

Exploring the sloped-to-peaked S_2/S_1 seam of intersection of thymine with static and quantum dynamical DD-vMCG calculations

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SUPPORTING INFORMATION

Run 1b

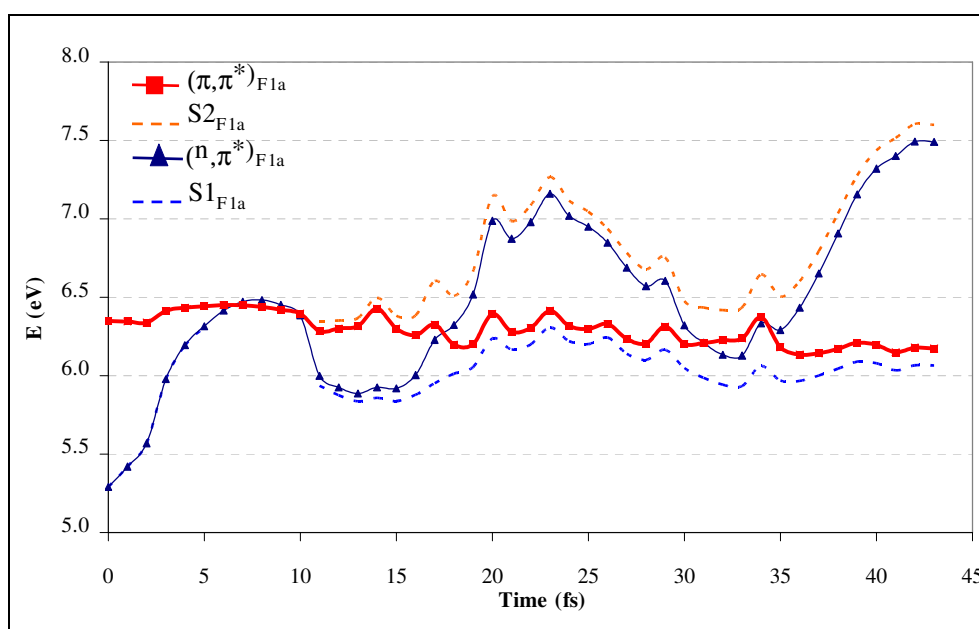


Figure SI-1a. Diabatic and adiabatic energies of the F1a function of run 1b.

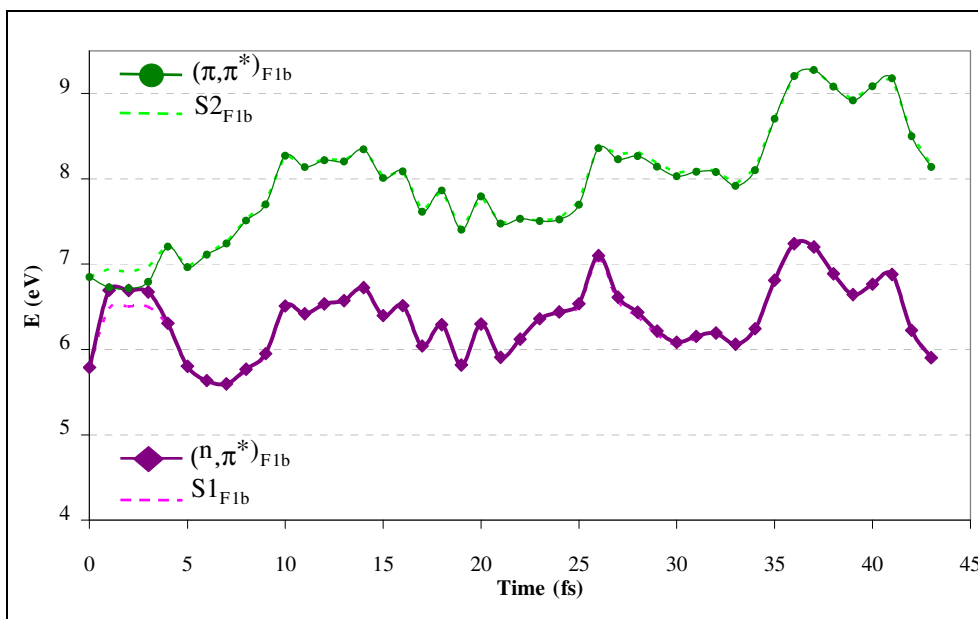


Figure SI-1b. Diabatic and adiabatic energies of the F1b function of run 1b.

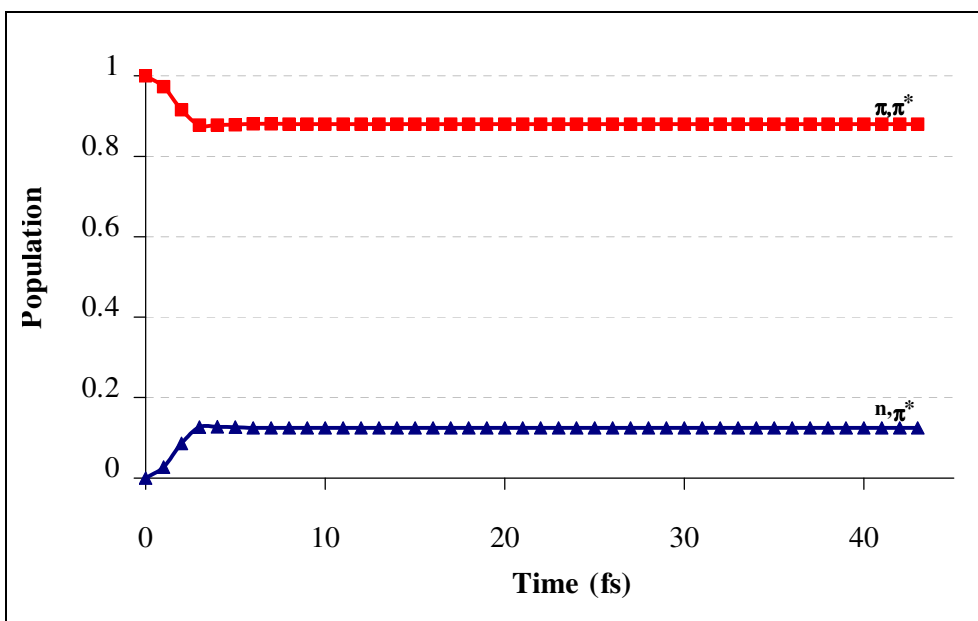


Figure SI-2. Quasi-diabatic populations of the (π, π^*) and (n, π^*) states of run 1b.

Run 1c

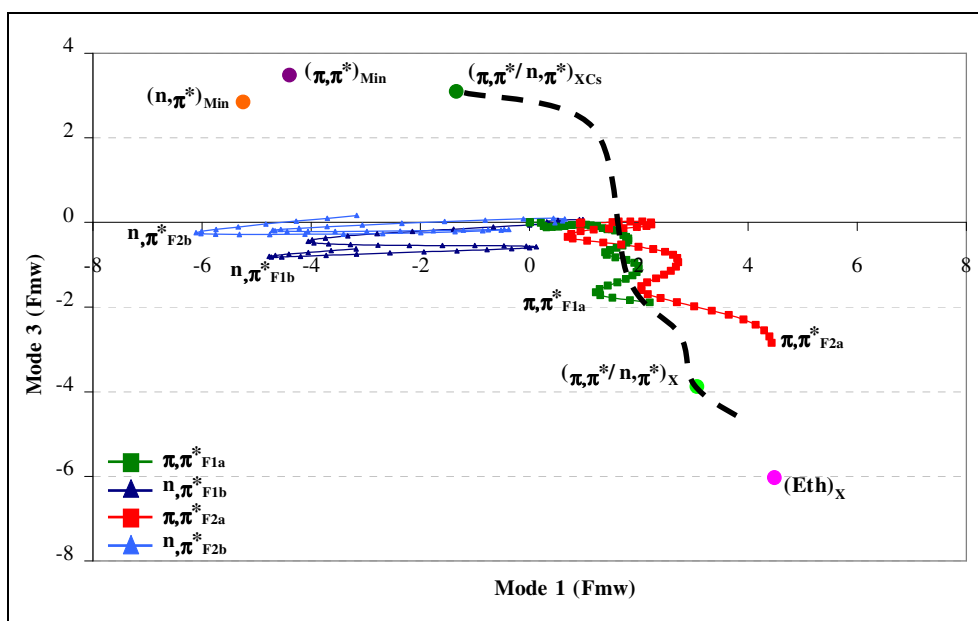


Figure SI-3. Position of the center of the Gaussian functions of run 1c (position relative to $(\pi, \pi^*)_{TS}$).

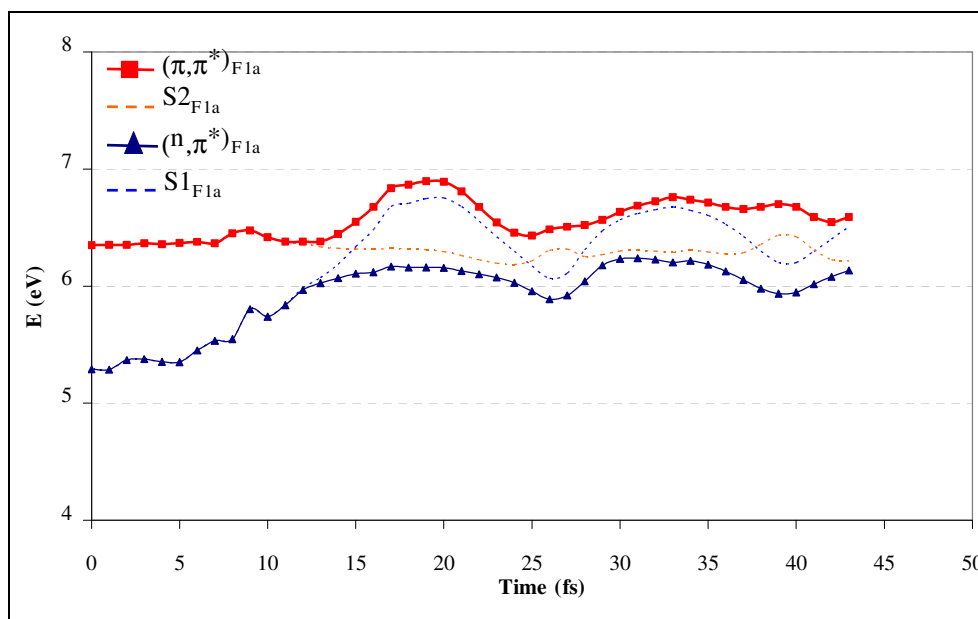


Figure SI-4a. Diabatic and adiabatic energies at the center of function F1a of run 1c.

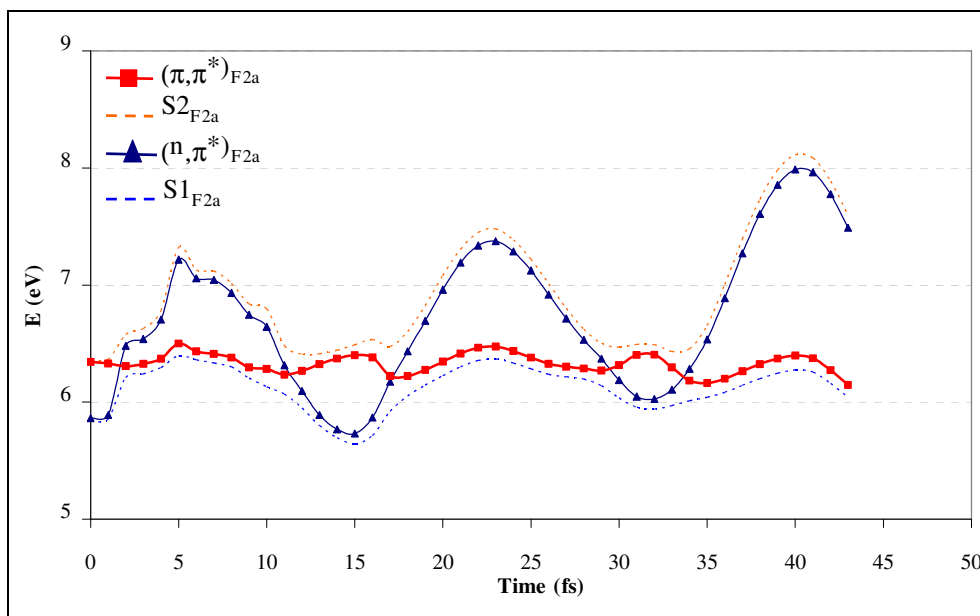


Figure SI-4b. Diabatic and adiabatic energies at the center of function F2a of run 1c.

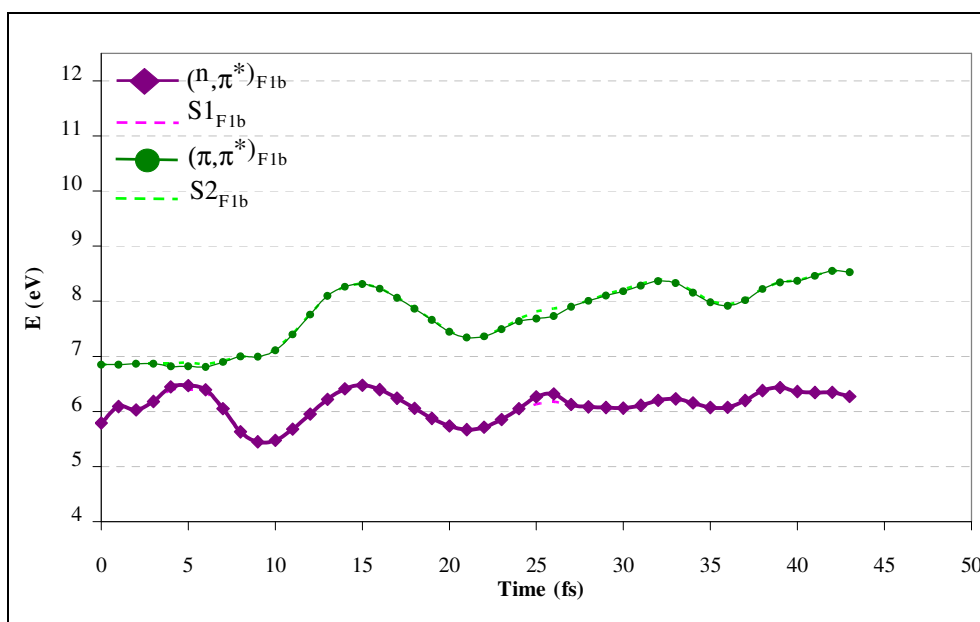


Figure SI-4c. Diabatic and adiabatic energies at the center of function F1b of run 1c.

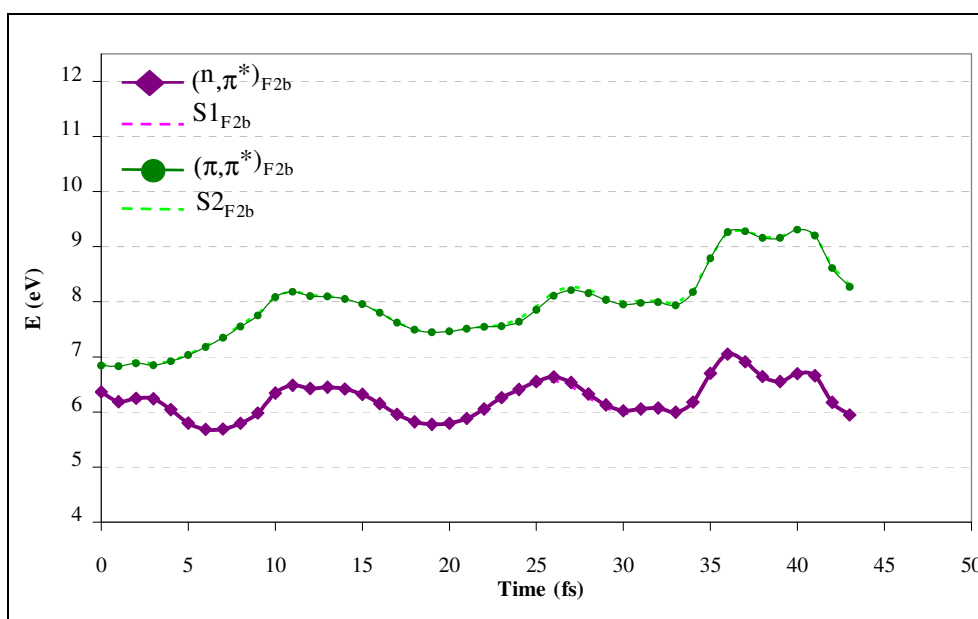


Figure SI-4d. Diabatic and adiabatic energies at the center of function F2b of run 1c.

