

Figure 1: HOMO and LUMO of PT\* form, N,N'-dimethylamino derivative

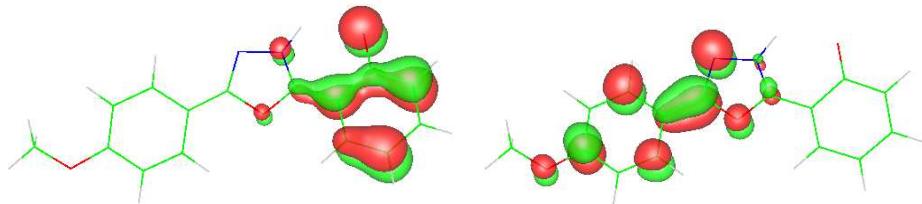


Figure 2: HOMO and LUMO of PT\* form, methoxy derivative

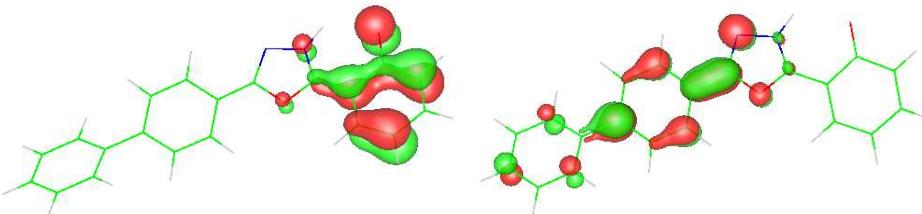


Figure 3: HOMO and LUMO of PT\* form, phenyl derivative

Table 1: Calculated spectra of the normal form, R = (CH<sub>3</sub>)<sub>2</sub>N

Exc. energy(cm <sup>-1</sup> )	Osc. str. $\times 10^{-2}$	Main transitions(%) <sup>a</sup>
28760	73.3	74—75 (98.0)
36014	17.0	74—76 (47.9)
		74—77 (31.7)
39609	10.8	72—75 (48.7)
		73—76 (44.6)
34631	6.53	74—77 (53.5)
		74—76 (30.1)
33276	5.84	73—75 (84.6)
41034	3.36	74—78 (71.8)
		73—76 (11.3)
39052	3.05	73—76 (38.8)
		72—75 (24.0)
		74—78 (19.5)
42030	2.33	71—75 (79.0)
43501	2.19	74—79 (96.1)
42457	1.22	73—77 (82.2)

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<sup>a</sup>74 is HOMO, 75 is LUMO

Table 2: Calculated spectra of the normal form, R = CH<sub>3</sub>O

Exc. energy (cm <sup>-1</sup> )	Osc. str. × 10 <sup>-2</sup>	Main transitions(%) <sup>a</sup>
30788	68.2	70—71 (96.4)
34347	13.1	69—71 (91.4)
44181	7.50	70—74 (29.4) 69—73 (29.1) 68—72 (17.7) 67—71 (12.7)
39885	6.99	69—72 (56.2) 68—71 (37.3)
46039	5.92	68—72 (61.8) 69—74 (15.9) 70—74 (10.9)
41163	3.04	68—71 (36.4) 69—72 (18.5) 70—72 (14.1) 70—74 (13.2)
36471	2.35	70—72 (68.2) 70—73 (11.9)
47463	1.87	68—73 (55.5) 67—72 (19.8) 69—74 (15.9)
43784	1.68	67—71 (34.3) 70—74 (30.5) 69—73 (14.8)
41783	1.30	69—73 (37.0) 67—71 (26.1) 70—73 (24.6)

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<sup>a</sup>70 is HOMO, 71 is LUMO

Table 3: Calculated spectra of the normal form, R = Ph

Exc. energy (cm <sup>-1</sup> )	Osc. str. $\times 10^{-2}$	Main transitions(%) <sup>a</sup>
29464	82.2	82—83 (97.7)
32945	28.0	81—83 (95.5)
42868	11.3	80—84 (35.7) 77—83 (32.0)
38805	7.84	81—84 (74.0)
45349	4.37	82—88 (41.3) 80—84 (21.2)
37477	2.67	80—83 (69.9)
41537	2.18	82—86 (47.6) 82—85 (11.8)
43408	1.95	81—85 (55.2)
42551	1.52	82—87 (30.6) 80—84 (20.2) 77—83 (20.2) 82—88 (15.8)
45691	1.32	79—84 (35.7) 81—86 (26.5) 78—84 (16.7)

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<sup>a</sup>82 is HOMO, 83 is LUMO

Table 4: Calculated spectra of the phototautomeric form, R = (CH<sub>3</sub>)<sub>2</sub>N

Exc. energy(cm <sup>-1</sup> )	Osc. str. $\times 10^{-2}$	Main transitions(%) <sup>a</sup>
24619	37.3	74—75 (98.3)
34758	26.3	73—76 (74.8)
30794	21.4	73—75 (80.8)
28727	18.8	74—76 (84.3) 73—75 (12.6)
36271	5.27	73—77 (73.9)
42701	5.10	70—75 (87.0)
37534	5.03	71—75 (80.2)
43781	4.88	74—79 (75.7)
41118	4.54	71—76 (88.2)
45469	1.63	73—78 (78.8) 74—78 (11.0)

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<sup>a</sup>74 is HOMO, 75 is LUMO

Table 5: Calculated spectra of the phototautomeric form, R = CH<sub>3</sub>O

Exc. energy (cm <sup>-1</sup> )	Osc. str. $\times 10^{-2}$	Main transitions(%) <sup>a</sup>
33239	40.3	68—71 (89.7)
24019	23.0	70—71 (98.1)
28504	14.9	70—72 (95.3)
41875	10.8	67—72 (88.6)
44079	9.69	70—74 (52.1) 66—71 (13.8)
39630	7.34	67—71 (31.9) 68—72 (29.9) 68—73 (12.6)
32060	3.92	70—73 (93.5)
38565	1.42	67—71 (39.8) 68—73 (35.6) 66—71 (16.6)
37315	1.10	68—72 (62.2) 67—71 (20.5)
43634	1.08	66—71 (35.5) 70—74 (24.5) 68—73 (23.5) 67—73 (11.6)

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<sup>a</sup>70 is HOMO, 71 is LUMO

Table 6: Calculated spectra of the phototautomeric form, R = Ph

Exc. energy (cm <sup>-1</sup> )	Osc. str. $\times 10^{-2}$	Main transitions(%) <sup>a</sup>
31541	57.3	80—83 (90.3)
28052	27.9	82—84 (94.2)
22141	20.7	82—83 (99.2)
40751	11.7	79—84 (90.0)
42573	9.44	76—83 (77.1) 80—87 (13.2)
42956	4.25	80—85 (31.0) 80—86 (20.4) 77—83 (19.8)
35367	4.11	79—83 (93.0)
36992	3.79	80—84 (41.9) 77—83 (27.6) 80—85 (13.7)
32634	1.82	82—85 (92.8)
37875	1.54	80—84 (46.6) 77—83 (29.1) 80—85 (14.1)

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<sup>a</sup>82 is HOMO, 83 is LUMO