A Theoretical Survey of the UV-Visible of Axially and Peripherally Substituted Boron Subphtalocyanines.

Al Mokhtar Lamsabhi, M. Merced Montero-Campillo, Otilia Mó and Manuel Yáñez *

Departamento de Química, Módulo 13, Facultad de Ciencias and Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Supporting Information

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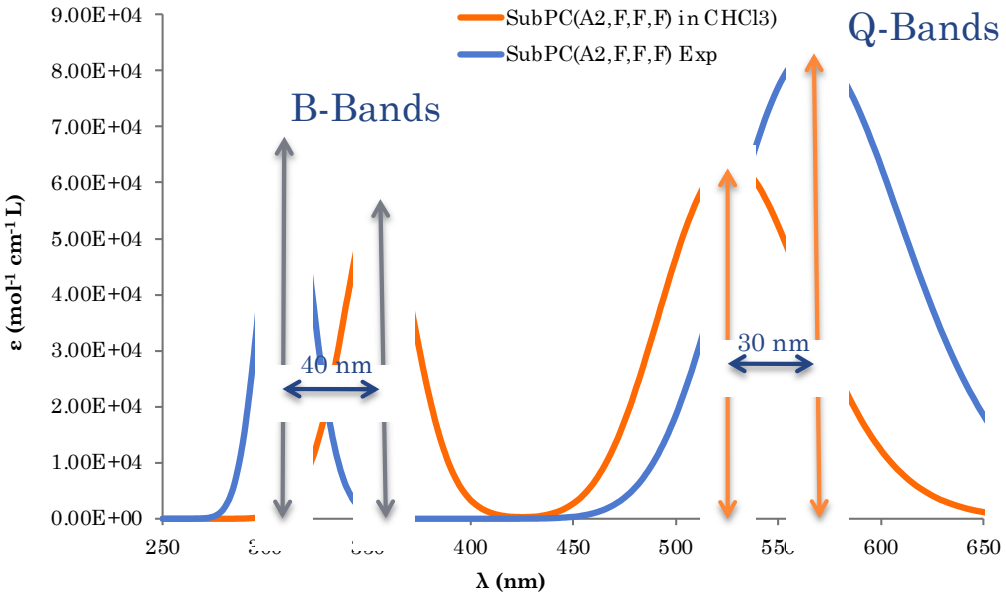


Figure S1. Comparison between the calculated (red curve) and the experimental (blue curve) UV-visible spectra for SubPc (A2,F,F,F) dissolved in $CHCl_3$.

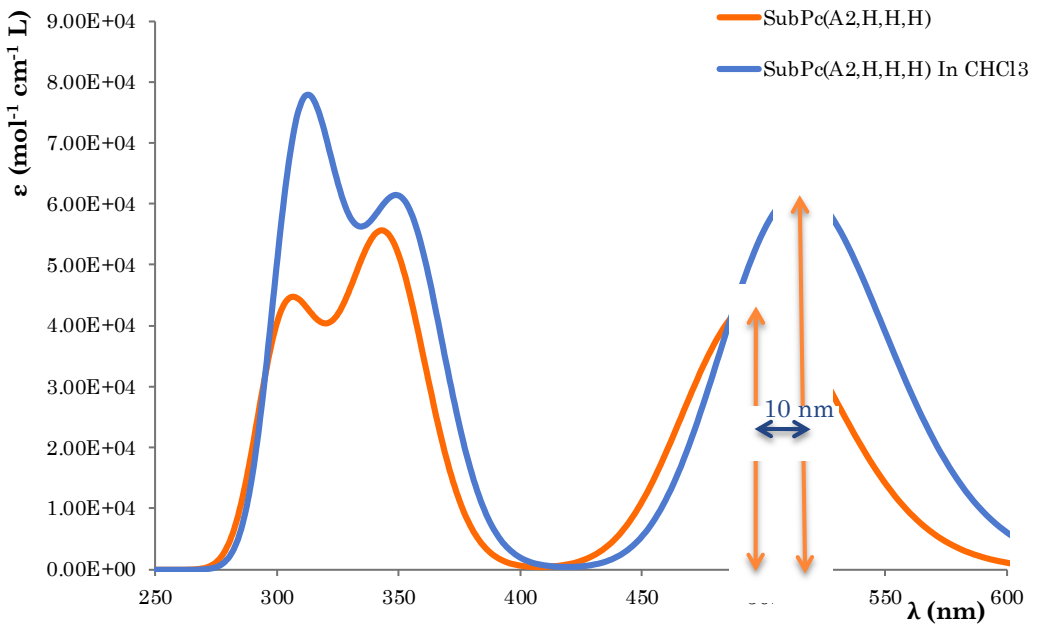


Figure S2. Comparison between the UV-visible spectrum of SubPc(A2,H,H,H) in the gas phase (red curve) and in $CHCl_3$ solution (blue curve).