Run 1d

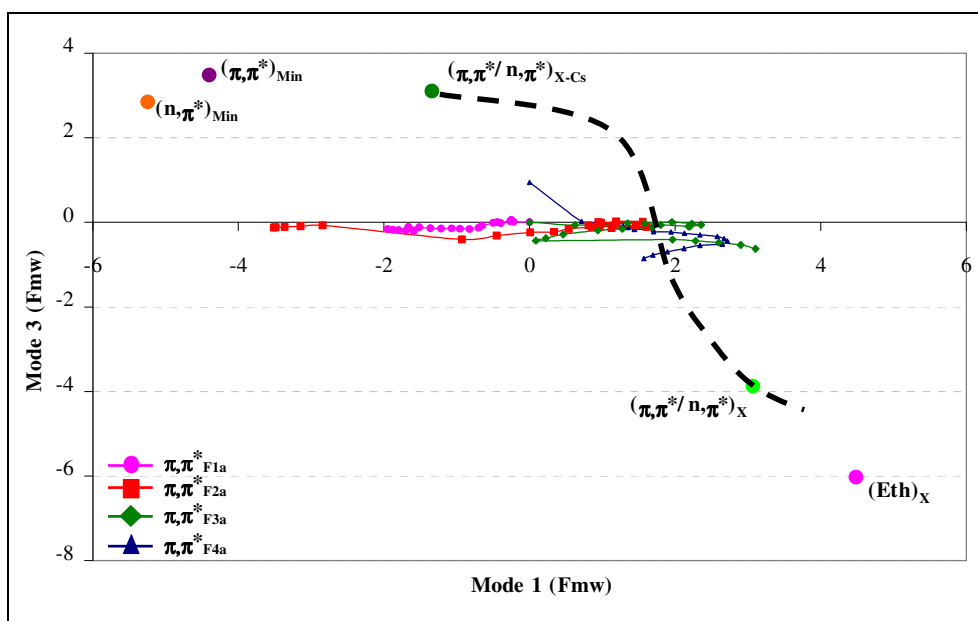


Figure SI-5a. Position of the center of the F1a-4a Gaussian functions of run 1d (position relative to $(\pi, \pi^*)_{\text{TS}}$).

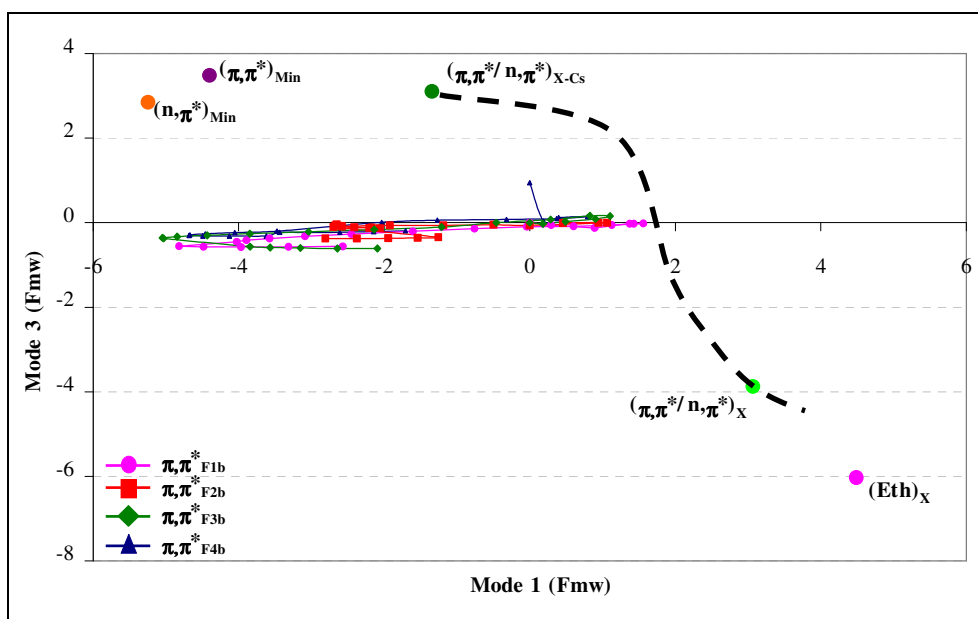


Figure SI-5b. Position of the center of the F1b-4b Gaussian functions of run 1d (position relative to $(\pi, \pi^*)_{\text{TS}}$).

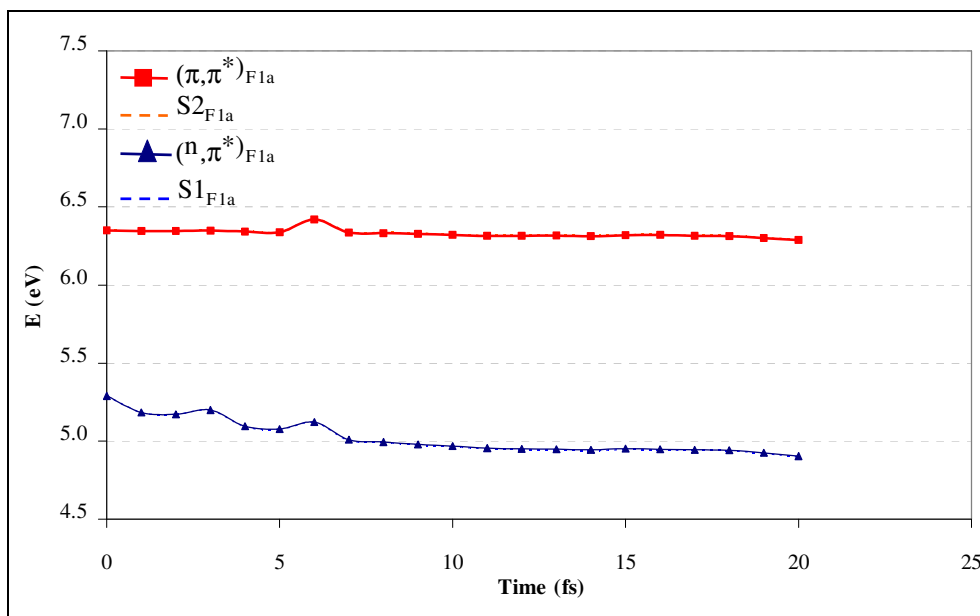


Figure SI-6a. Diabatic and adiabatic energies at the center of function F1a of run 1d.

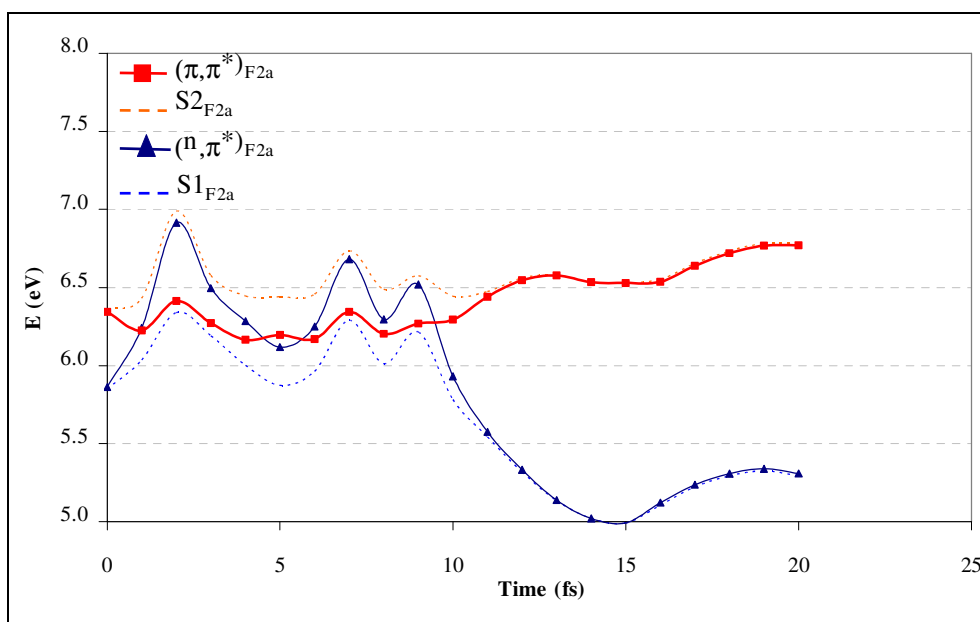


Figure SI-6b. Diabatic and adiabatic energies at the center of function F2a of run 1d.

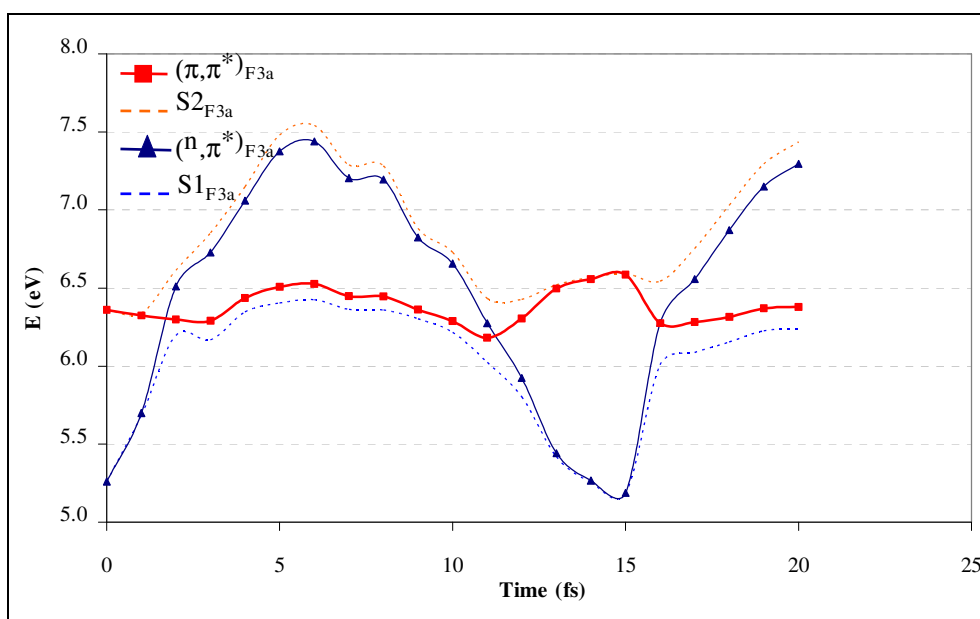


Figure SI-6c. Diabatic and adiabatic energies at the center of function F3a of run 1d.

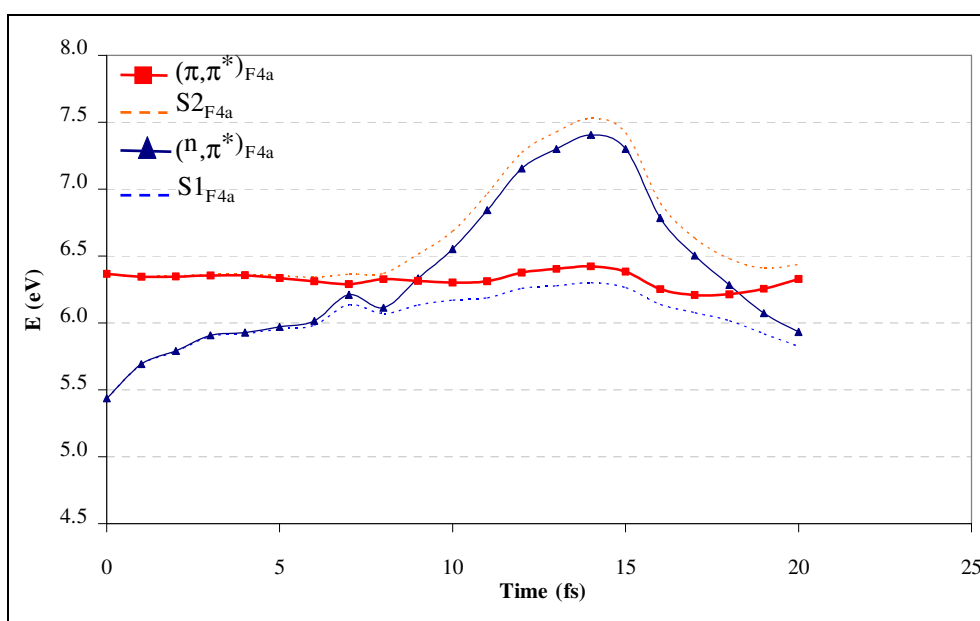


Figure SI-6d. Diabatic and adiabatic energies at the center of function F4a of run 1d.

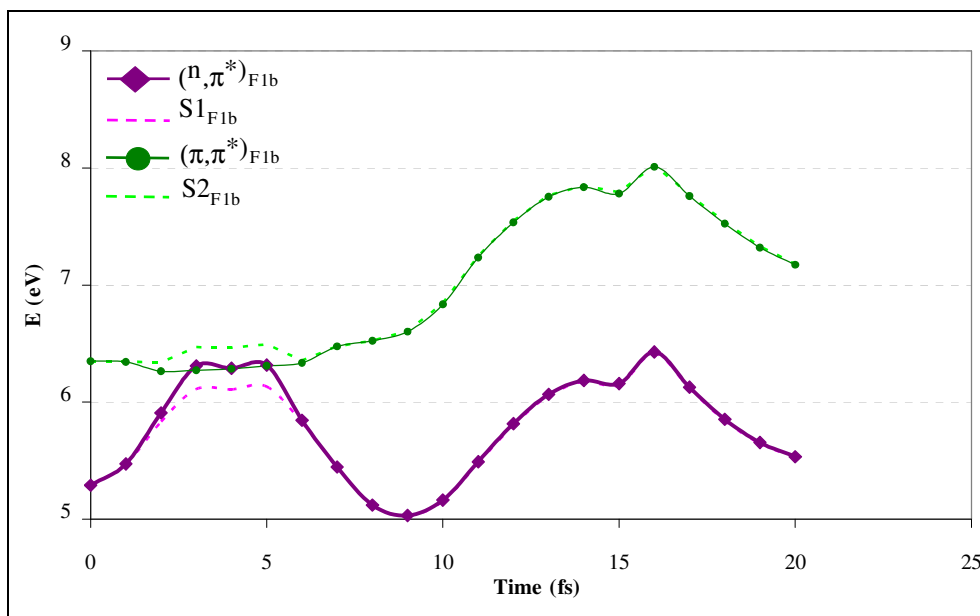


Figure SI-6e. Diabatic and adiabatic energies at the center of function F1b of run 1d.

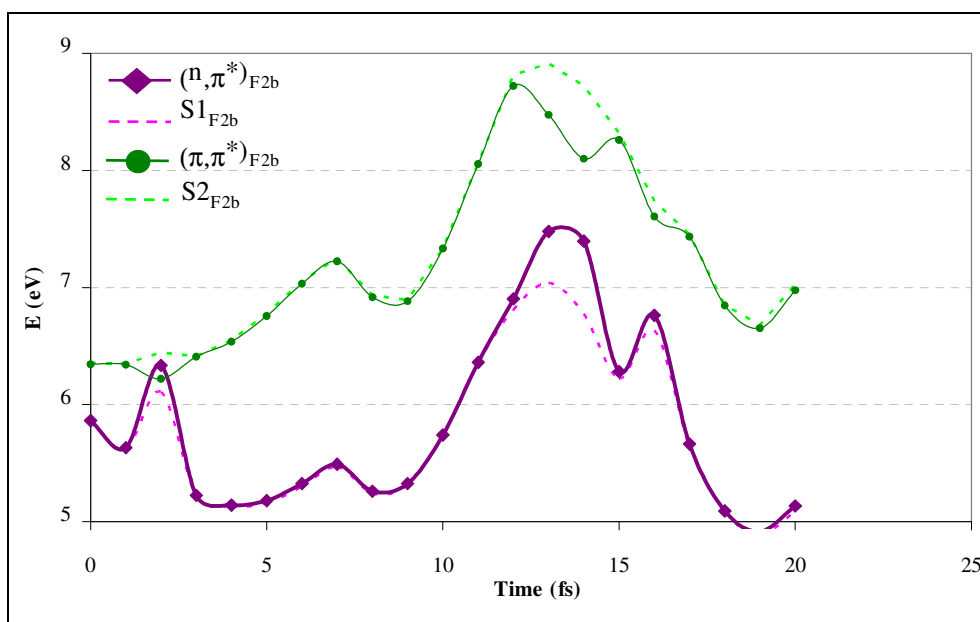


Figure SI-6f. Diabatic and adiabatic energies at the center of function F2b of run 1d.

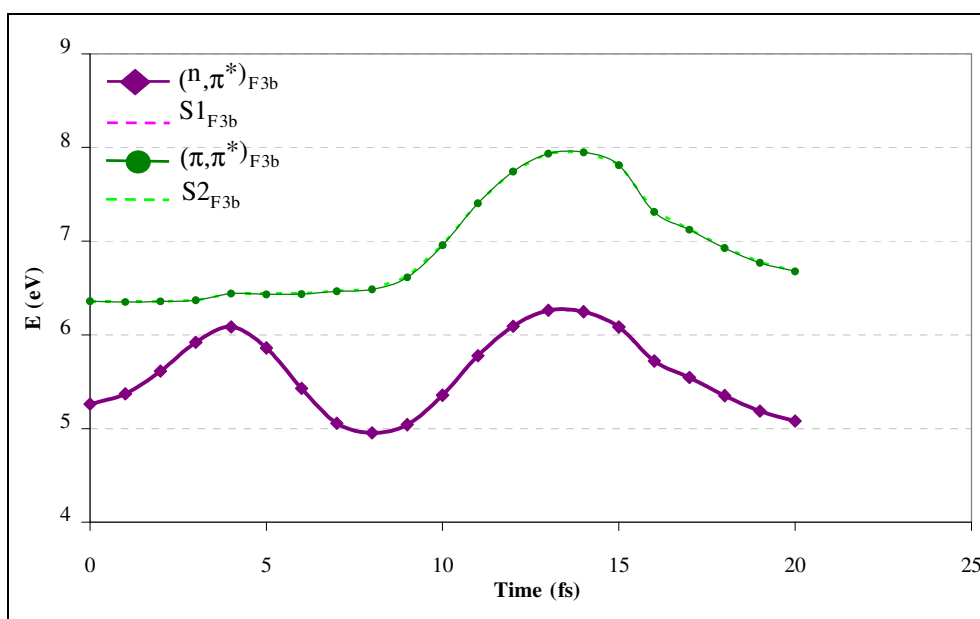


Figure SI-6g. Diabatic and adiabatic energies at the center of function F3b of run 1d.

