state	transition	Δ **E** [eV]	$t_1/\|\|t\|\|$ (%)	**f**
S_1	$\pi \rightarrow \pi^* +$ Ryd	4.984	-.447 (20.0) 0.400 (16.0) 0.361 (13.0) 0.317 (10.0)	0.13151
S_2	$\pi \rightarrow$ Ryd	5.079	0.695 (48.4)	0.02776
S_3	n $\rightarrow$ Ryd + π^*	5.379	-.3678 (13.5) -.336 (11.3)	0.00281
S_4	$\pi \rightarrow$ Ryd	5.429	0.646 (41.7)	0.14133
S_5	$\pi \rightarrow$ Ryd + π^*	5.466	0.595 (35.3) -.335 (11.2)	0.17925
S_6	$\pi \rightarrow$ Ryd	5.993	0.755 (57.0)	0.00335
S_7	n $\rightarrow$ Ryd	6.073	0.444 (19.8) 0.331 (11.0)	0.00587
S_8	n $\rightarrow$ Ryd	6.130	0.361 (13.0)	0.00770

state	transition	Δ **E** [eV]	$t_1/\|\|t\|\|$ (%)
T_1	$\pi \rightarrow \pi^* +$ Ryd	4.289	0.520 (27.0) -.411 (16.9) -.402 (16.2) 0.333 (11.1)
T_2	$\pi \rightarrow \pi^*$ $\pi \rightarrow$ Ryd	4.405	0.470 (22.1) 0.376 (14.1)
T_3	$\pi \rightarrow$ Ryd + π^*	5.030	0.789 (62.2)
T_4	n $\rightarrow$ Ryd + π^*	5.161	-.377 (14.2) -.326 (10.6)
T_5	$\pi \rightarrow$ Ryd $\pi \rightarrow \pi^*$	5.397	-.518 (26.8) 0.351 (12.3) -.332 (11.0)
T_6	$\pi \rightarrow$ Ryd	5.447	0.684 (46.7)
T_7	mix	5.896	-
T_8	$\pi \rightarrow$ Ryd	5.970	0.703 (49.4)