

The 14–electron ring model and the anomalous

Magnetic Circular Dichroism of

meso–Triarylsubporphyrins

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Supporting Information

Table S1: Orbital energies and delocalization of the Hartree-Fock and Kohn-Sham orbitals

	4PysubP			MosubP		
CASCI(HF)	E (eV)	Inner (%)	Outer (%)	E (eV)	Inner (%)	Outer (%)
c3	-7.22	99.3	0.6	-6.70	95.5	4.3
s3	-7.54	84.9	14.9	-6.63	78.3	21.5
c4	0.11	88.3	11.7	0.75	91.4	8.6
s4	0.16	88.6	11.3	0.80	91.5	8.5
CASCI(KS)	E (eV)	Inner (%)	Outer (%)	E (eV)	Inner (%)	Outer (%)
c3	-6.27	98.8	1.2	-5.66	99.4	0.4
s3	-6.11	82.4	17.4	-5.22	66.8	33.0
c4	-2.84	84.2	15.7	-2.13	89.2	10.7
s4	-2.81	84.8	15.1	-2.10	89.4	10.6

Table S2: Configurational composition of the electronic transitions.

CASCI(HF) 4PsubP	$ c3 \rightarrow c4\rangle$	$ s3 \rightarrow c4\rangle$	$ c3 \rightarrow s4\rangle$	$ s3 \rightarrow s4\rangle$
$ ^1S_x\rangle$	0.74298			-0.63834
$ ^1S_y\rangle$		0.65234	0.73069	
$ ^1B_x\rangle$	0.61764			0.72403
$ ^1B_y\rangle$		-0.71262	0.63172	

CASCI(KS) 4PsubP	$ c3 \rightarrow c4\rangle$	$ s3 \rightarrow c4\rangle$	$ c3 \rightarrow s4\rangle$	$ s3 \rightarrow s4\rangle$
$ ^1S_x\rangle$	0.71276			-0.64527
$ ^1S_y\rangle$		0.65728	0.70204	
$ ^1B_x\rangle$	0.63705			0.70283
$ ^1B_y\rangle$		-0.69227	0.64796	

CASCI(HF) MOsubP	$ c3 \rightarrow c4\rangle$	$ s3 \rightarrow c4\rangle$	$ c3 \rightarrow s4\rangle$	$ s3 \rightarrow s4\rangle$
$ ^1S_x\rangle$	0.68782			-0.69757
$ ^1S_y\rangle$		0.70957	0.67621	
$ ^1B_x\rangle + (^1B_y\rangle)$	0.57943	-0.34361	0.36162	0.57175
$ ^1B_y\rangle - (^1B_x\rangle)$	-0.35676	-0.56166	0.58998	-0.34901

CASCI(KS) MOsubP	$ c3 \rightarrow c4\rangle$	$ s3 \rightarrow c4\rangle$	$ c3 \rightarrow s4\rangle$	$ s3 \rightarrow s4\rangle$
$ ^1S_x\rangle + (^1S_y\rangle)$	0.59381	0.33805	0.33633	-0.60525
$ ^1S_y\rangle - (^1S_x\rangle)$	-0.34015	0.61552	0.58475	0.33473
$ ^1B_x\rangle$	0.67525			0.66503
$ ^1B_y\rangle$		-0.65562	0.68462	