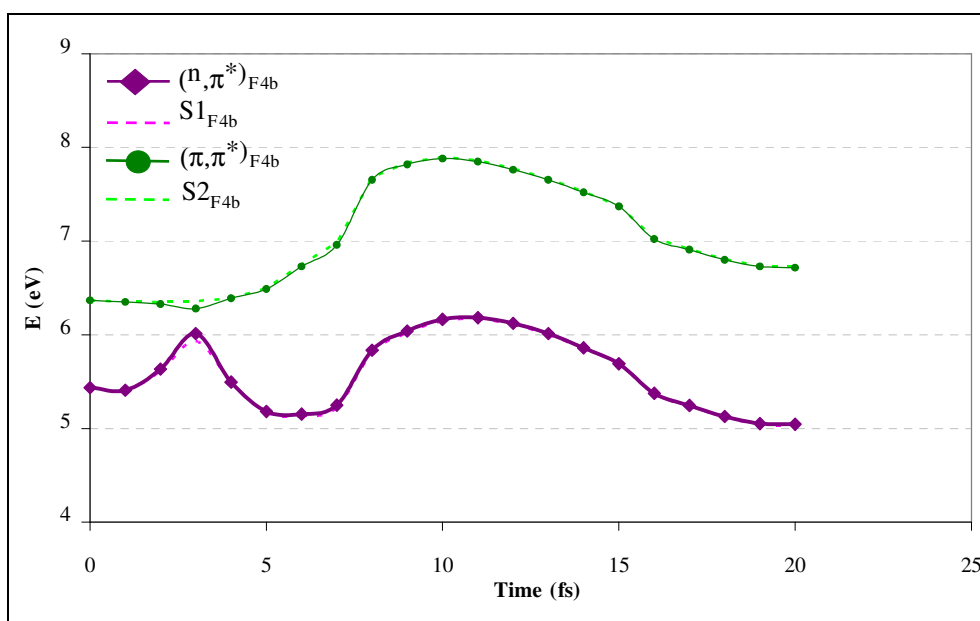


Figure SI-6h. Diabatic and adiabatic energies at the center of function F4b of run 1d.

Run 1e

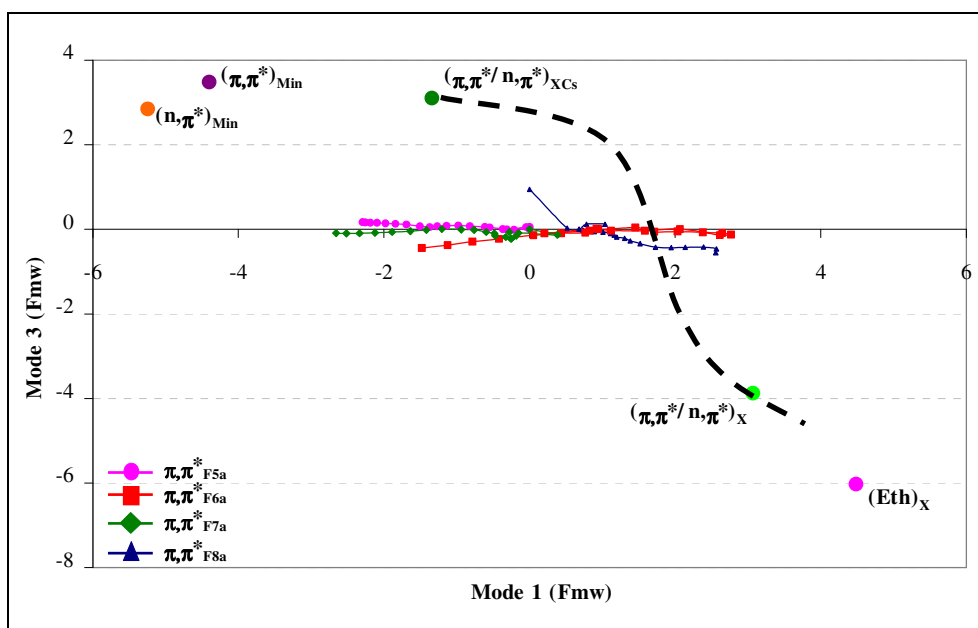


Figure SI-7a Position of the center of the F1a-F4a Gaussian functions of run 1e.

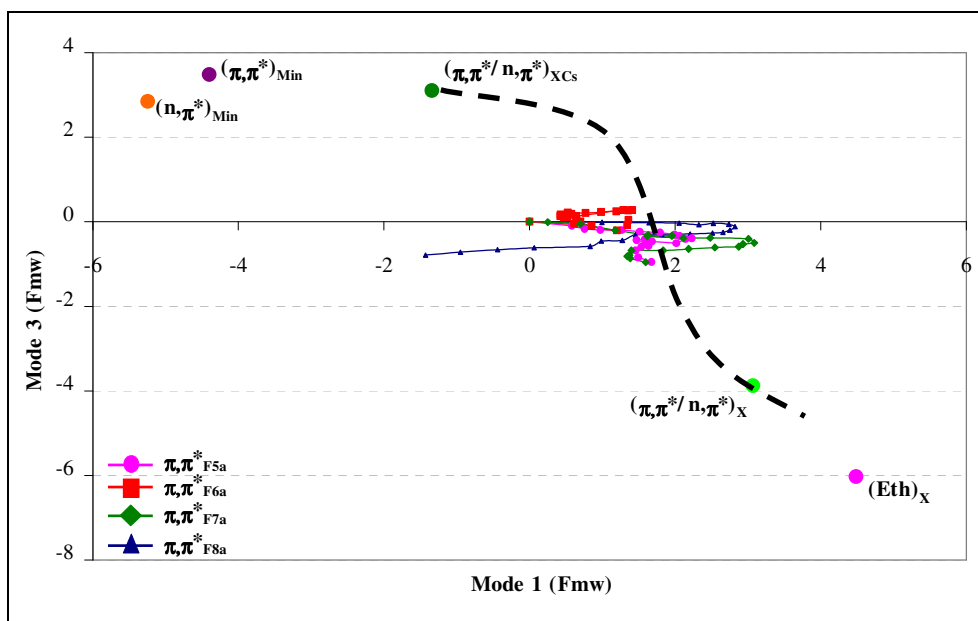


Figure SI-7b Position of the center of the F5a-F8a Gaussian functions of run 1e.

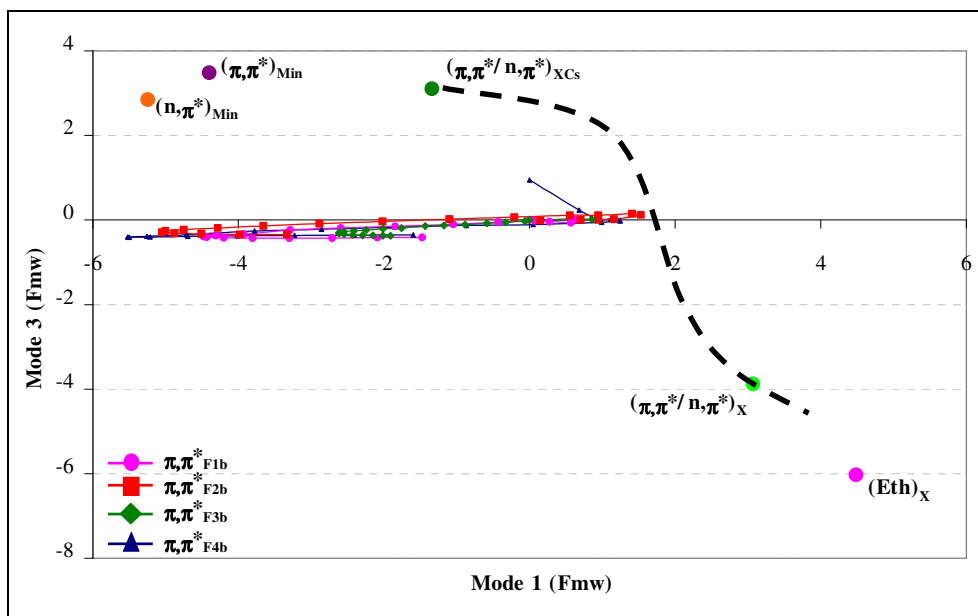


Figure SI-7c Position of the center of the F1b-F4b Gaussian functions of run 1e (positions relative to $(\pi, \pi^*)_{\text{TS}}$).

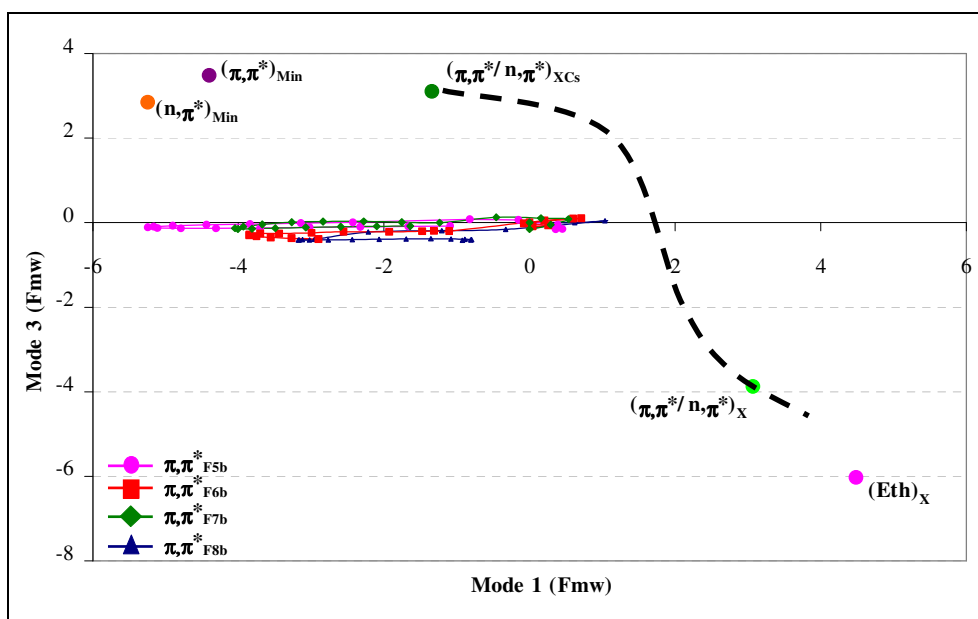


Figure SI-7d Position of the center of the F5b-F8b Gaussian functions of run 1e (positions relative to $(\pi, \pi^*)_{\text{TS}}$).

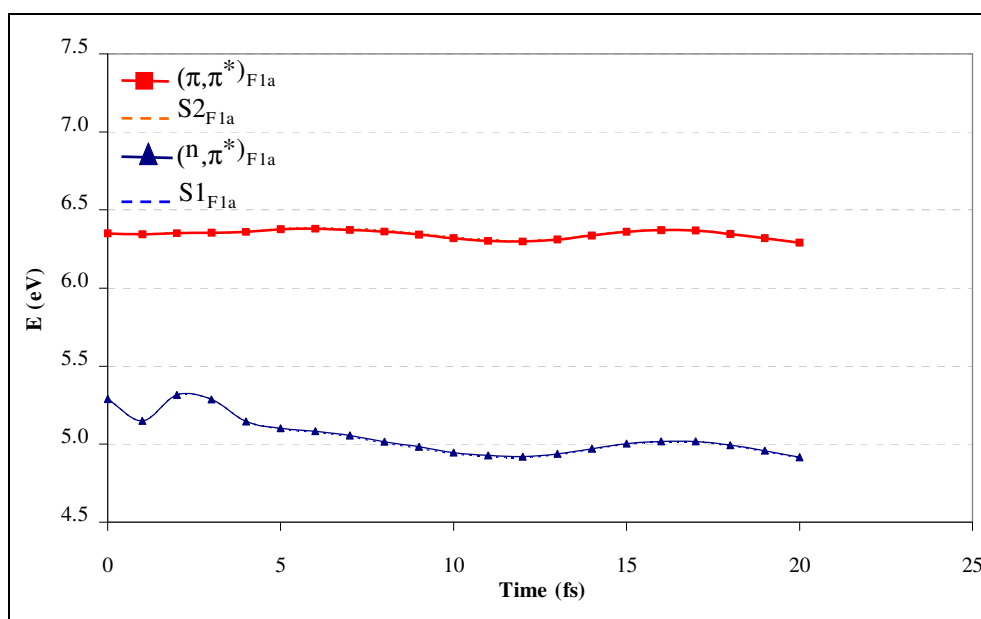


Figure SI-8a. Diabatic and adiabatic energies at the center of function F1a of run 1e.

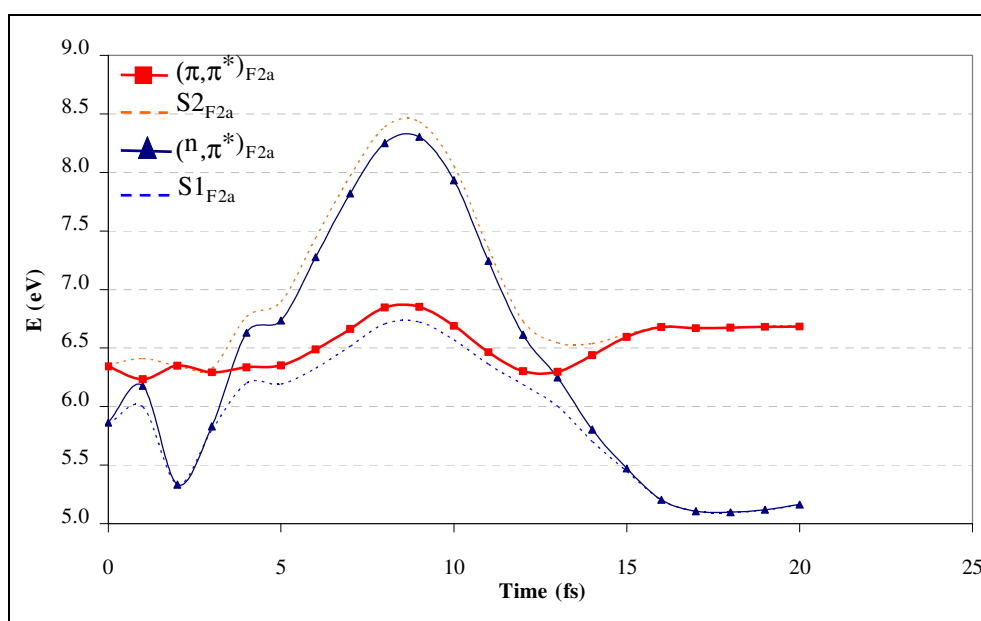


Figure SI-8b. Diabatic and adiabatic energies at the center of function F2a of run 1e.

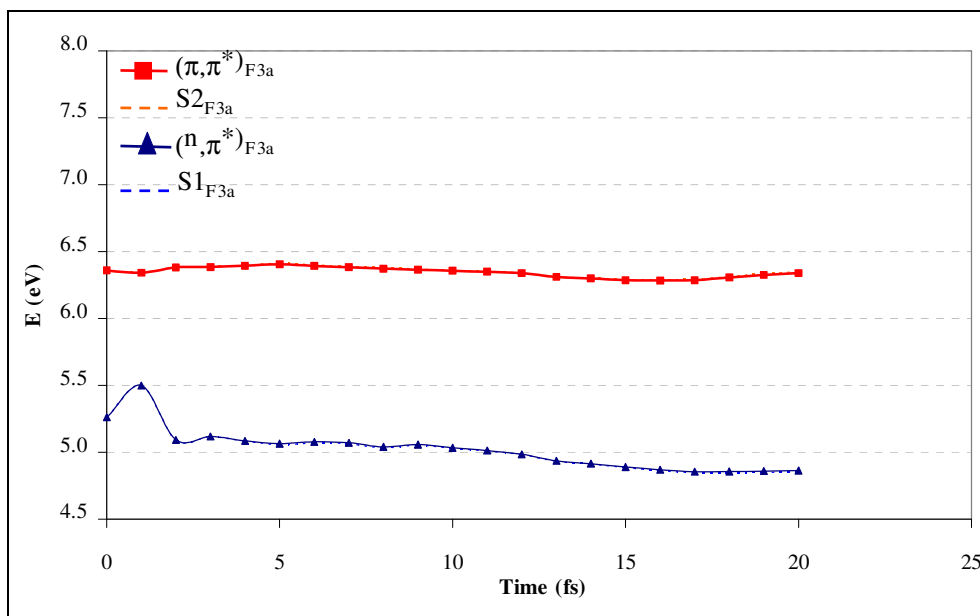


Figure SI-8c. Diabatic and adiabatic energies at the center of function F3a of run 1e.