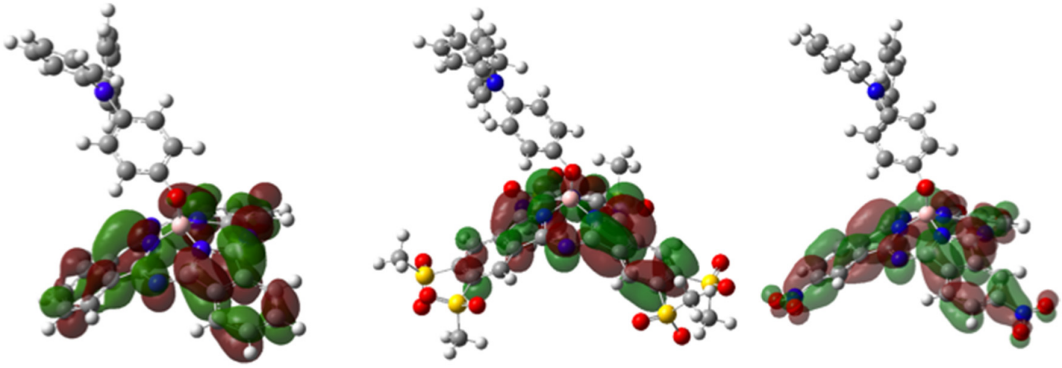
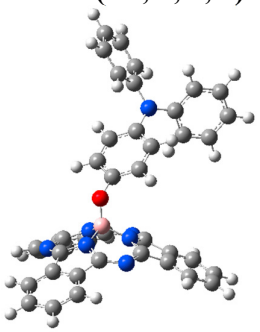


Figure S3: Lowest Unoccupied Molecular Orbital of SubPc(A1,H,H,H), SubPc(A1,SO_2CH_3,SO_2CH_3H,H) and SubPc(A1,NO_2,H,H).

Table S1. B3LYP/6-31G(d) optimized geometries (cartesian coordinates in Å) for the different SubPcs included in this study.

SubPc(A1,H,H,H)



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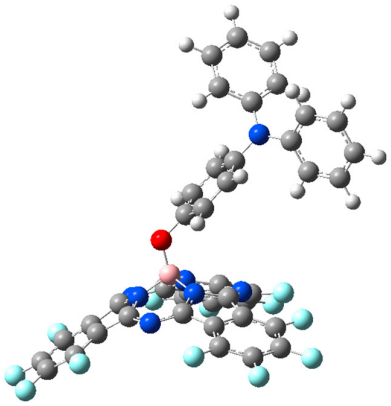

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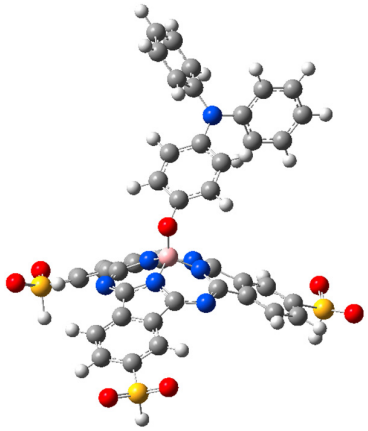

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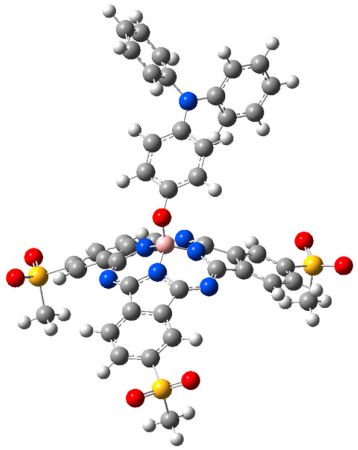
SubPc(A1,SO_2CH_3,H,H)



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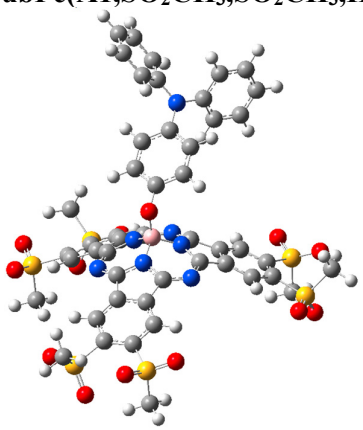

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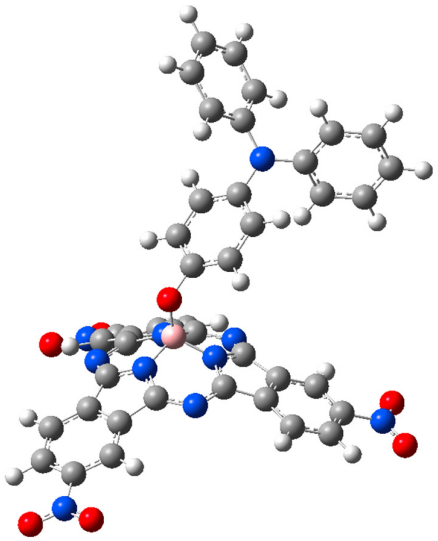

