Science Letters ISSN 2345-5463 DOI: https://doi.org/10.47262/SL/9.2.132021008

Supplementary Material

Tuning the Electronic and Nonlinear Optical Properties of (4-Methylphenyl) (4-methylpiperidin-1-yl) Methanone and Its Substituted Analogues

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Table S1 Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of MPMPM with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
			B3LYP					***BLYP***	
210.14	0.12	5.90	H-3-L+1 H-2-L H-1-L+1	39 21 17	234.88	0.22	5.28	H-2-L H+1-L	57 15
214.85	0.14	5.77	H-3-L H-2-L+1 H-1-L+1	30 20 17	252.52	0.00	4.91	H-3-L H-2-L+1	57 38
227.52	0.00	5.44	H-L+1 H-1-L+1	64 22	271.05	0.00	4.58	H-1-L+1	88
237.42	0.10	5.22	H-1-L H-L	60 19	285.48	0.06	4.34	H-1-L	83
240.74	0.02	5.15	H-2-L H-L+1 H-1-L+1	30 24 20	294.50	0.00	4.21	H-L+1	96
266.39	0.13	4.65	H-3-L H-L H-3-L	11 58 18	312.84	0.01	3.96	H-L	86

Exp: λ_{abs} = 296 nm; band gap = 4.19 eV [22]

Table S2 Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of 4-CHO derivative with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
			B3LYP					***BLYP***	
231.14	0.34	5.36	H-4-L H-L+1	41 32	291.78	0.01	4.25	H-3-L H-2-L+1 H-L+1 H-4-L	44 16 14 13
235.27	0.15	5.27	H-L+1 H-4-L	63 24	301.90	0.00	4.11	H-L+1	81
263.14	0.02	4.71	H-3-L	74	392.89	0.03	3.16	H-2-L	91
294.12	0.06	4.22	H-1-L	75	401.78	0.01	3.09	H-1-L	96
311.39	0.01	3.98	H-L	83	427.62	0.01	2.89	H-L	94

Table S3: Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of 4-CH=C(CN)COOH derivative with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
			B3LYP					***BLYP***	
240.45	0.02	5.15	H-L+1	48	302.82	0.09	4.09	H-L+1	81
			H-L+2	11					
283.71	0.97	4.37	H-2-L	56	309.79	0.93	4.00	H-2-L	71
			H-1-L	28					
295.48	0.02	4.19	H-3-L	86	340.61	0.01	3.64	H-4-L	89
341.02	0.15	3.64	H-1-L	64	487.27	0.06	2.54	H-1-L	82
			H-2-L	33					
364.22	0.01	3.40	H-L	91	534.73	0.02	2.32	H-L	88

Table S4 Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of 4-CN derivative with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
			B3LYP					***BLYP***	
220.74	0.26	5.62	H-1-L+1	33	243.86	0.34	5.08	H-2-L	56
			H-2-L	32				H-L+2	14
			H-3-L+1	13				H-1-L+2	13
			H-2-L+1	13					
224.55	0.27	5.52	H-2-L	30	264.29	0.01	4.69	H-3-L	58
			H-1-L+1	22				H-2+L+1	38
			H-2-L+1	18					
			H-3-L	14					
238.81	0.00	5.19	H-L+1	81	309.65	0.00	4.00	H-L+1	97
249.62	0.01	4.97	H-3-L	44	350.59	0.04	3.54	H-1-L	94
			H-1-L+1	23					
			H-L+1	17					
277.11	0.06	4.47	H-1-L	62	374.91	0.01	3.31	H-L	93
			H-L	28					
294.21	0.02	4.21	H-L	66					
			H-1-L	17					

Table S5 Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of 4-NO_2 derivative with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
			B3LYP					***BLYP***	
251.21	0.34	4.94	H-3-L	74	308.66	0.00	4.02	H-L+1	90
277.55	0.02	4.47	H-2-L	85	325.75	0.01	3.81	H-3-L	83
319.17	0.06	3.88	H-1-L	90	461.90	0.03	2.68	H-1-L	94
340.03	0.01	3.65	H-L	92	508.90	0.01	2.44	H-L	94

Table S6 Absorption wavelengths (λ_{abs}), excitation energies (E_{ex}) and the electronic transitions and their corresponding orbital contributions of 4-NC derivative with the TD-DFT calculations.

λ_{abs}	*f*	E_{ex}	Transitions	Contribution %	λ_{abs}	*f*	E_{ex}	Transitions	Contribution %
B3LYP					***BLYP***				
220.25	0.25	5.63	H-2-L	27	248.90	0.01	4.98	H-4-L	95
			H-1-L+1	26					
			H-2-L+1	24					
			H-3-L+1	11					
224.28	0.31	5.52	H-2-L	33	263.22	0.00	4.71	H-3-L	57
			H-2-L+1	21				H-2-L+1	40
			H-1-L+1	15					
			H-1-L	14					
238.72	0.00	5.19	H-L+1	72	311.00	0.00	3.99	H-L+1	96
			H-1-L+1	15					
248.75	0.00	4.98	H-3-L	42	337.13	0.05	3.68	H-1-L	92
			H-L+1	25					
			H-1-L+1	25					
267.13	0.08	4.64	H-1-L	60	363.41	0.01	3.41	H-L	92
			H-L	27					
286.36	0.02	4.33	H-L	64					
			H-2-L	16					
			H-1-L	13					