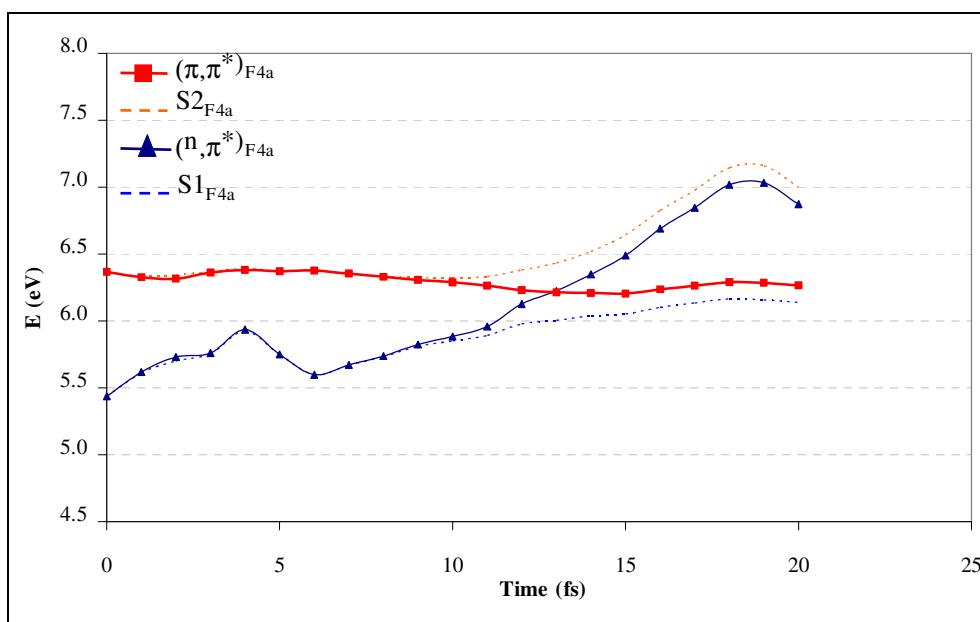


Figure SI-8d. Diabatic and adiabatic energies at the center of function F4a of run 1e.

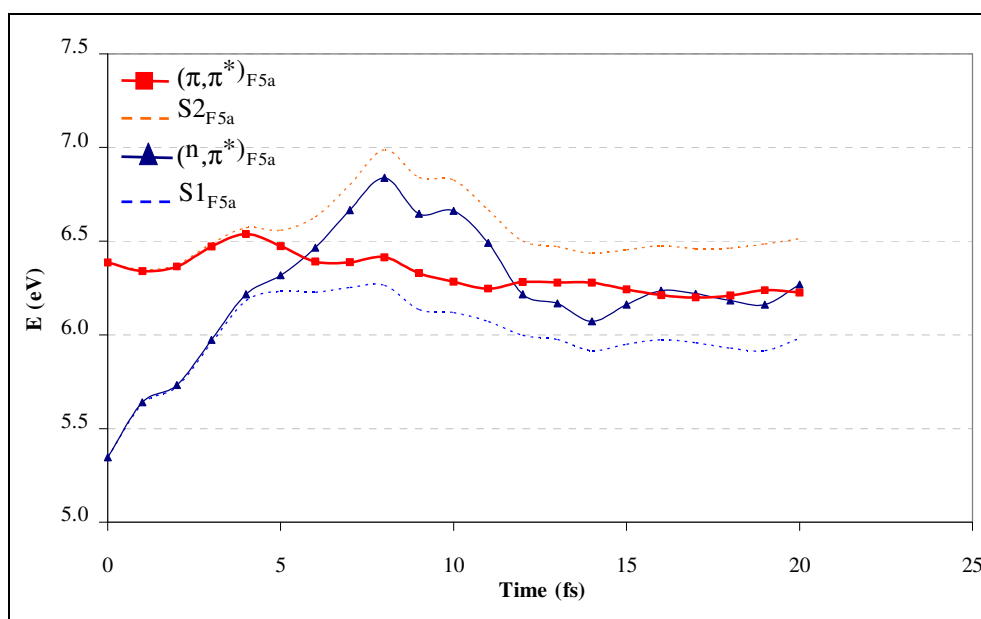


Figure SI-8e. Diabatic and adiabatic energies at the center of function F5a of run 1e.

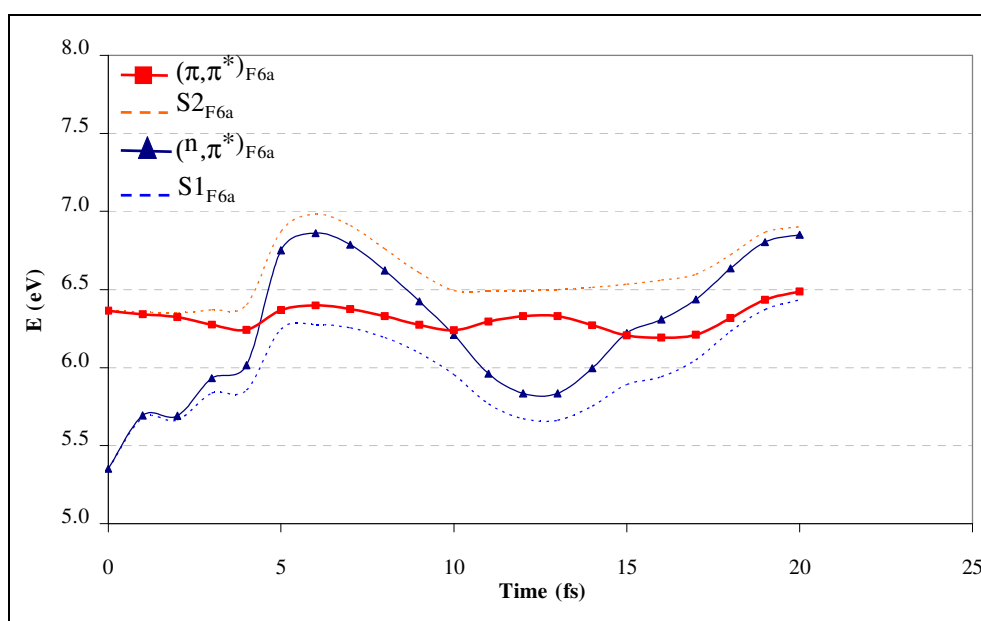


Figure SI-8f. Diabatic and adiabatic energies at the center of function F6a of run 1e.

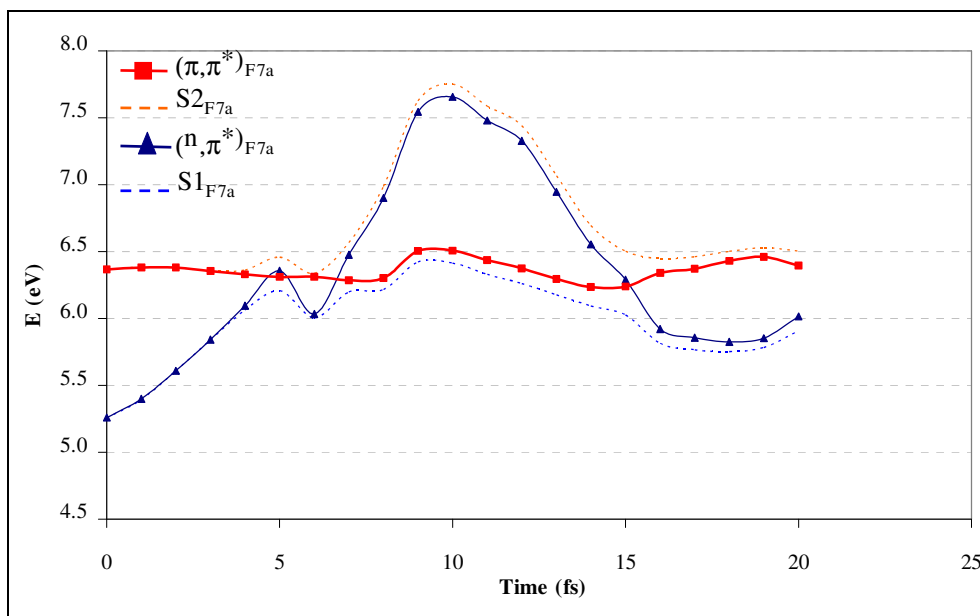


Figure SI-8g. Diabatic and adiabatic energies at the center of function F7a of run 1e.

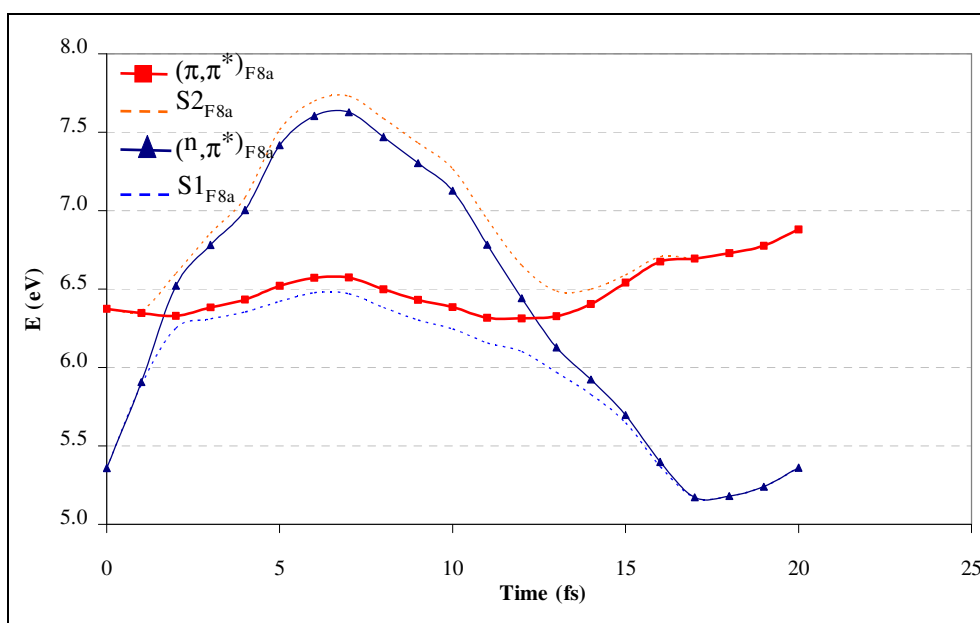


Figure SI-8h. Diabatic and adiabatic energies at the center of function F8a of run 1e.

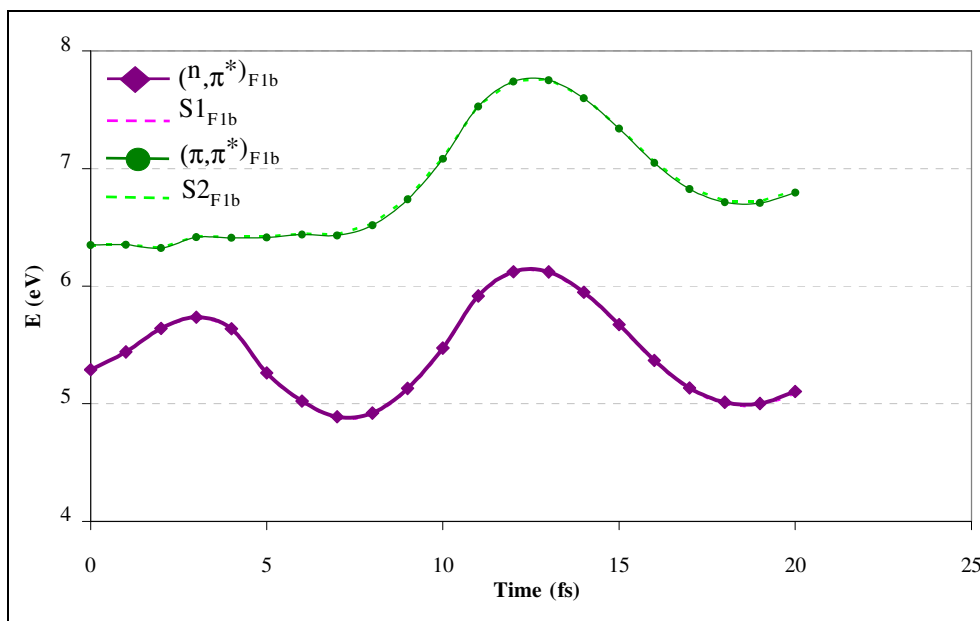


Figure SI-8i. Diabatic and adiabatic energies at the center of function F1b of run 1e.

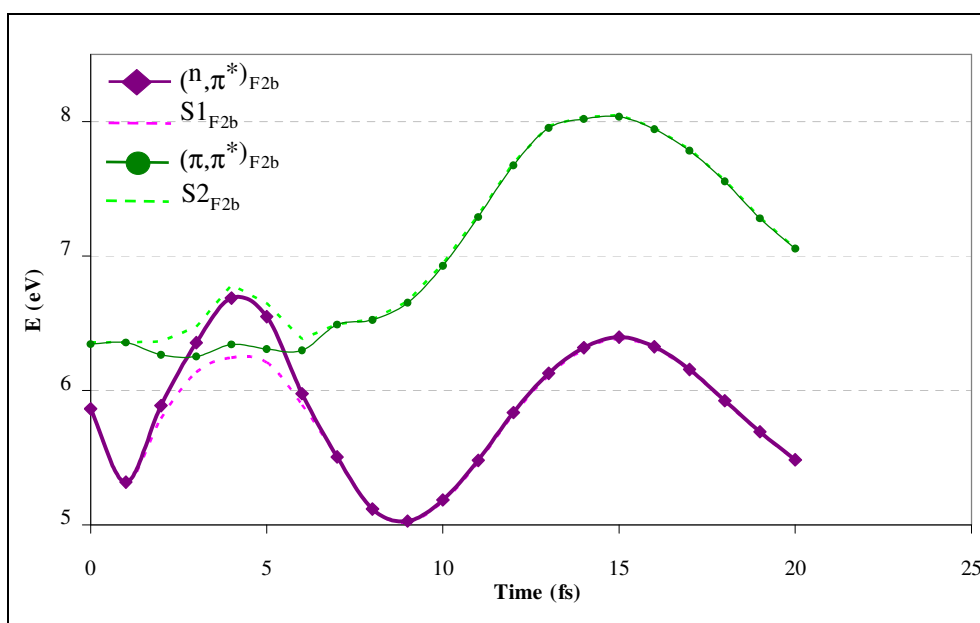


Figure SI-8j. Diabatic and adiabatic energies at the center of function F2b of run 1e.

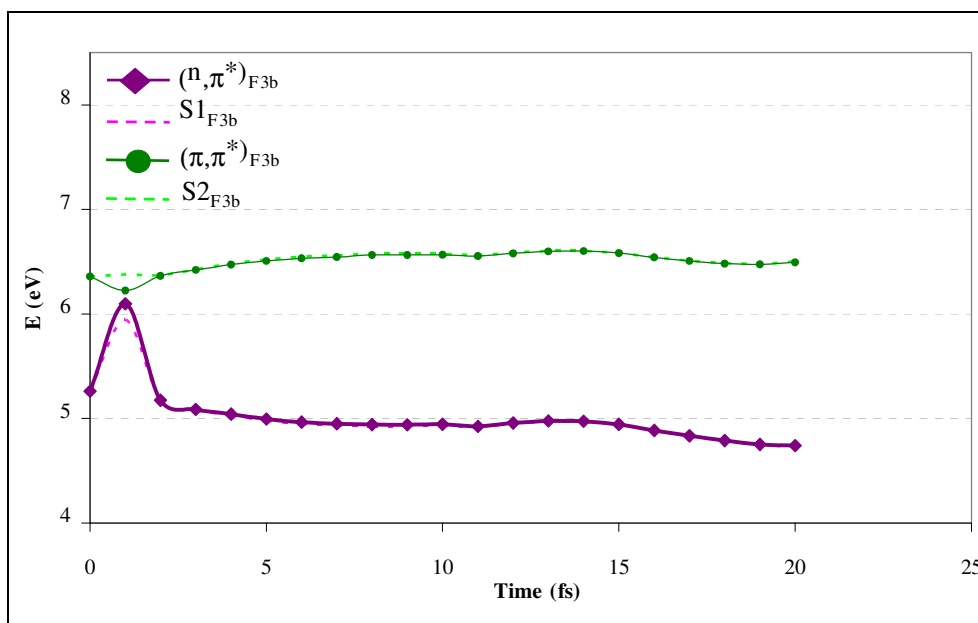


Figure SI-8k. Diabatic and adiabatic energies at the center of function F3b of run 1e.

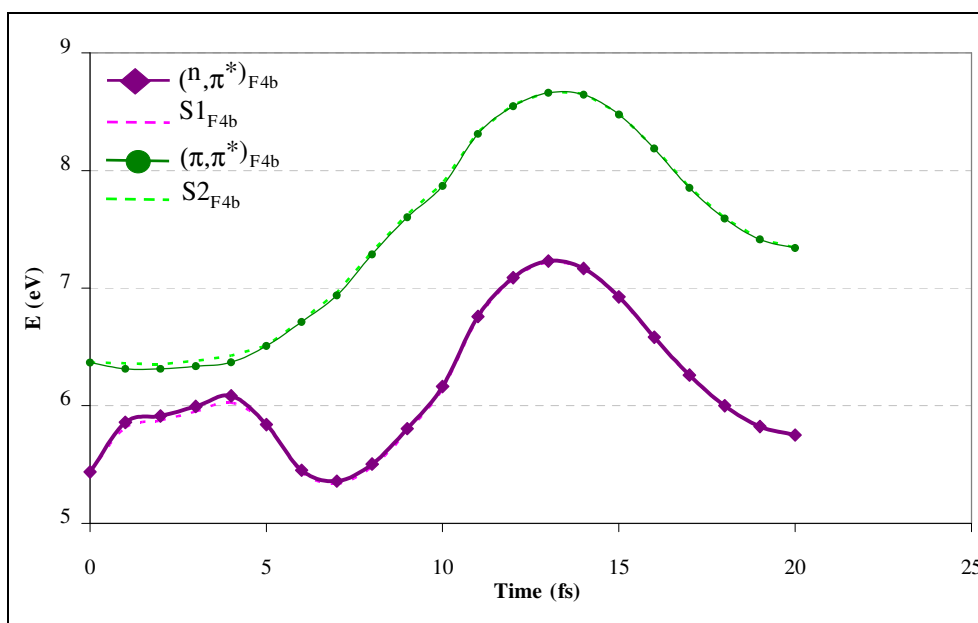


Figure SI-8l. Diabatic and adiabatic energies at the center of function F4b of run 1e.