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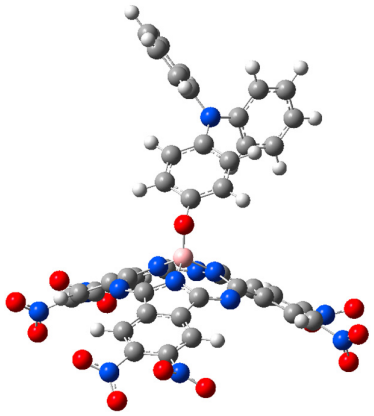

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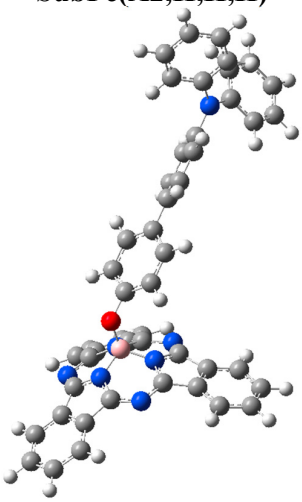

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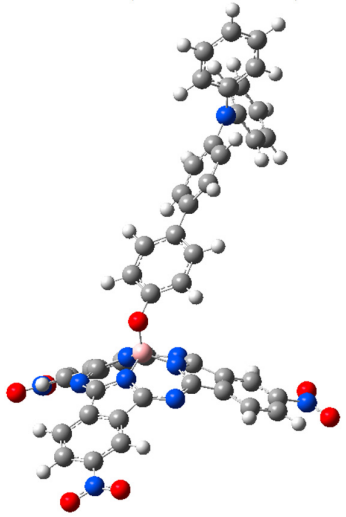

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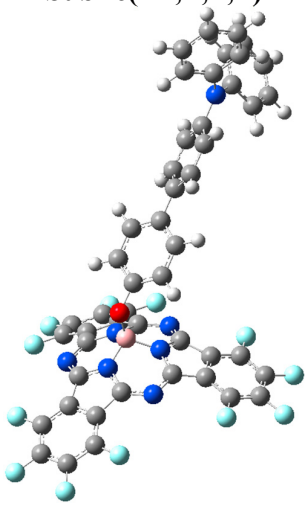

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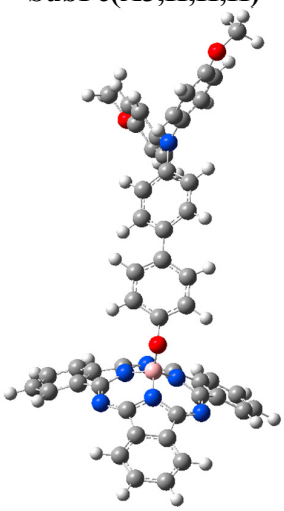

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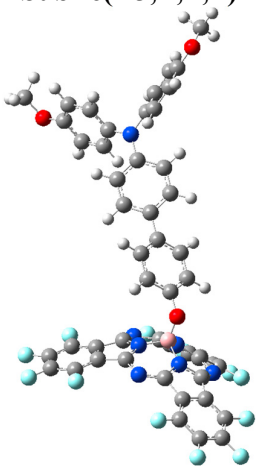

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Table S2. Q-Band (λ_{max}) excitation energies in vacuum, oscillator strengths *f* and dominant electronic transitions, for the SubPcs included in this study

An	R_1	R_2	R_3	λmax (eV)	nm	f	Main Configuration
A1	H	H	H	2.49	498.9	0.2856	H-1->L+0(+85%)
				2.50	496.70	0.3125	H-1->L+1(+85%)
A1	F	F	F	2.42	512.9	0.2997	H-1->L+0(+85%)
				2.43	510.4	0.3276	H-1->L+1(+85%)
A1	SO_2H	H	H	2.46	504.4	0.3401	H-1->L+0(+96%)
				2.47	502.0	0.3726	H-1->L+1(+95%)
A1	SO_2CH_3	SO_2CH_3	H	2.42	511.8	0.4257	H-1->L+0(+96%)
				2.43	509.2	0.4623	H-1->L+1(+95%)
A1	SO_2CH_3	H	H	2.46	504.0	0.3456	H-1->L+0(+96%)
				2.47	501.5	0.3774	H-1->L+1(+96%)
A1	NO_2	H	H	2.31	536.6	0.3316	H-1->L+0(+96%)
				2.32	534.1	0.3567	H-1->L+1(+96%)
A1	NO_2	NO_2	H	2.31	536.9	0.3058	H-1->L+0(+82%)
				2.33	532.4	0.3875	H-1->L+1(+91%)
A2	H	H	H	2.49	498.6	0.2886	H-1->L+0(+96%)
				2.5	496.8	0.3186	H-1->L+1(+95%)
A2	NO_2	H	H	2.31	535.8	0.3331	H-1->L+0(+95%)
				2.32	534.0	0.3598	H-1->L+1(+95%)
A2	F	F	F	2.42	511.9	0.293	H-1->L+0(+92%)
				2.43	509.5	0.3247	H-1->L+1(+92%)
A3	H	H	H	2.49	498.4	0.2872	H-1->L+0(+95%)
				2.5	496.8	0.3199	H-1->L+1(+95%)
A3	F	F	F	2.42	512.1	0.3025	H-2->L+0(+95%)
				2.43	509.9	0.3378	H-2->L+1(+95%)