10.1071/CH18449_AC

Australian Journal of Chemistry 2019, 72(4), 244-251

Supplementary Material

Theoretical study of phenothiazine organic dyes with different spacers for dye sensitized solar cells

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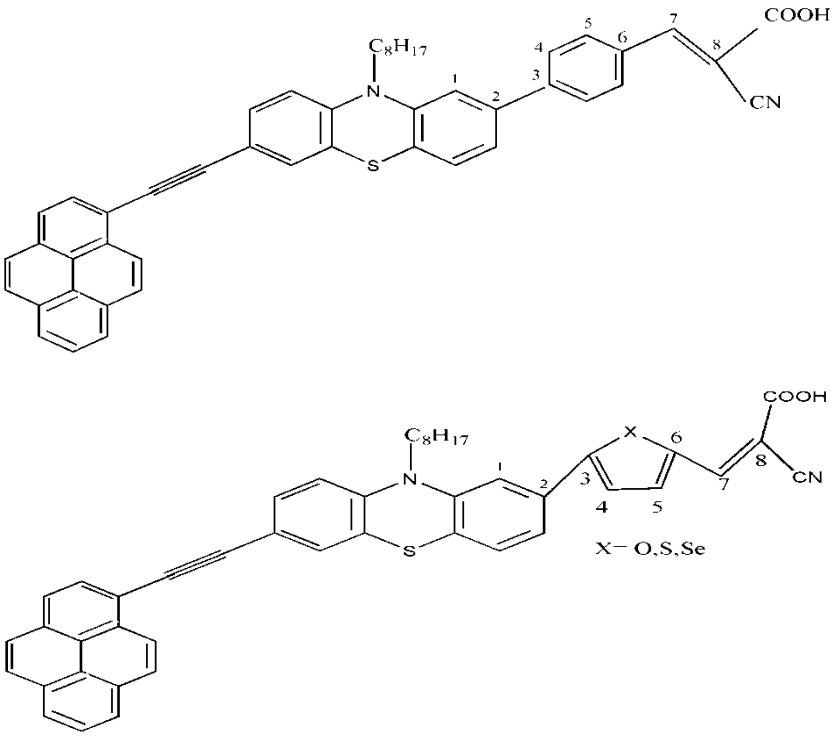

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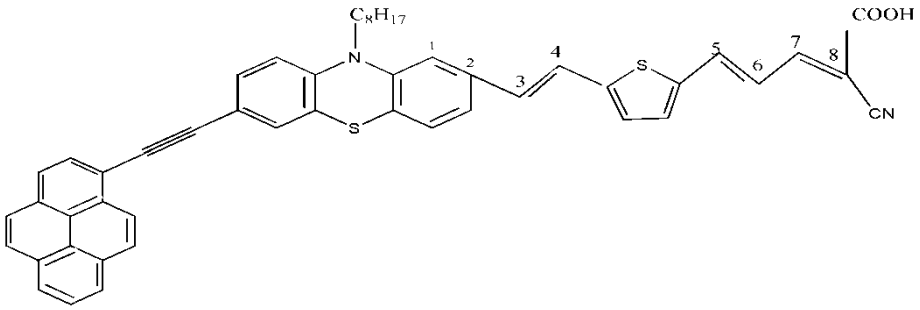

	dye2	dye3	dye4	dye5	dye6	dye7
Bond lengths						
C2-C3	1.46	1.45	1.48	1.46	1.46	1.46
C6-C7	1.42	1.42	1.45	1.43	1.42	1.42
Dihedral angles [a]						
θ1	35.88	-0.12	33.47	21.42	21.05	-1.54
θ2	153.87	179.92	-0.06	179.13	179.22	-179.96

a: θ1: C1-C2-C3-C4 θ2: C5-C6-C7-C8

Table S1: Selected bond lengths and dihedral angles of the optimized sensitizers calculated using B3LYP functional with 6-311G(d,p) basis set in gas phase .

	dye2	dye3	dye4	dye5	dye6	dye7
Bond lengths						
C2-C3	1.46	1.45	1.48	1.46	1.46	1.46
C6-C7	1.42	1.41	1.45	1.42	1.42	1.42
Dihedral angles [a]						
θ1	34.14	-0.61	31.39	19.36	16.06	-2.28
θ2	156.11	-179.93	-179.02	179.56	179.50	-179.89

a: θ1: C1-C2-C3-C4 θ2: C5-C6-C7-C8

Table S2: Selected bond lengths and dihedral angles of the optimized sensitizers calculated using B3LYP functional with 6-311G(d,p) basis set in acetonitrile solvent .