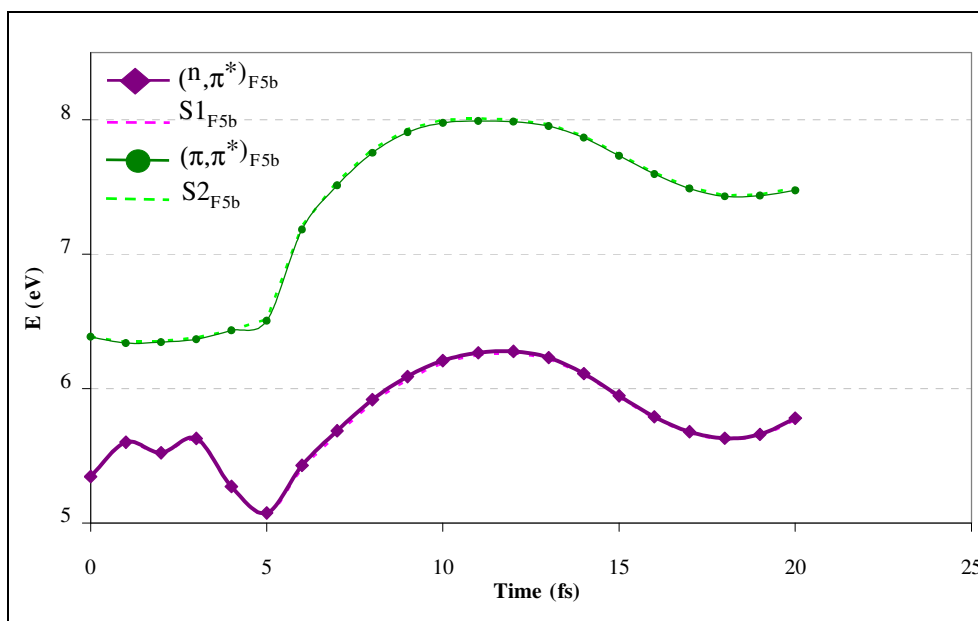


Figure SI-8m. Diabatic and adiabatic energies at the center of function F5b of run 1e.

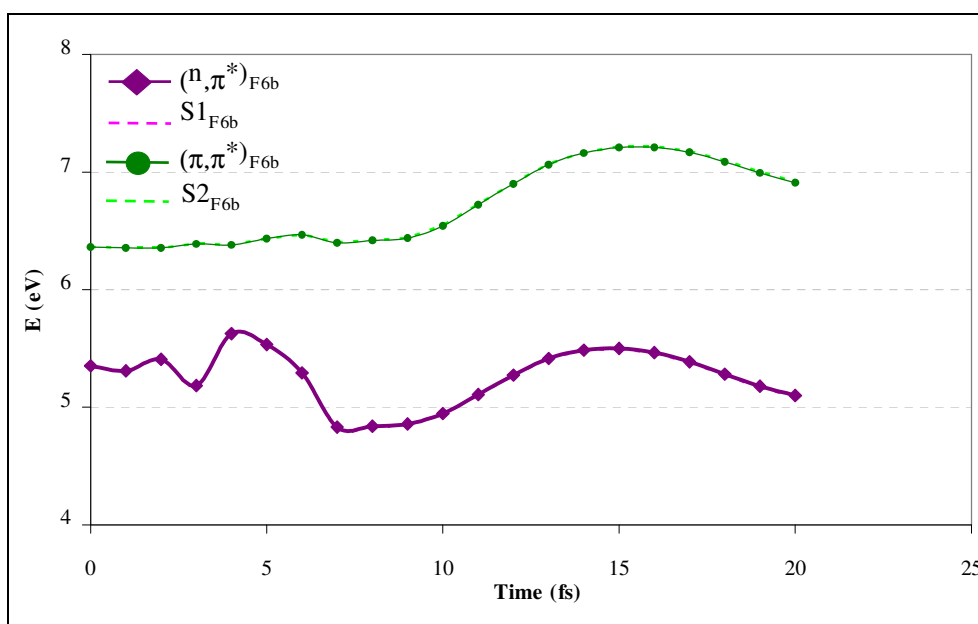


Figure SI-8n. Diabatic and adiabatic energies at the center of function F6b of run 1e.

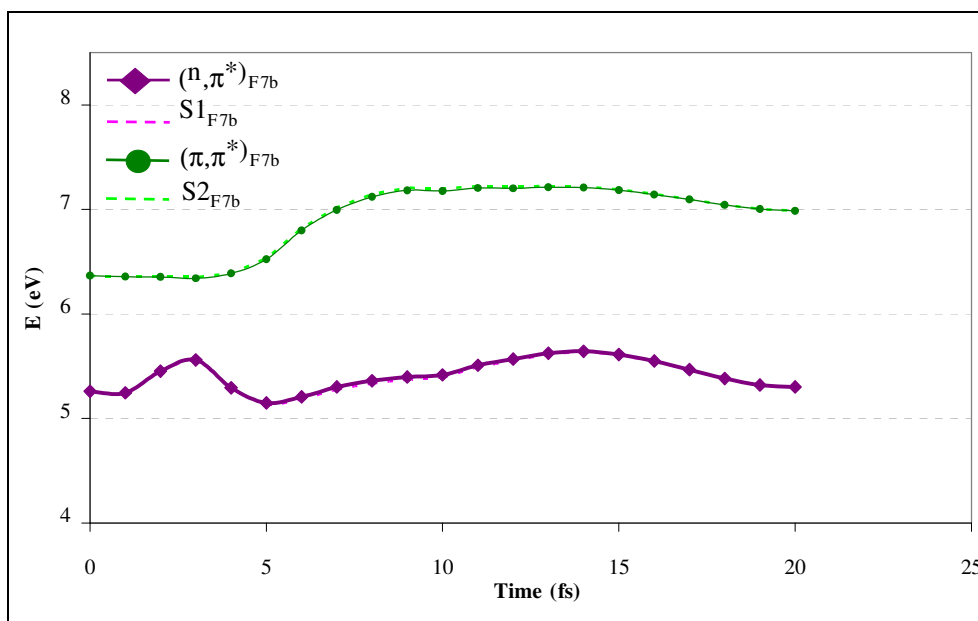


Figure SI-8o. Diabatic and adiabatic energies at the center of function F7b of run 1e.

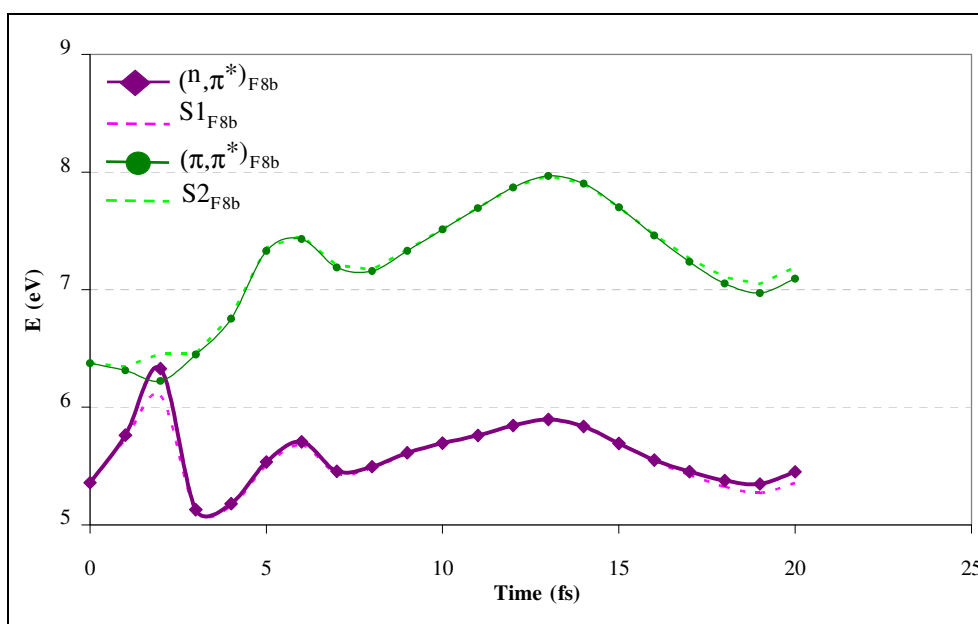


Figure SI-8p. Diabatic and adiabatic energies at the center of function F8b of run 1e.

Run 2a

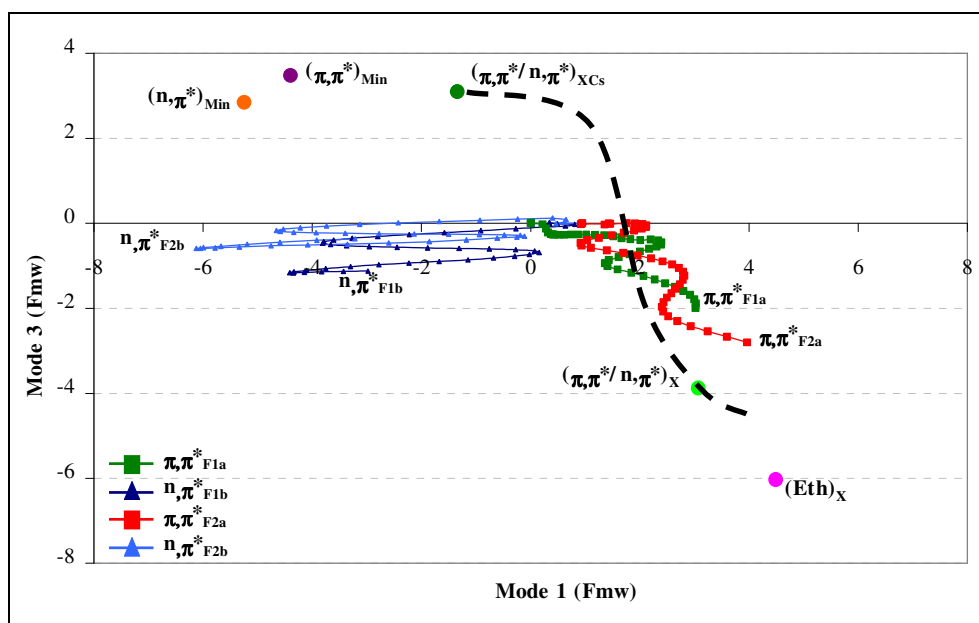


Figure SI-9 Position of the center of the Gaussian functions of run 2a.

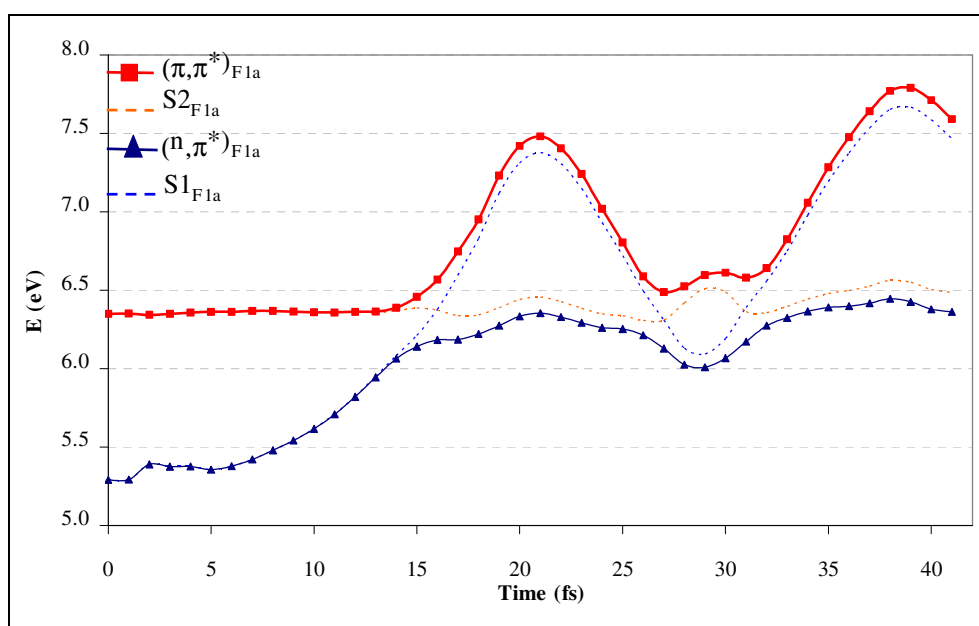


Figure SI-10a. Diabatic and adiabatic energies at the center of function F1a of run 2a.

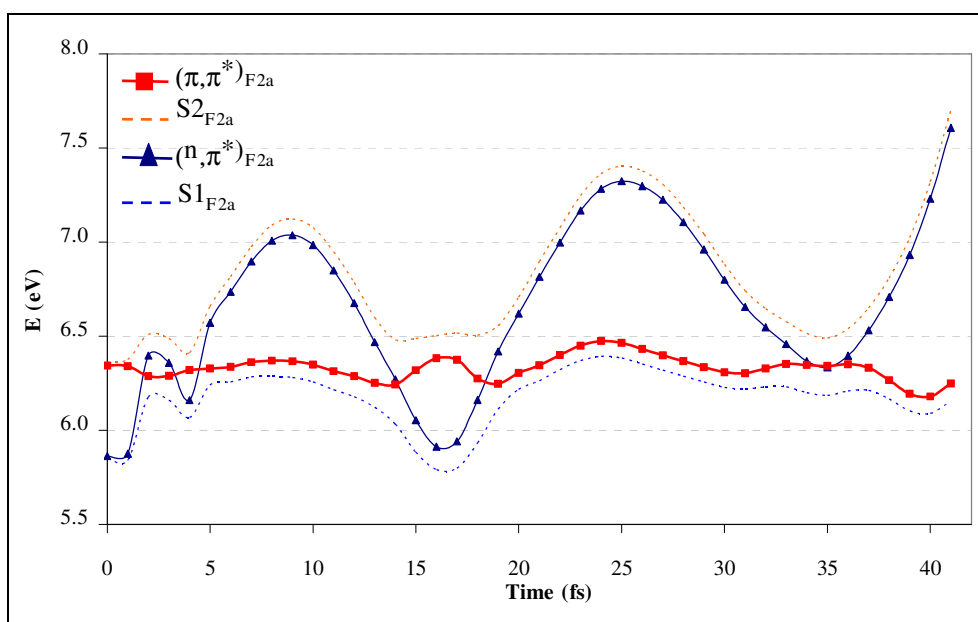


Figure SI-10b. Diabatic and adiabatic energies at the center of function F2a of run 2a.

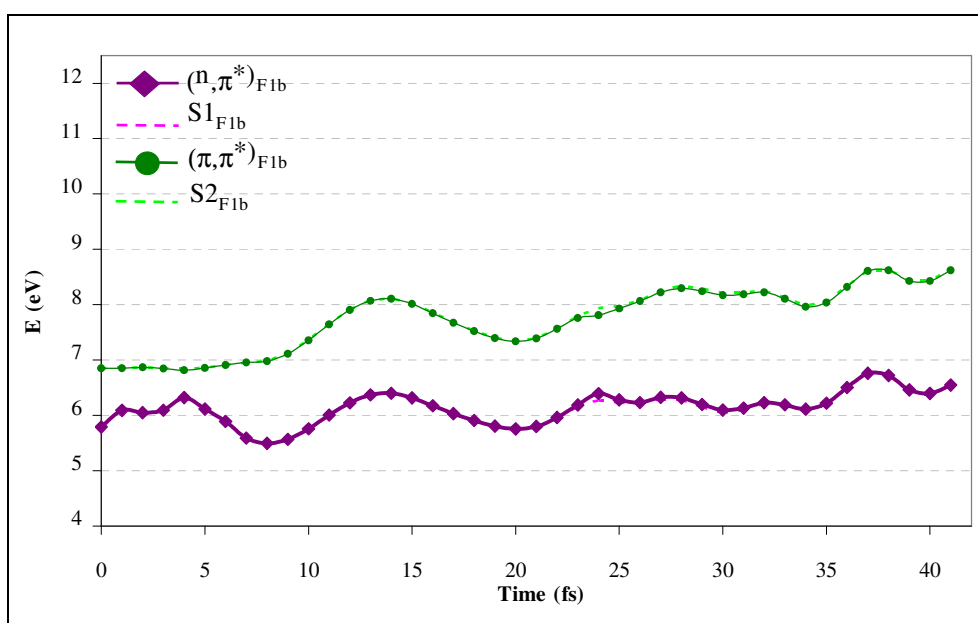


Figure SI-10c. Diabatic and adiabatic energies at the center of function F1b of run 2a.

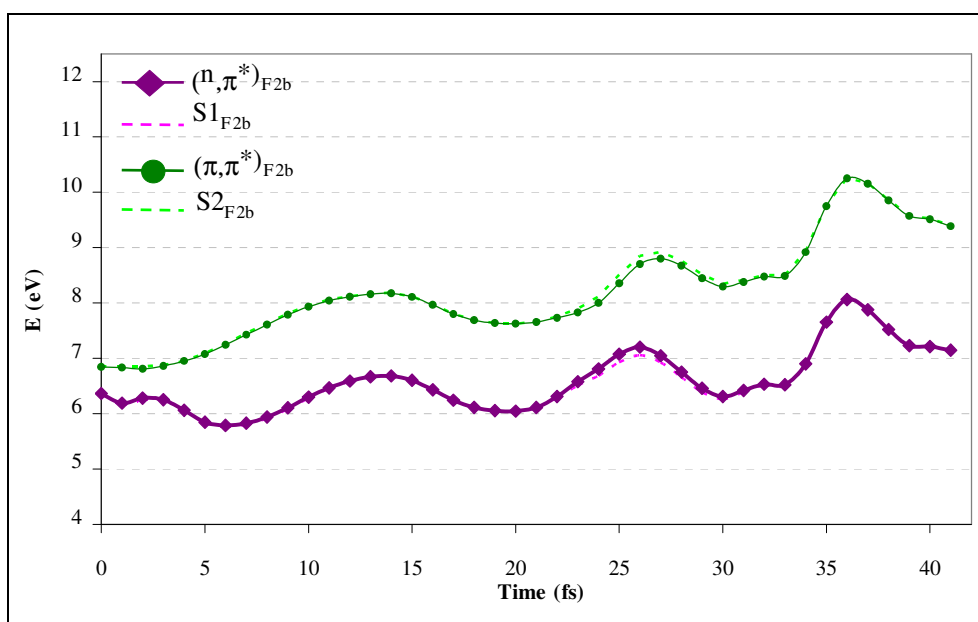


Figure SI-10d. Diabatic and adiabatic energies at the center of function F2b of run 2a.

