Electronic Supplementary Information for:

Exploring the excited-state nonadiabatic effects in the semisaturated planar tetracoordinated carbon molecule C_7H_4

Chithra M J, Probal Nag, Sai Vamsi Krishna Isukapalli, and Sivaranjana Reddy Vennapusa*

School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Maruthamala PO, Vithura, Thiruvananthapuram 695551, India.
Email: siva@iisertvm.ac.in

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Table S1: Symmetry and harmonic frequency (ω) of the vibrational modes of C_7H_4 at B3LYP/6-311++G(d,p) level of theory.

No.(Sym.)	Freq (in cm^{-1})
ν_1 (A_2)	94.7224
ν_2 (B_1)	270.633
ν_3 (A_2)	330.7573
ν_4 (A_1)	469.7463
ν_5 (B_1)	525.6469
ν_6 (B_2)	553.6491
ν_7 (B_2)	615.8429
ν_8 (A_1)	645.2011
ν_9 (B_1)	783.8379
ν_{10} (B_2)	799.5259
ν_{11} (A_1)	836.9950
ν_{12} (B_2)	901.4518
ν_{13} (A_1)	917.5521
ν_{14} (A_2)	1008.0332
ν_{15} (A_1)	1155.5285
ν_{16} (B_1)	1158.9089
ν_{17} (A_2)	1241.0244
ν_{18} (A_1)	1287.1241
ν_{19} (B_2)	1310.9198
ν_{20} (B_2)	1467.2474
ν_{21} (A_1)	1485.3490
ν_{22} (A_1)	1717.8870
ν_{23} (B_2)	1728.9691
ν_{24} (B_2)	3054.5545
ν_{25} (A_1)	3059.9059
ν_{26} (A_2)	3085.1980
ν_{27} (B_1)	3102.6907

Table S2: Ground-state (S_0) equilibrium geometry of C_7H_4 optimized at B3LYP/6-311++G(d,p) level of theory.

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.000000	0.000000	1.021207
C	0.000000	1.104283	0.103105
C	-0.000000	-1.104283	0.103105
C	0.000000	0.787934	-1.364183
C	-0.000000	-0.787934	-1.364183
C	0.000000	-1.511469	1.369436
C	0.000000	1.511469	1.369436
H	-0.879753	1.208785	-1.856883
H	0.879753	1.208785	-1.856883
H	0.879753	-1.208785	-1.856883
H	-0.879753	-1.208785	-1.856883

Table S3: Linear intrastate coupling parameters (κ) (in eV) for the singlet electronic states of C_7H_4 obtained at (TD)ωB97XD/6-311++G(d,p) level of theory. Excitation strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in parenthesis.

a_1 mode (Freq, eV)	κ^{S_1}	κ^{S_2}	κ^{S_3}
ν_4 (0.0582)	-0.0745 (0.8183)	0.0223 (0.0731)	-0.1152 (1.9603)
ν_8 (0.0800)	-0.2542 (5.0466)	0.0637 (0.3168)	0.0204 (0.0325)
ν_{11} (0.1038)	-0.0040 (0.0008)	-0.0191 (0.0170)	0.0026 (0.0003)
ν_{13} (0.1138)	0.0183 (0.0129)	0.0085 (0.0028)	-0.0648 (0.1620)
ν_{15} (0.1433)	-0.5829 (8.2728)	-0.0452 (0.0497)	-0.3079 (2.3085)
ν_{18} (0.1596)	-0.0867 (0.1475)	-0.0098 (0.0019)	-0.0379 (0.0282)
ν_{21} (0.1842)	0.0288 (0.0122)	0.0109 (0.0018)	0.0245 (0.0089)
ν_{22} (0.2130)	-0.0287 (0.0091)	0.0165 (0.0030)	0.1672 (0.3083)
ν_{25} (0.3794)	0.0250 (0.0022)	0.0168 (0.0010)	-0.0041 (0.0001)

Table S4: Quadratic intrastate coupling parameters (γ) (in eV) for the singlet electronic states of C_7H_4 obtained at (TD)ωB97XD/6-311++G(d,p) level of theory.

a_1 mode (Freq, eV)	γ^{S_1}	γ^{S_2}	γ^{S_3}
ν_4 (0.0582)	-0.0387	0.0735	-0.0265
ν_8 (0.0800)	-0.1431	0.0904	-0.0417
ν_{11} (0.1038)	-0.0025	-0.0050	-0.0081
ν_{13} (0.1138)	-0.0001	0.0004	-0.0302
ν_{15} (0.1433)	0.0148	-0.0111	-0.0932
ν_{18} (0.1596)	-0.0117	0.0020	-0.0211
ν_{21} (0.1842)	-0.0008	0.0021	-0.0083
ν_{22} (0.2130)	-0.0891	0.0725	-0.0031
ν_{25} (0.3794)	-0.0092	-0.0010	-0.0015

Table S5: Linear interstate coupling parameters (λ) (in eV) computed along a_2 modes for singlet electronic states of C_7H_4 obtained at (TD)ωB97XD/6-311++G(d,p) level of theory. Excitation strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

a_2 mode (Freq, eV)	$\lambda_{S_1-S_3}$	$\lambda_{S_2-S_3}$
ν_1 (0.0117)	0.1443 (76.0236)	0.1137 (47.2600)
ν_3 (0.0410)	0.2055 (12.5575)	0.2049 (12.4839)
ν_{14} (0.1250)	0.0437 (0.0612)	0.0349 (0.0389)
ν_{17} (0.1539)	0.0640 (0.0864)	0.0450 (0.0427)
ν_{26} (0.3825)	0.0509 (0.0088)	0.0265 (0.0024)

