

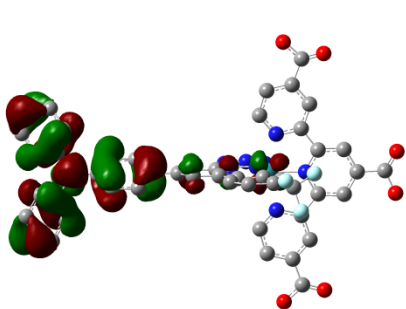
Highly Robust Tetrazolate Based Complexes for Efficient and Long-term Stable Dye Sensitized Solar Cells

Tharallah A. Shoker, Ralph Tanios, Remi Fayyad and Tarek H. Ghaddar*

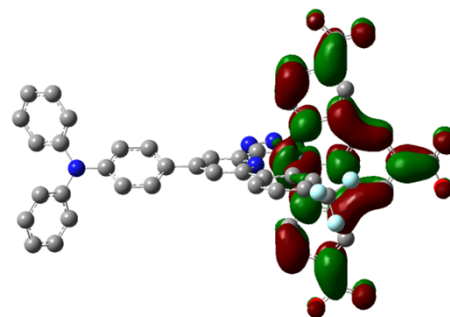
Department of Chemistry, American University of Beirut, Beirut 11-0236, Lebanon

Supporting Information:

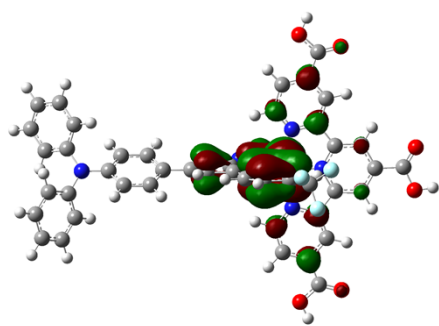
T120



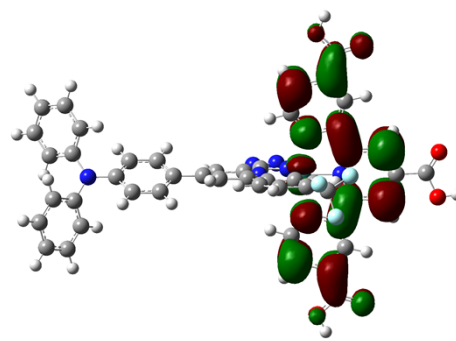
HOMO



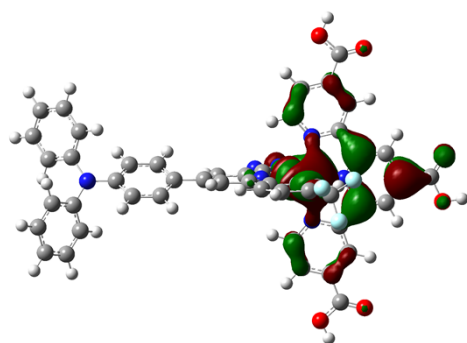
LUMO



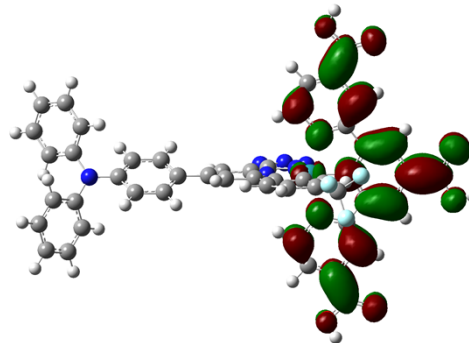
HOMO-1



LUMO+1

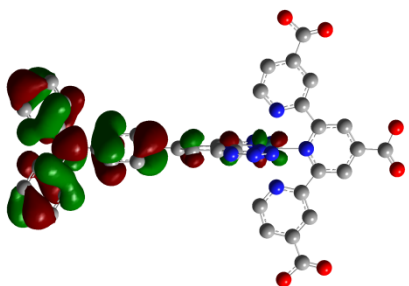


HOMO-2

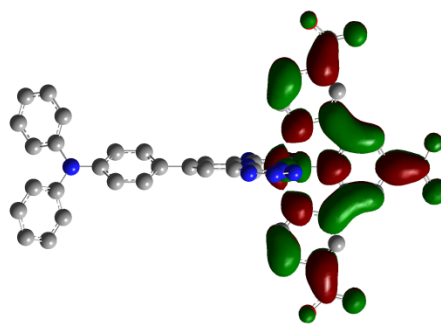


LUMO+2

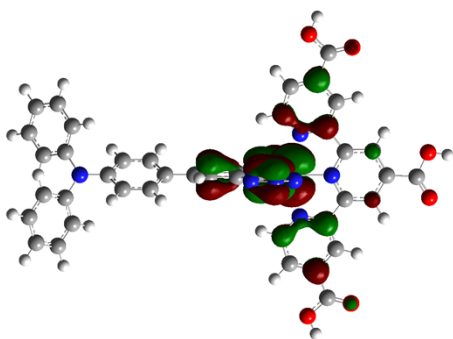
T147



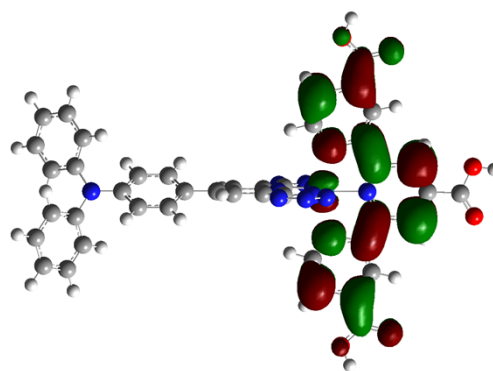
HOMO



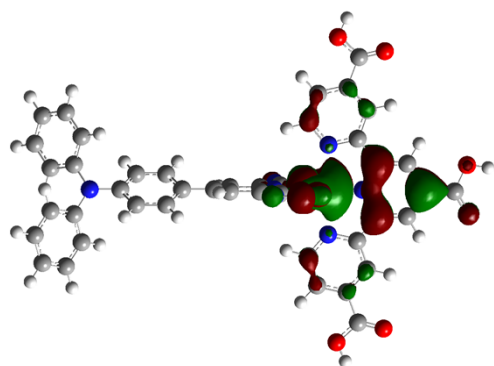
LUMO



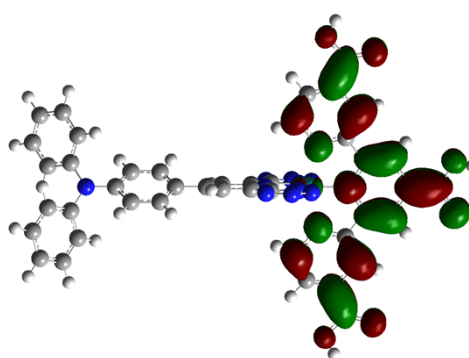
HOMO-1



LUMO+1

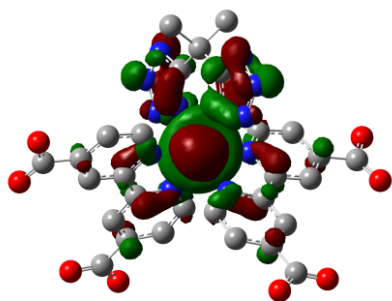


HOMO-2

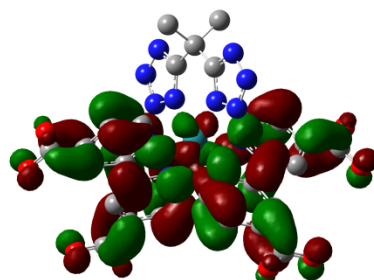


LUMO+2

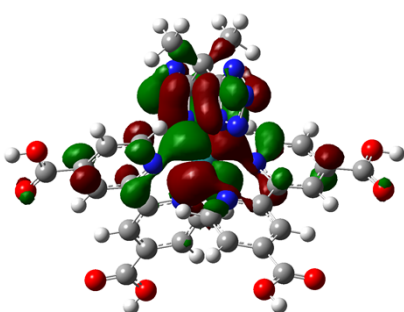
T162



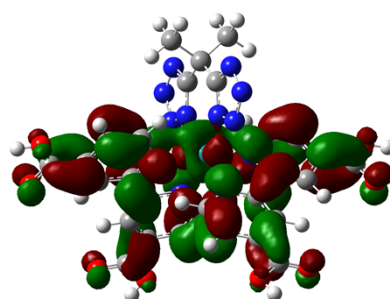
HOMO



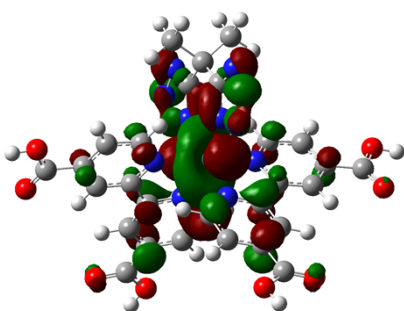
LUMO



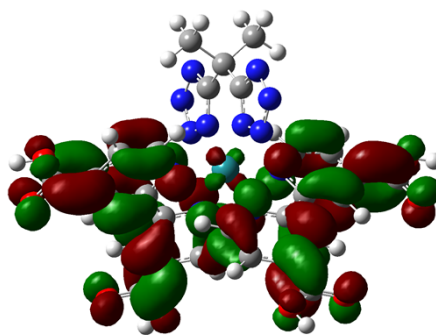
HOMO-1



LUMO+1



HOMO-2



LUMO+2

Scheme S1: The isodensity plots shown are for the HOMO and LUMO of T120, T147 and T162.

Table S1: Calculated spectra of T120, T147 and T162 above 460 nm