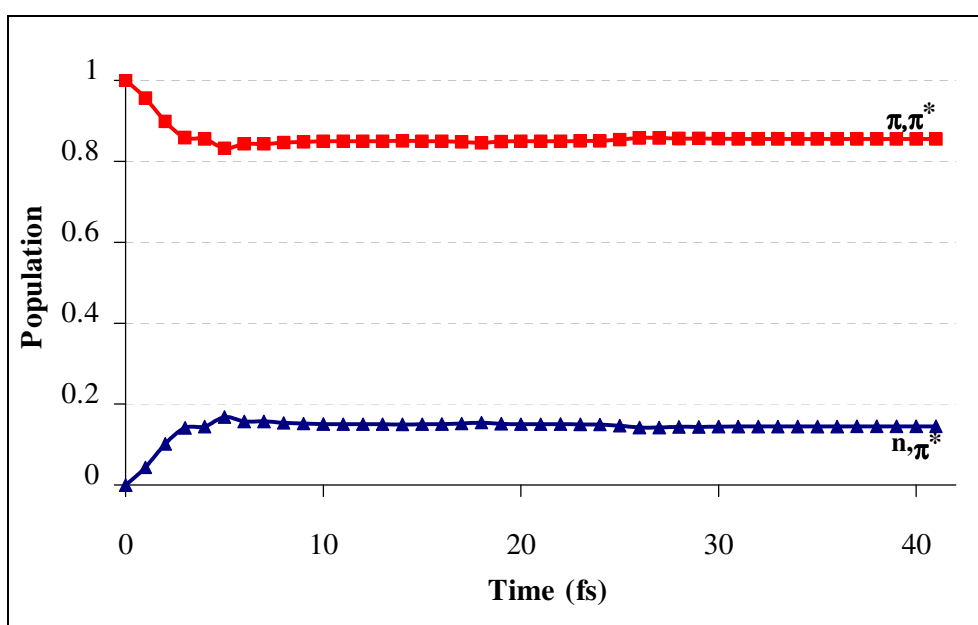


Figure SI-11. Populations of the π, π^* and n, π^* states of run 2a.

Run 2b

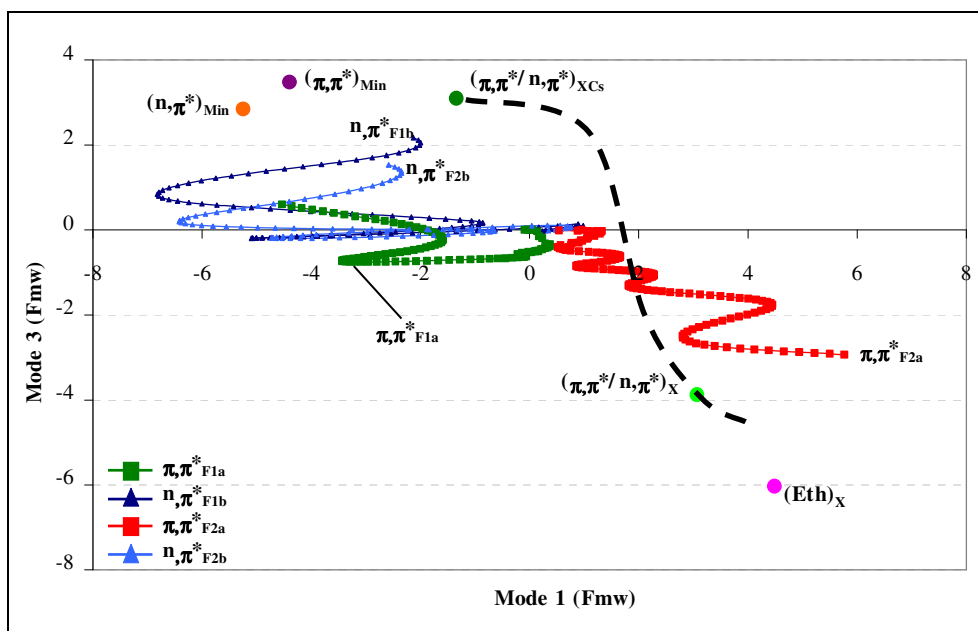


Figure SI-12 Position of the center of the Gaussian functions of run 2b.

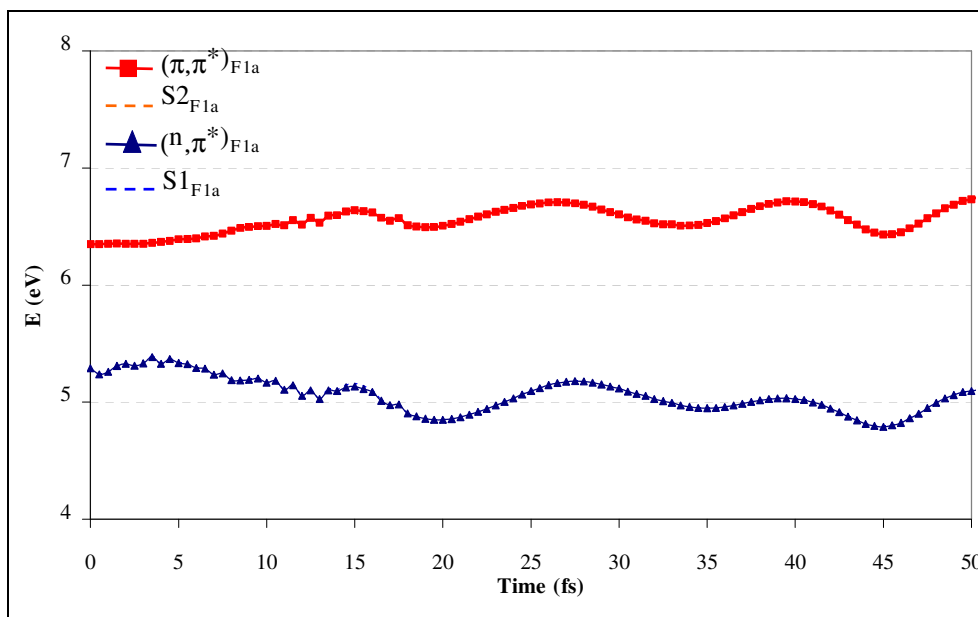


Figure SI-13a. Diabatic and adiabatic energies at the center of function F1a of run 2b.

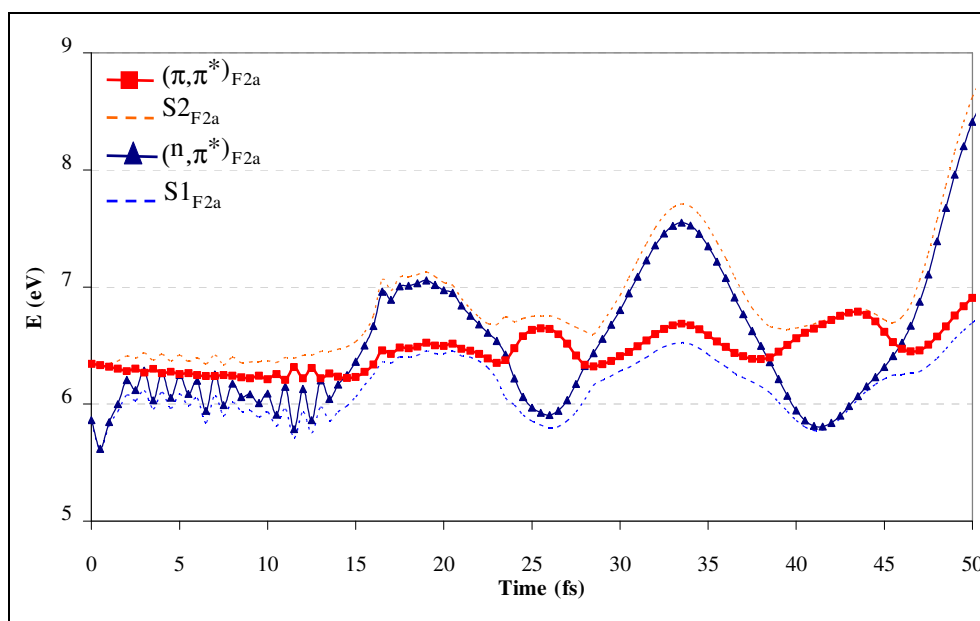


Figure SI-13b. Diabatic and adiabatic energies at the center of function F2a of run 2b.

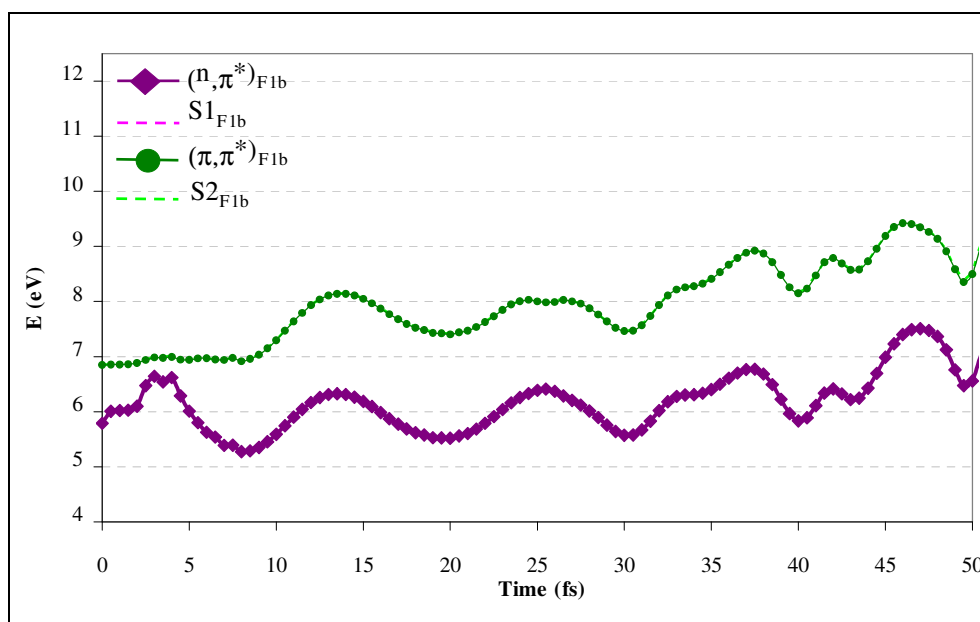


Figure SI-13c. Diabatic and adiabatic energies at the center of function F1b of run 2b.

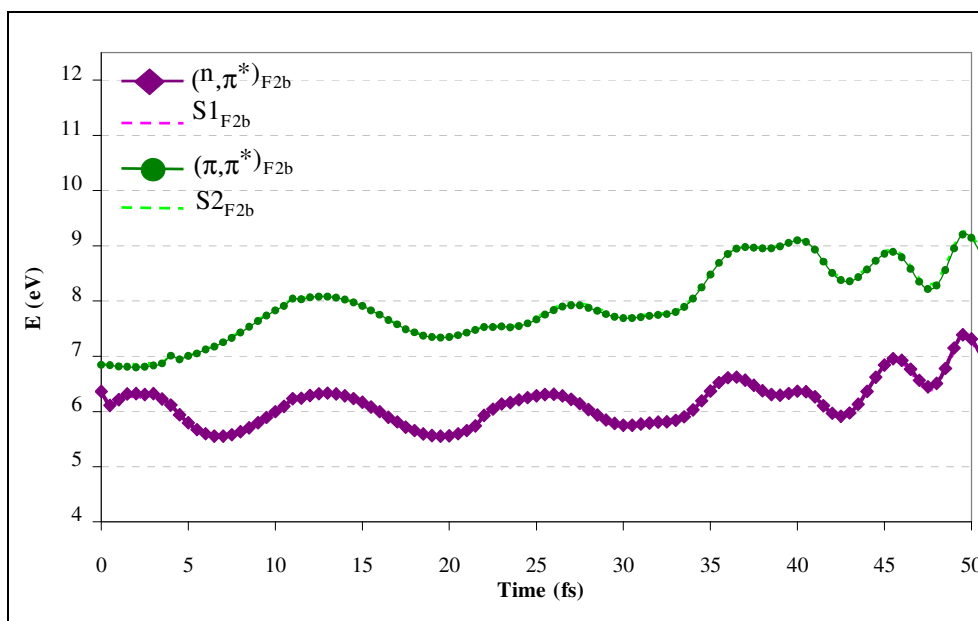


Figure SI-13d. Diabatic and adiabatic energies at the center of function F2b of run 2b.

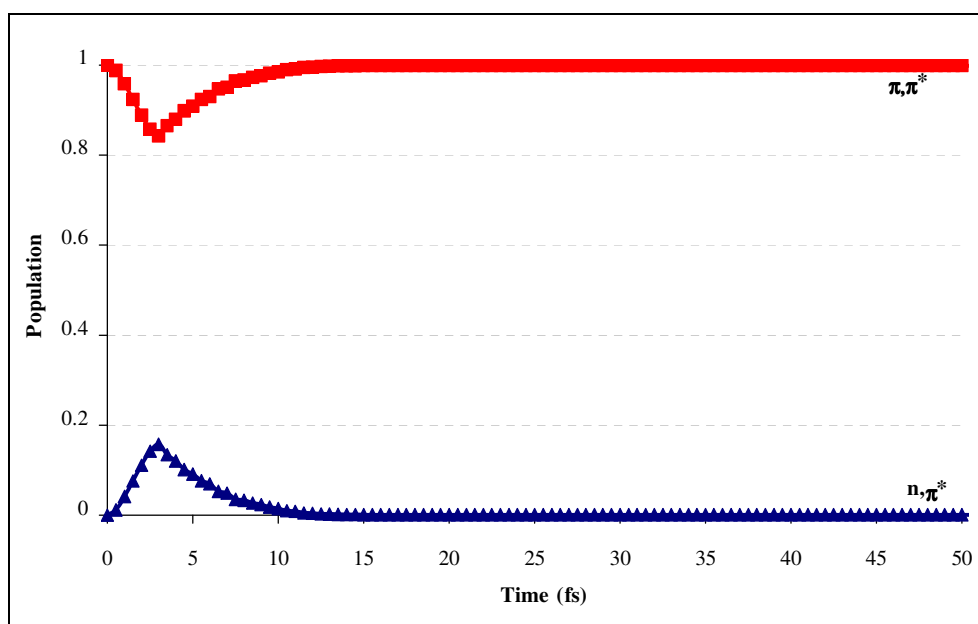


Figure SI-14. Populations of the π, π^* and n, π^* states of run 2b.

Run 3a

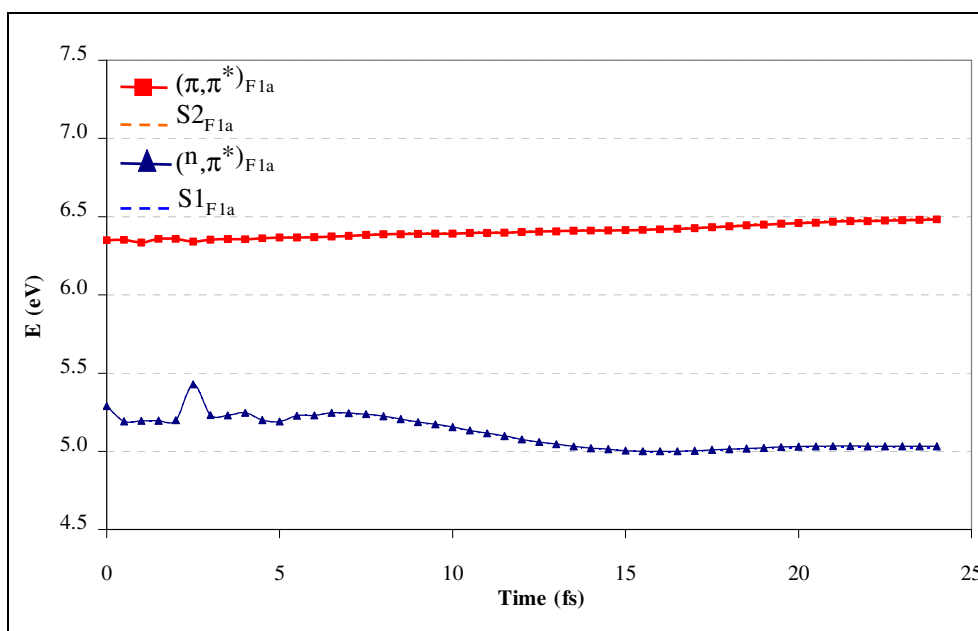


Figure SI-15a. Diabatic and adiabatic energies at the center of function F1a of run 3a.

