a_2$)	9.7($11a_1$)	10.5($2b_1$)	12.5($7b_2$)	14.5($6b_2$)	
pyrimidine	9.7($7b_2$)	10.4($2b_1$)	11.3($11a_1$)	11.4($1a_2$)		
pyrrole	8.2($1a_2$)	9.2($2b_1$)				
furan	8.9($1a_2$)	10.4($2b_1$)				

Figure 1: Molecular orbitals. HF/4-31G.

benzene	pyrazine	pyrimidine	pyridine	pyrrole	furan
					
$1e_{1g}(xz)$	$1b_{2g}$	$2b_1$	$2b_1$	$2b_1$	$2b_1$
					
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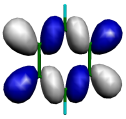	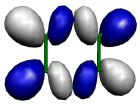	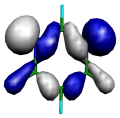	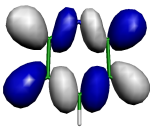		
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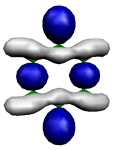	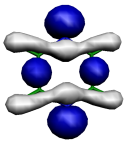	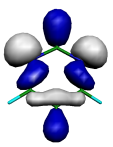	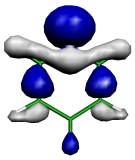		
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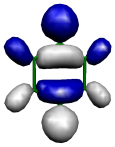	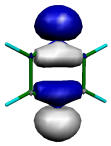	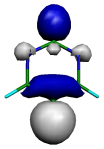	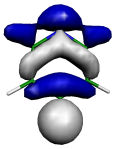		
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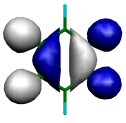	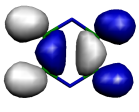	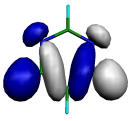	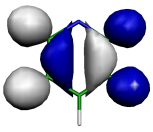		
$3e_{1u}(y)$	$4b_{2u}$	$6b_2$	$6b_2$		