Dye	nm	Oscillator Strength	(Assignment; H=HOMO and L=LUMO)
T120	696.9	0.028	H-1->L+0(+94%)
	585.8	0.0273	H-2->L+0(+53%) H-1->L+1(45%)
			H-2->L+1(6%)
	530.7	0.0877	H-2->L+1(+84%)
	494.5	0.1895	H-1->L+1(+43%) H-2->L+0(+32%)
			H-1->L+3(+10%) H-2->L+2(+10%)
	454.6	0.2001	H-1->L+2(+88%)
	443.6	0.0391	H-1->L+4(+91%)
	434	0.7877	H-2->L+2(+50%) H-0->L+4(+39%)
	430.8	0.1304	H-1->L+3(+46%) H-0->L+4(+29%)
			H-2->L+2(19%)
	426.4	0.0112	H-2->L+3(+82%) H-2->L+4(+16%)
	422.7	0.0114	H-0->L+3(+79%) H-3->L+3(+13%)
	T147	626.5	0.0354
525		0.0353	H-2->L+0(+54%) H-1->L+1(44%)
466.9		0.0632	H-2->L+1(+95%)
461.4		0.6183	H-1->L+1(+39%) H-2->L+0(+26%)
			H-0->L+4(+25%)
435.1		0.4077	H-0->L+4(+70%) H-1->L+3(9%)
			H-2->L+0(9%) H-1->L+1(8%)
415.5		0.1717	H-1->L+2(+93%)
T162	569.6	0.0201	H-1->L+1(+83%) H-2->L+0(14%)
	507	0.2109	H-2->L+0(+82%) H-1->L+1(+14%)
	474.7	0.0179	H-2->L+1(+62%) H-0->L+3(23%)
			H-1->L+0(+9%)
	430.9	0.0396	H-0->L+2(+67%) H-1->L+3(+29%)
	427	0.0119	H-1->L+2(+68%) H-0->L+3(+26%)
421.7	0.2004	H-1->L+3(+65%) H-0->L+2(29%)	