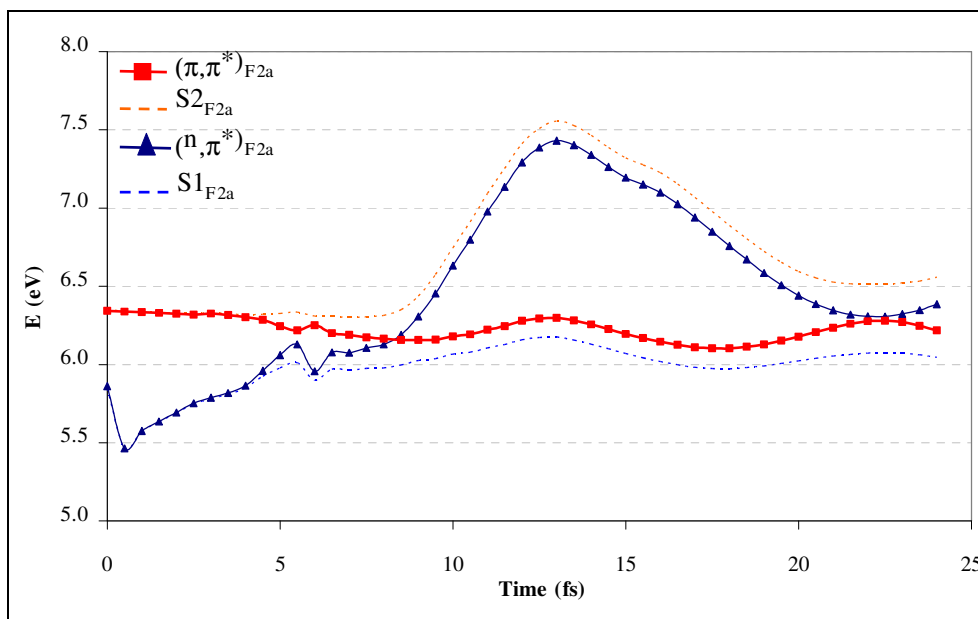


Figure SI-15b. Diabatic and adiabatic energies at the center of function F2a of run 3a.

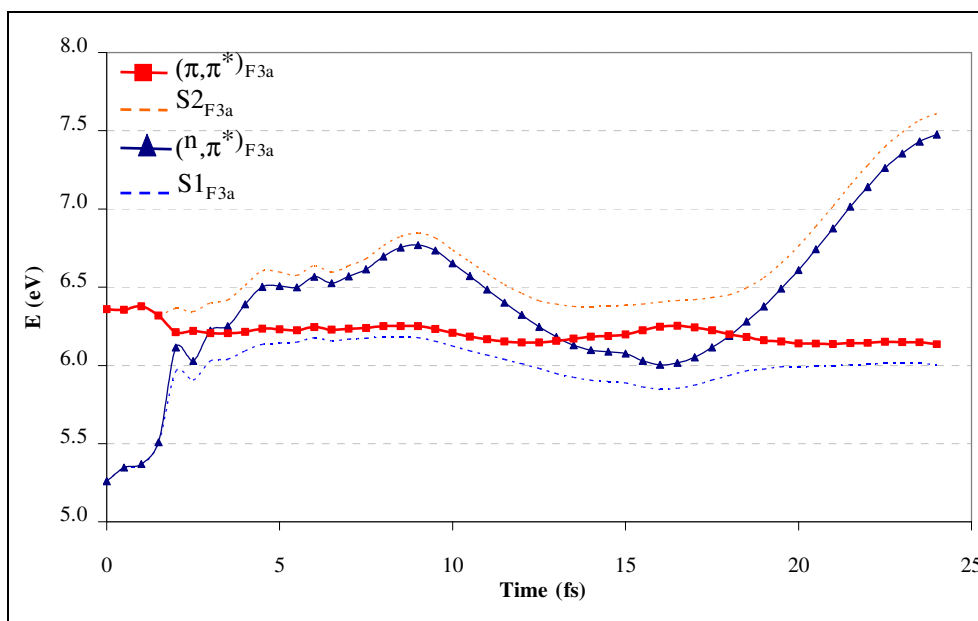


Figure SI-15c. Diabatic and adiabatic energies at the center of function F3a of run 3a.

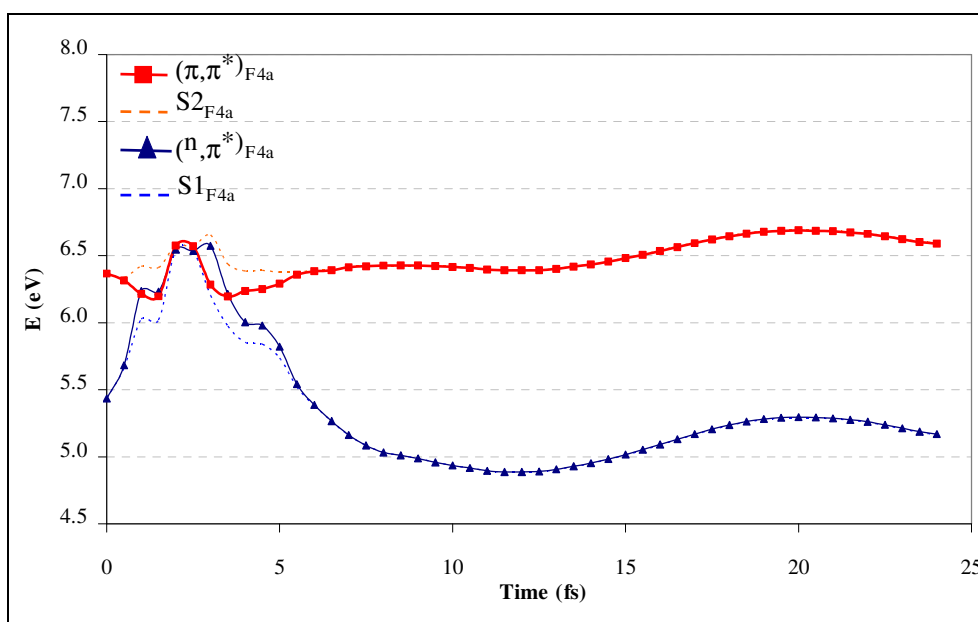


Figure SI-15d. Diabatic and adiabatic energies at the center of function F4a of run 3a.

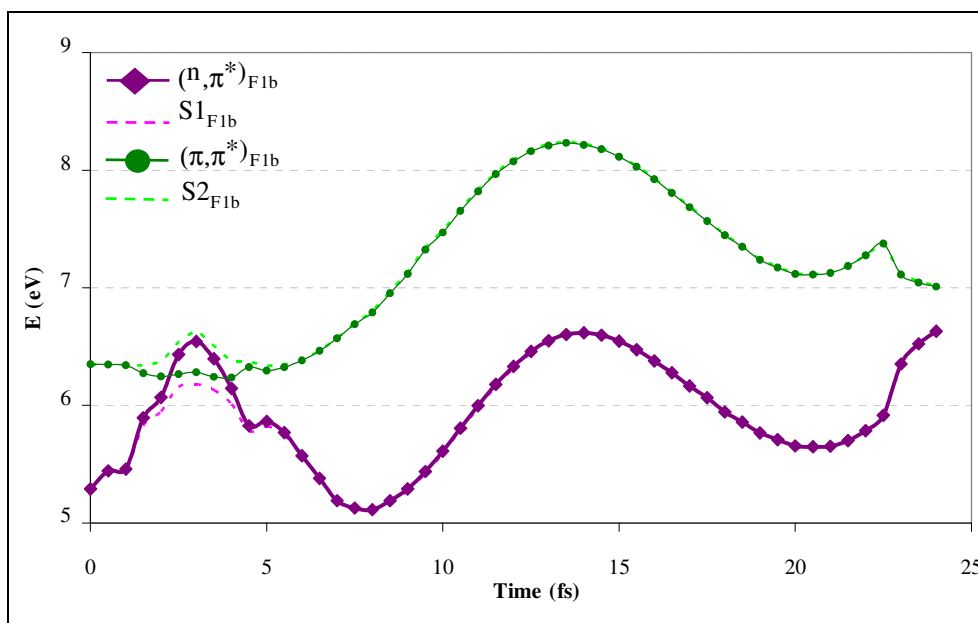


Figure SI-15e. Diabatic and adiabatic energies at the center of function F1b of run 3a.

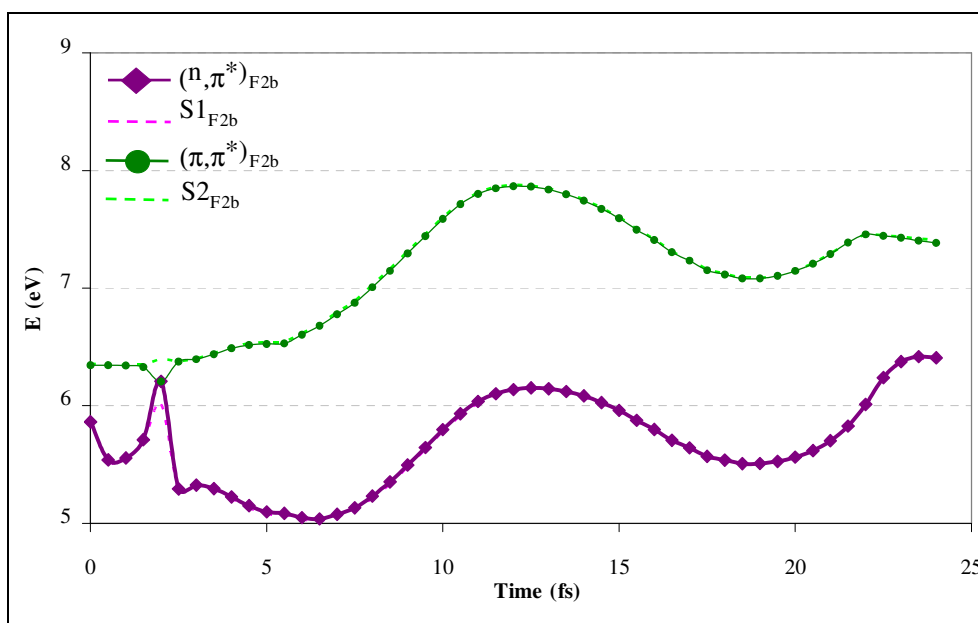


Figure SI-15f. Diabatic and adiabatic energies at the center of function F2b of run 3a.

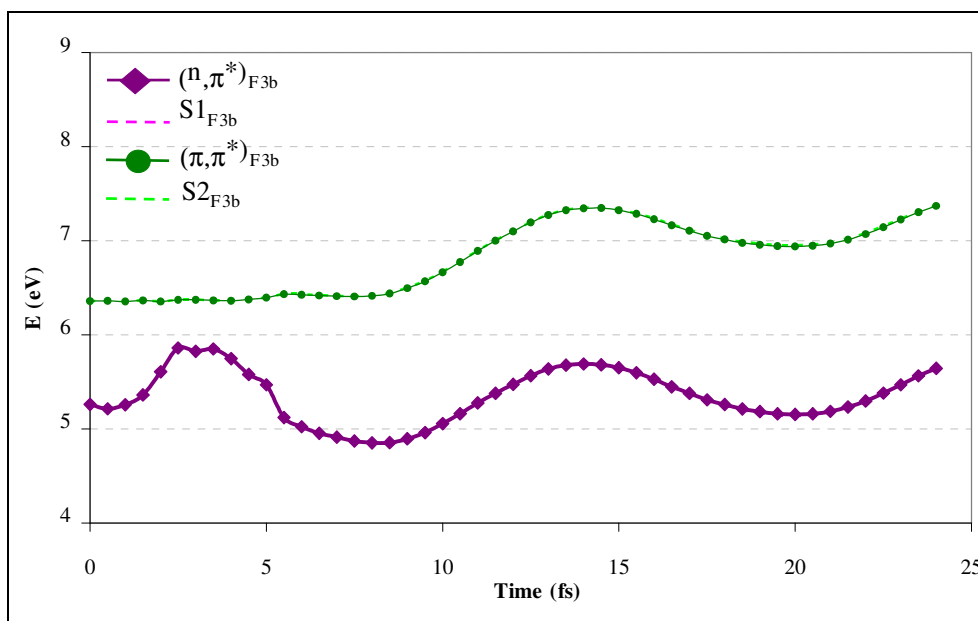


Figure SI-15g. Diabatic and adiabatic energies at the center of function F3b of run 3a.

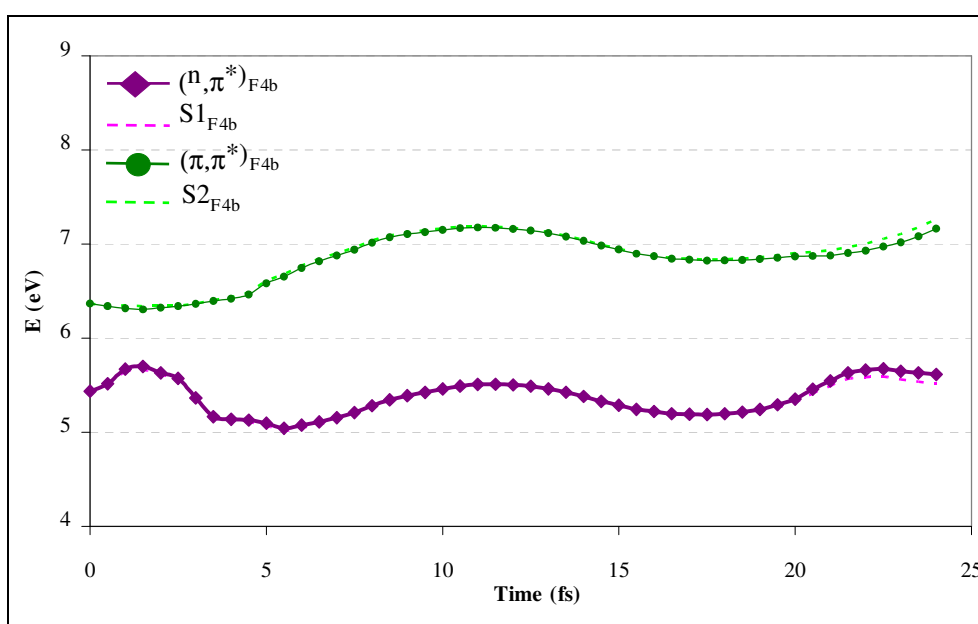


Figure SI-15h. Diabatic and adiabatic energies at the center of function F4b of run 3a.

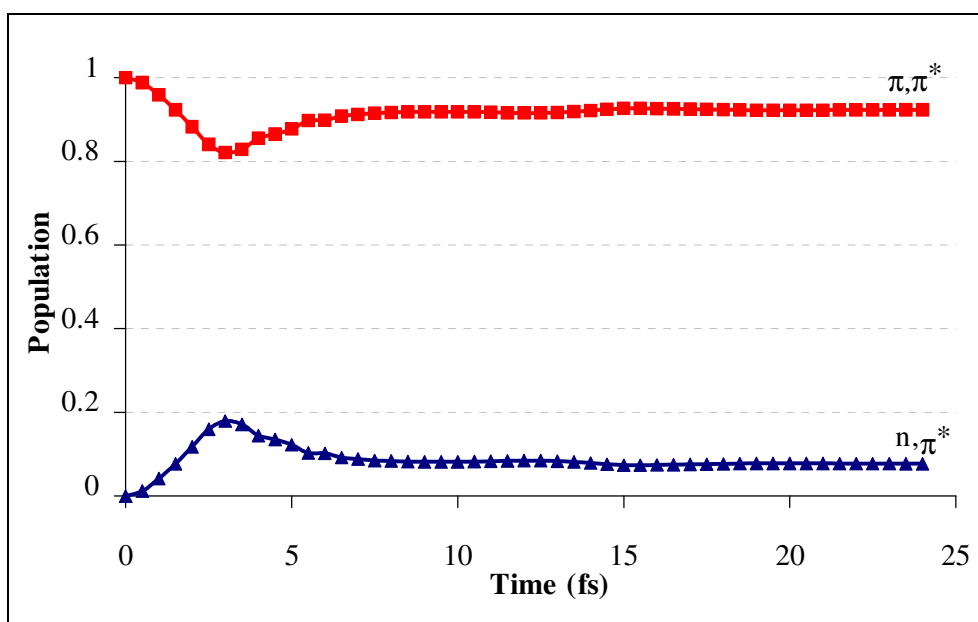


Figure SI-16. Populations of the π, π^* and n, π^* states of run 3a.

Run 3b

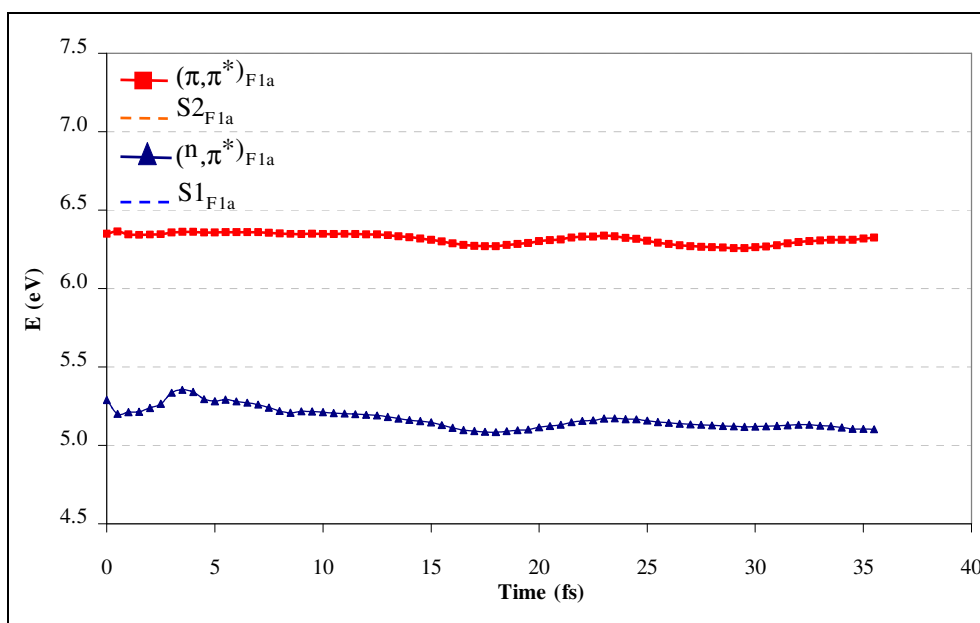


Figure SI-17a. Diabatic and adiabatic energies at the center of function F1a of run 3b.