Table S6: Linear interstate coupling parameters (λ) (in eV) computed along a_1 modes for the singlet electronic states of C_7H_4 obtained at (TD)ωB97XD/6-311++G(d,p) level of theory. Excitation strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

a_1 mode (Freq, eV)	$\lambda_{S_1-S_2}$
ν_4 (0.0582)	0.2340 (8.0826)
ν_8 (0.0800)	0.4439 (15.3924)
ν_{11} (0.1038)	0.0708 (0.2327)
ν_{13} (0.1138)	0.0592 (0.1355)
ν_{15} (0.1433)	0.5087 (6.3013)
ν_{18} (0.1596)	0.1755 (0.6043)
ν_{21} (0.1842)	0.0820 (0.0992)
ν_{22} (0.2130)	0.1578 (0.2743)
ν_{25} (0.3794)	0.0623 (0.0135)

Table S7: MCTDH details of normal modes combination, size of the primitive and single particle bases used in the S_1-S_2-S_3 vibronic dynamics of C_7H_4.

Normal modes	Primitive basis	SPF
(ν_1, ν_3, ν_4)	(8, 10, 9)	[9, 6, 10]
(ν_8, ν_{11}, ν_{13})	(9, 5, 6)	[9, 7, 6]
(ν_{14}, ν_{15}, ν_{17})	(6, 10, 6)	[12, 6, 11]
(ν_{18}, ν_{21}, ν_{22})	(6, 5, 6)	[6, 4, 7]
(ν_{25}, ν_{26})	(4, 5)	[4, 4, 4]

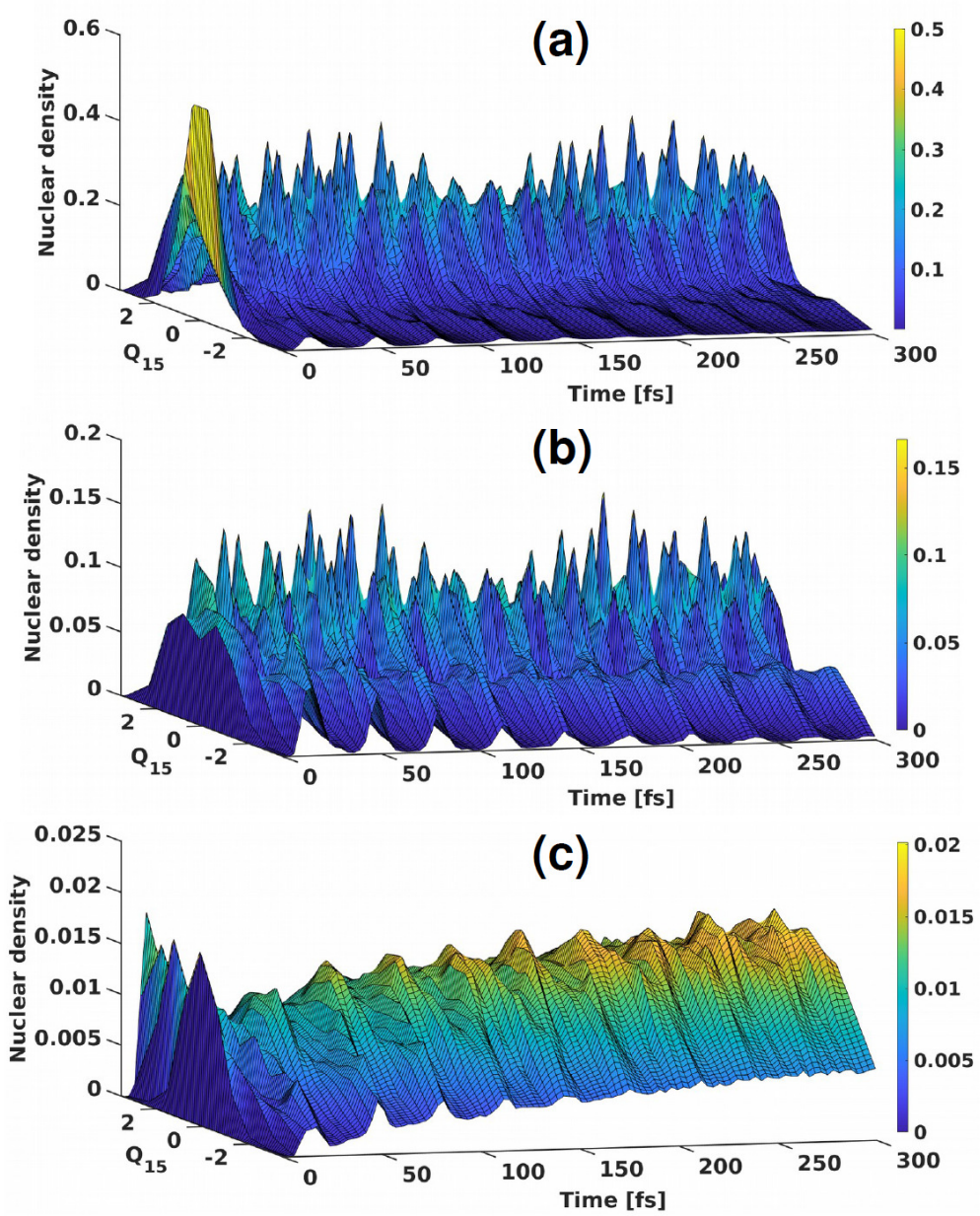

Figure S1: Nuclear densities variation of (a) S_1, (b) S_2 and (c) S_3 along Q_{15} of C_7H_4 obtained by propagating intital wavepacket on the S_1 state.