^a Only bands with oscillator strength > 0.01 are listed

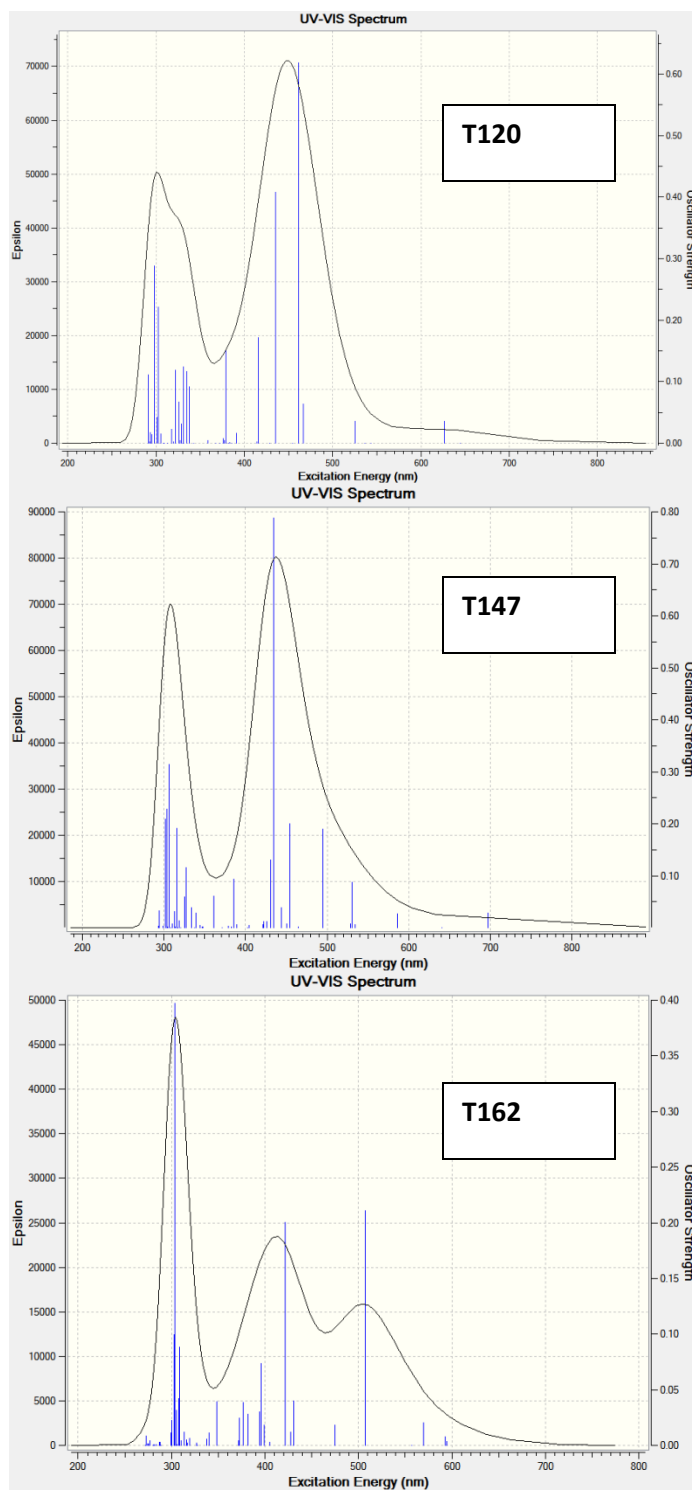


Figure S1: The computed absorption spectra of T120, T147 and T162 as measured in water.