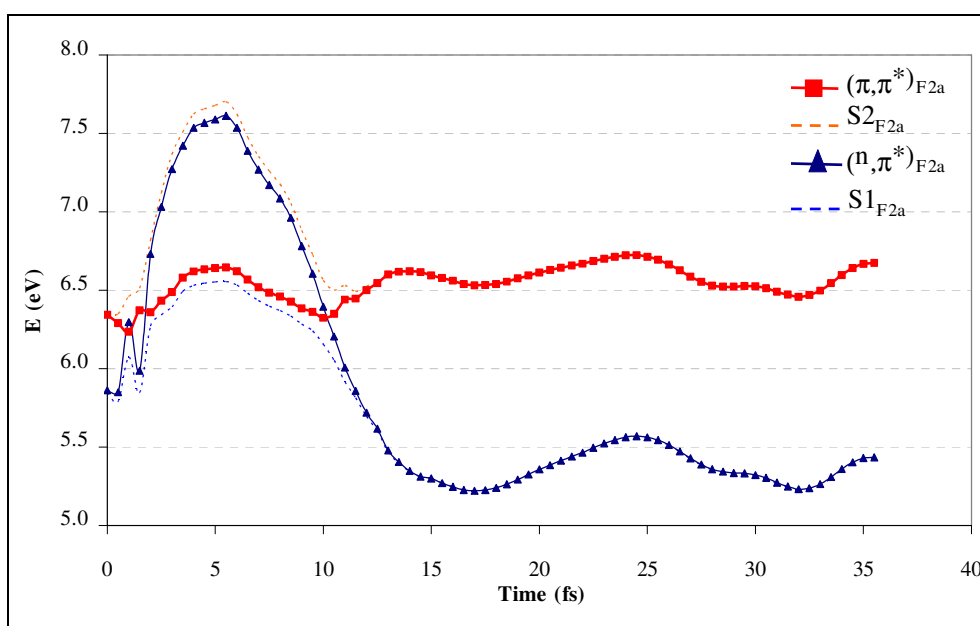


Figure SI-17b. Diabatic and adiabatic energies at the center of function F2a of run 3b.

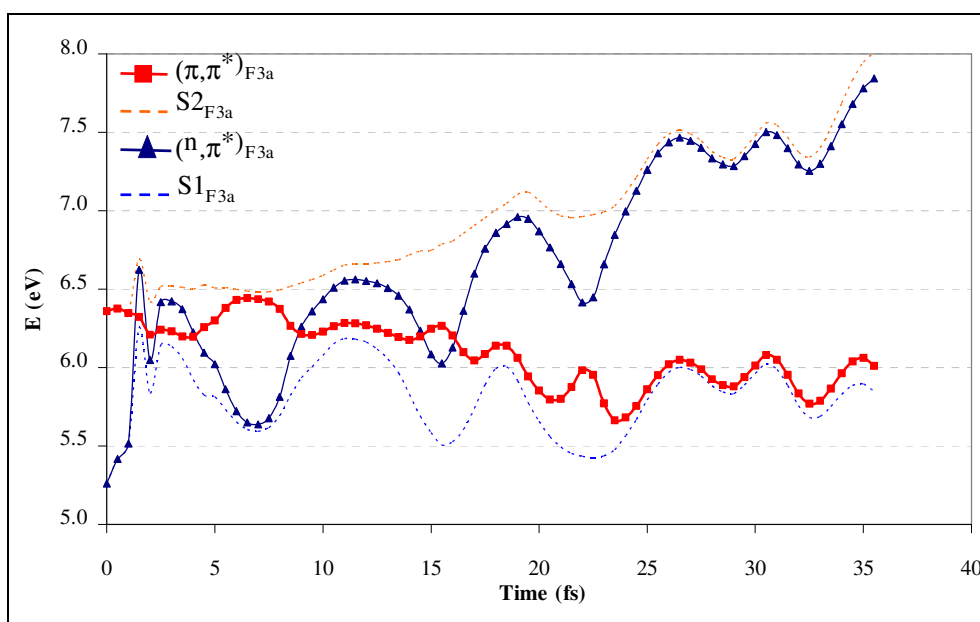


Figure SI-17c. Diabatic and adiabatic energies at the center of function F3a of run 3b.

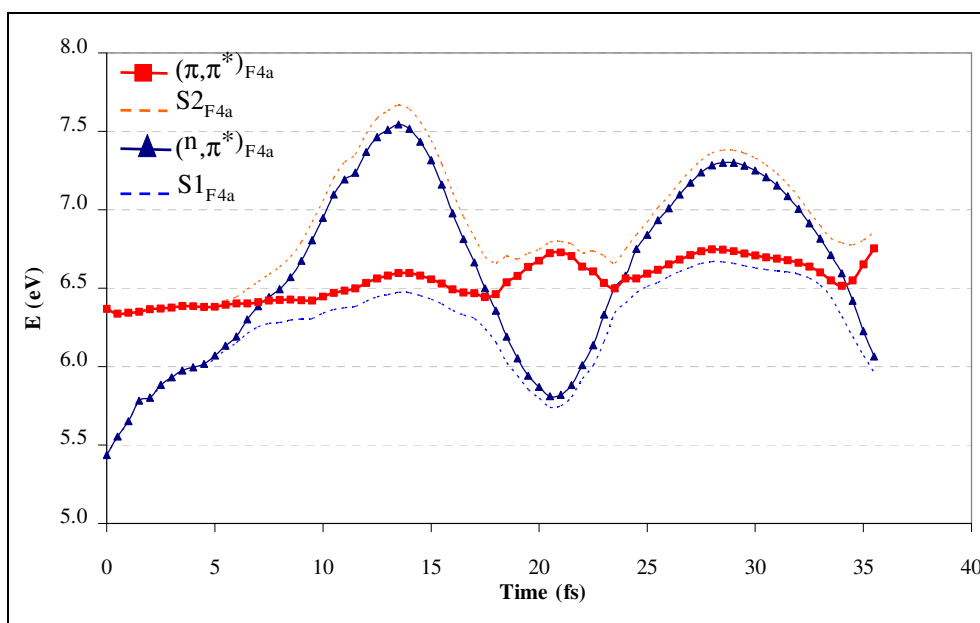


Figure SI-17d. Diabatic and adiabatic energies at the center of function F4a of run 3b.

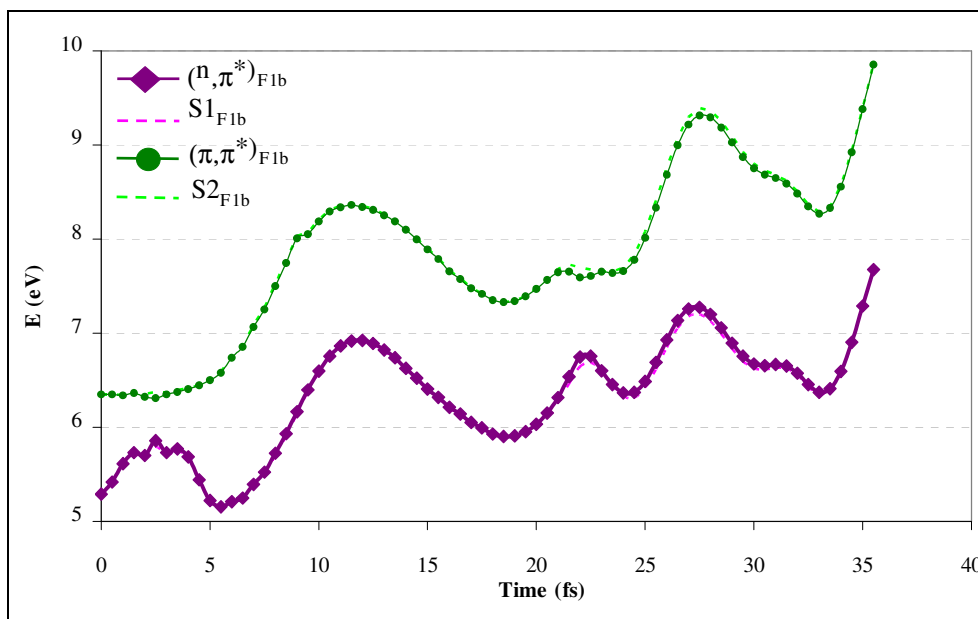


Figure SI-17e. Diabatic and adiabatic energies at the center of function F1b of run 3b.

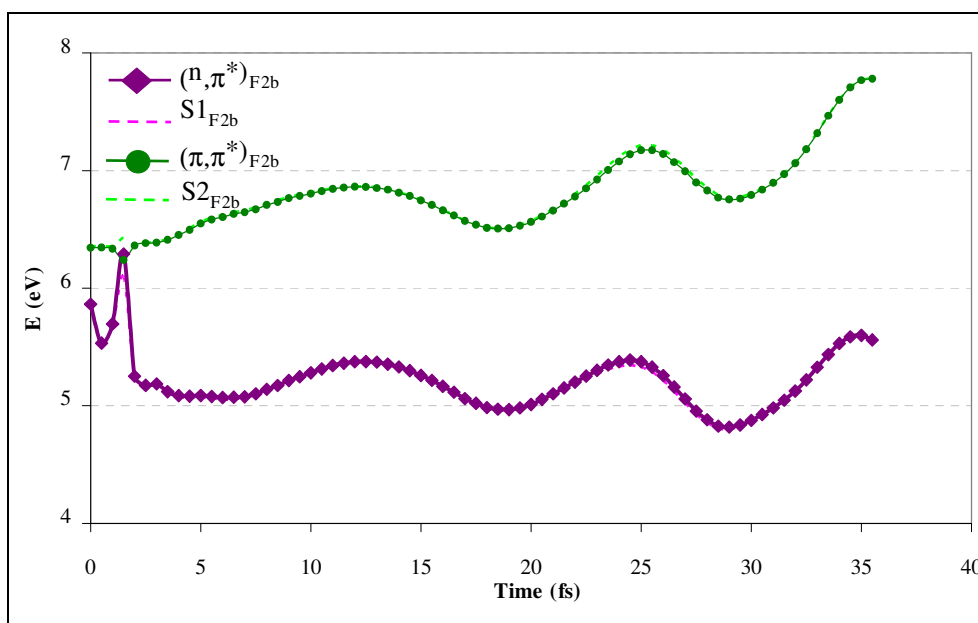


Figure SI-17f. Diabatic and adiabatic energies at the center of function F2b of run 3b.

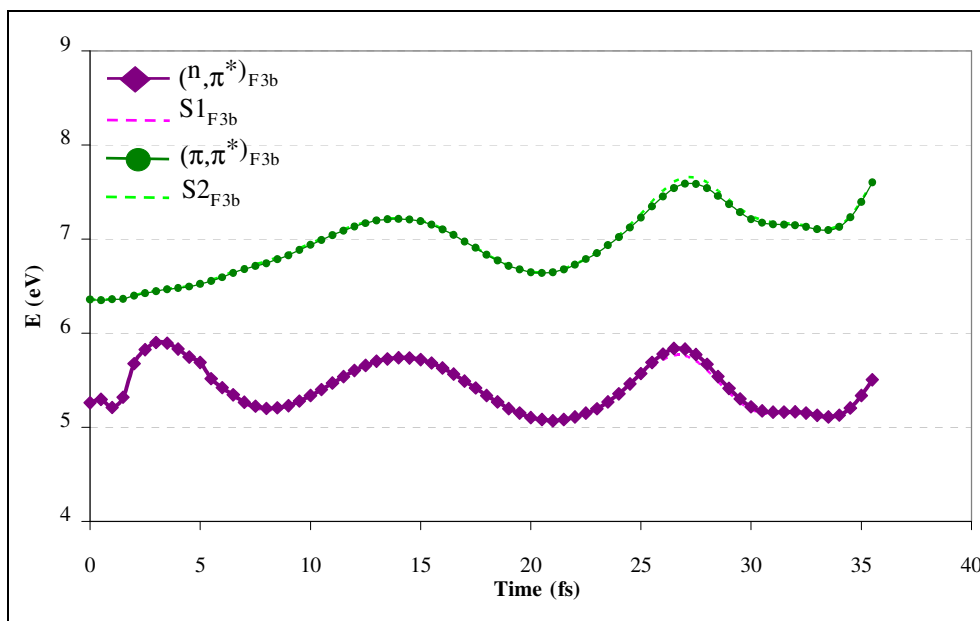


Figure SI-17g. Diabatic and adiabatic energies at the center of function F3b of run 3b.

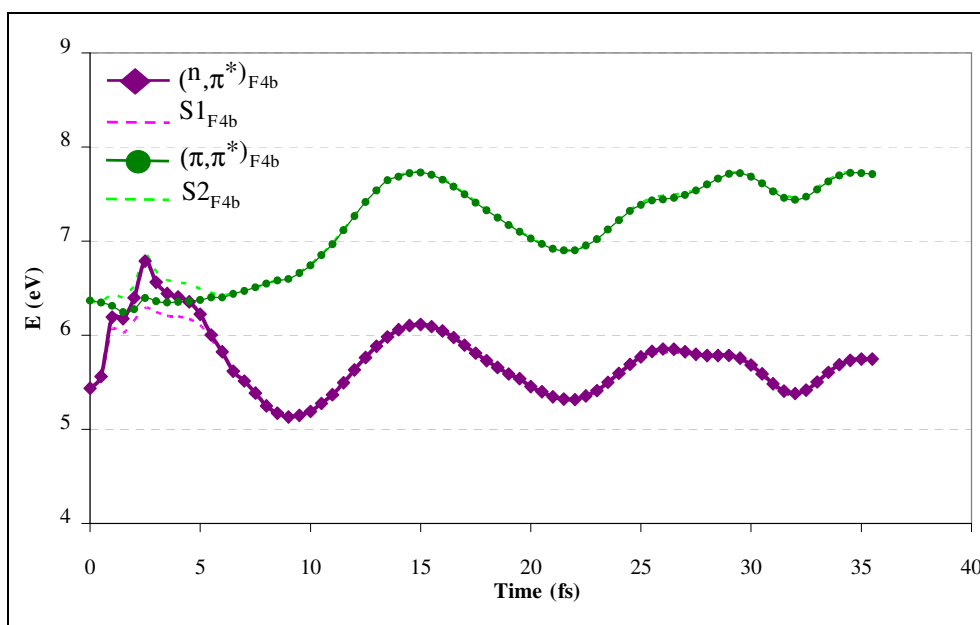


Figure SI-17h. Diabatic and adiabatic energies at the center of function F4b of run 3b.

Cartesian Coordinates of structures

$(\pi, \pi^*/n, \pi^*)_X\text{-Cs}$

7	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.302709000
6	0.000000000	1.465361900	1.937465570
6	0.000000000	2.620541940	1.110255100
7	0.000000000	2.307922600	-0.348109220
6	0.000000000	1.131579260	-0.928101470
1	0.000000080	-0.920472000	1.844497450
6	0.000000120	1.506772450	3.409858360
8	0.000000080	3.768817100	1.394786130
1	0.000000080	3.110482740	-0.940283240
8	-0.000000090	0.819461510	-2.077281940
1	-0.000000080	-0.863508190	-0.513019530
1	0.873205760	0.992791980	3.830699200
1	0.000000200	2.530292160	3.752859730
1	-0.873205420	0.992791920	3.830699340

$(\pi, \pi^*/n, \pi^*)_X\text{-PT2-1}$

7	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.377437000
6	0.000000000	1.413634760	1.989083600
6	-0.001595800	2.485760800	1.175738810
7	-0.002224950	2.333692750	-0.252630070
6	-0.001534020	1.098659320	-0.855160710
1	0.001739070	-0.958137730	1.872139080
6	0.000522910	1.438897100	3.484213100
8	-0.003550930	3.810128580	1.517850830
1	-0.003287960	3.117075500	-0.846495390
8	-0.001404420	0.858871890	-2.023624320
1	0.001184130	-0.858859480	-0.484772780
1	0.872756770	0.921328230	3.888034570
1	-0.000814320	2.457628560	3.841088460
1	-0.871282550	0.919536450	3.888473460

$(\pi, \pi^*/n, \pi^*)_X$ -PT2-2

7	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.359190000
6	0.000000000	1.349341880	2.002504090
6	-0.431260620	2.364136720	1.226471580
7	-0.519532700	2.226813990	-0.144503450
6	-0.183869460	1.084568720	-0.827438790
1	-0.415441340	-0.877247430	1.825830010
6	0.361833280	1.456808140	3.448553170
8	-0.694023590	3.622875530	1.595869910
1	-0.774084150	3.026617120	-0.681394270
8	-0.113589100	0.994005340	-2.018635600
1	0.033535920	-0.868226200	-0.491204830
1	1.343834860	1.028307800	3.625912570
1	0.384708230	2.488853970	3.764237830
1	-0.338065860	0.930825910	4.094097480