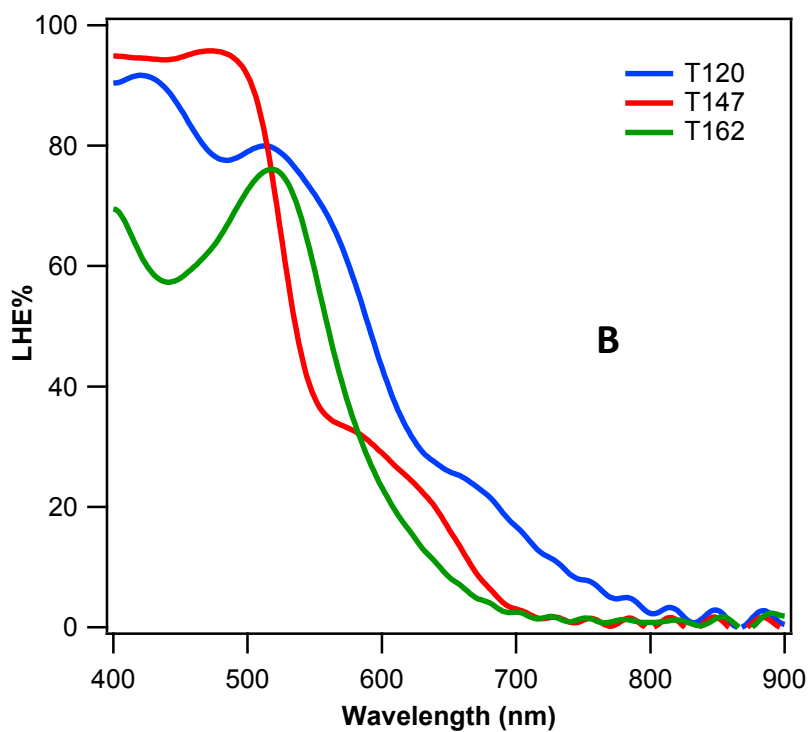
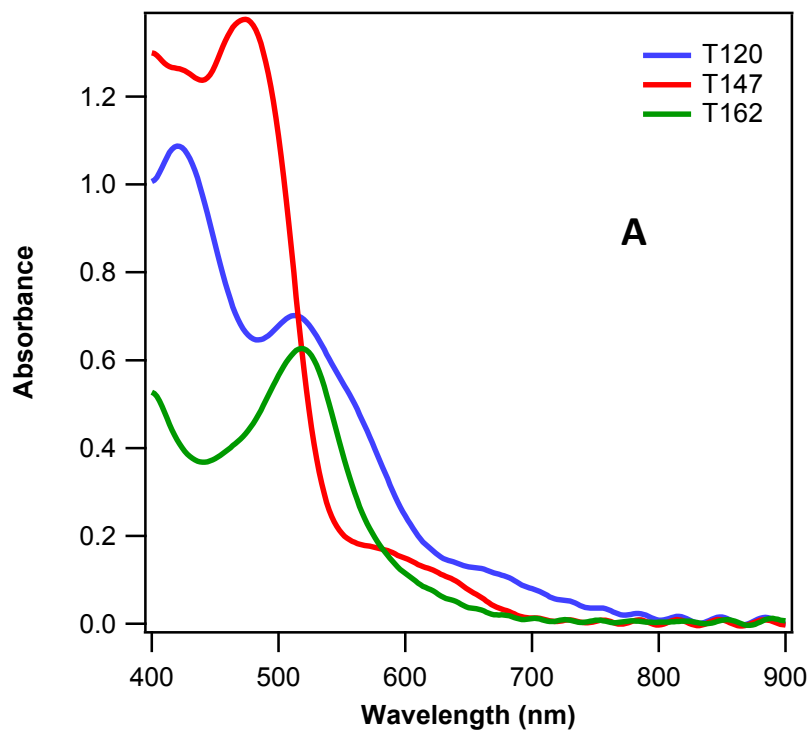


Figure S2: **A)** Absorption spectra of 6 μm TiO₂ films of T120, T147 and T162. **B)** The calculated light harvesting efficiencies (LHE%) of 6 μm TiO₂ films of T120, T147 and T162.

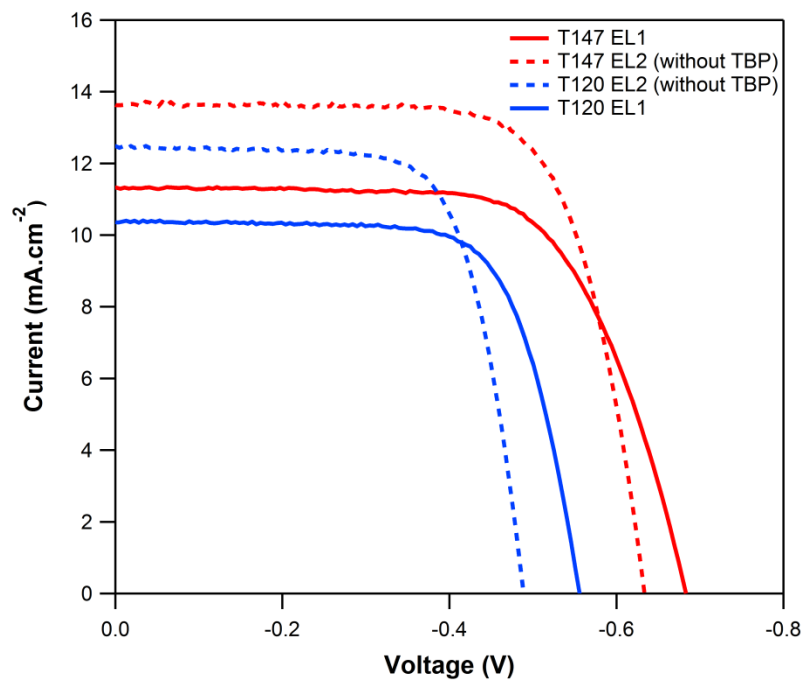


Figure S3: Photocurrent–voltage characteristics of DSSCs sensitized with dyes: T147 (red) and T120 (blue), assembled with electrolyte EL1 (solid) and EL2 (dashed).