Supplementary Information: Carbon K-edge X-ray Emission Spectroscopy of Gas Phase Ethylenic Molecules

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1 Supplementary Information

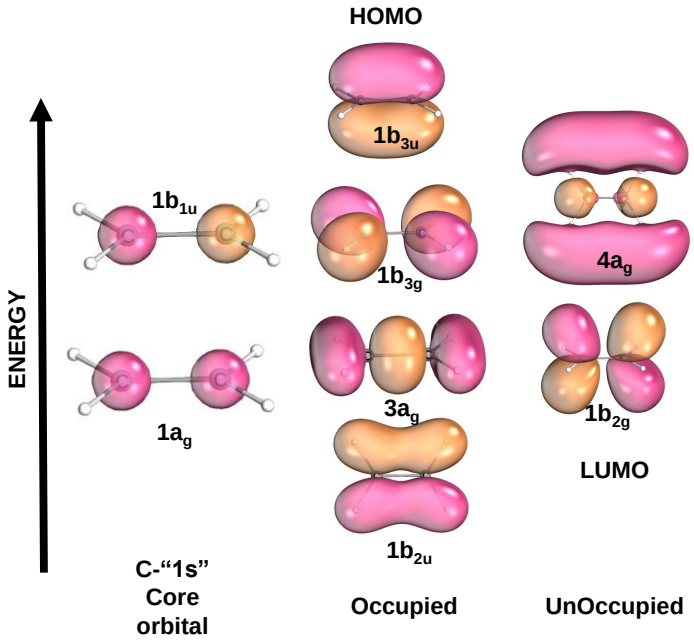

Figure S1: Kohn-Sham molecular orbitals of ethylene

Energy / eV	Oscillator Strength	Dominant Configuration
263.791	0.03393	HOMO-3($1b_{2u}$) $\rightarrow$ $1a_g$"1s"
264.638	0.04222	HOMO-2($3a_g$) $\rightarrow$ $1b_{1u}$"1s"
266.969	0.02475	HOMO-1($1b_{3g}$) $\rightarrow$ $1b_{1u}$"1s"
268.836	0.05458	HOMO($1b_{3u}$) $\rightarrow$ $1a_g$"1s"

Table S1: Calculated NXES energies and oscillator strengths for ethylene. The energies reported in this table are uncorrected with respect to the experimental values.

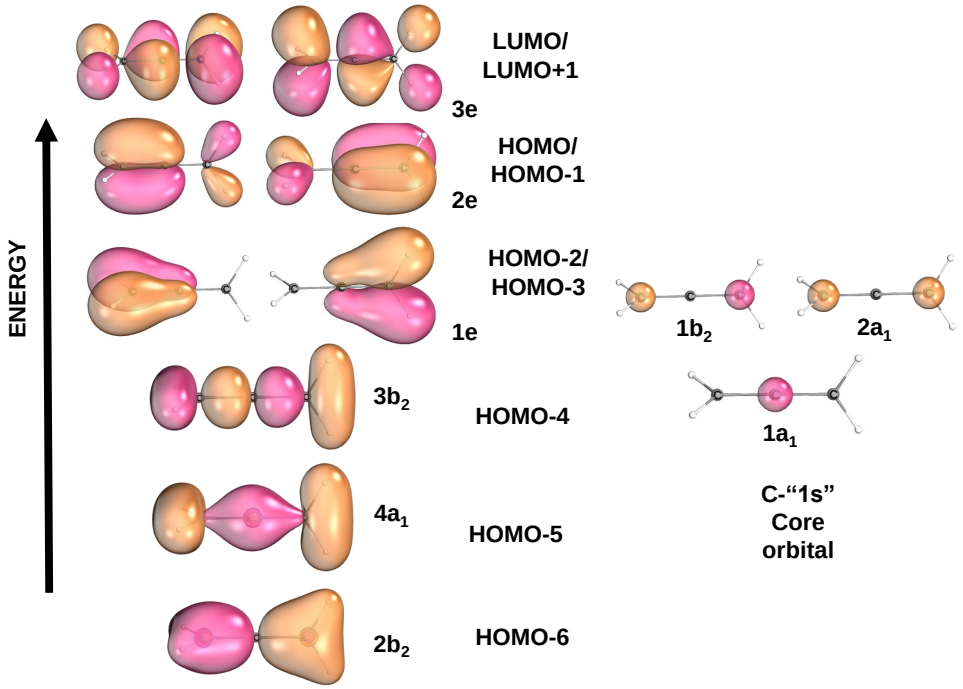

Figure S2: Kohn-Sham molecular orbitals of allene

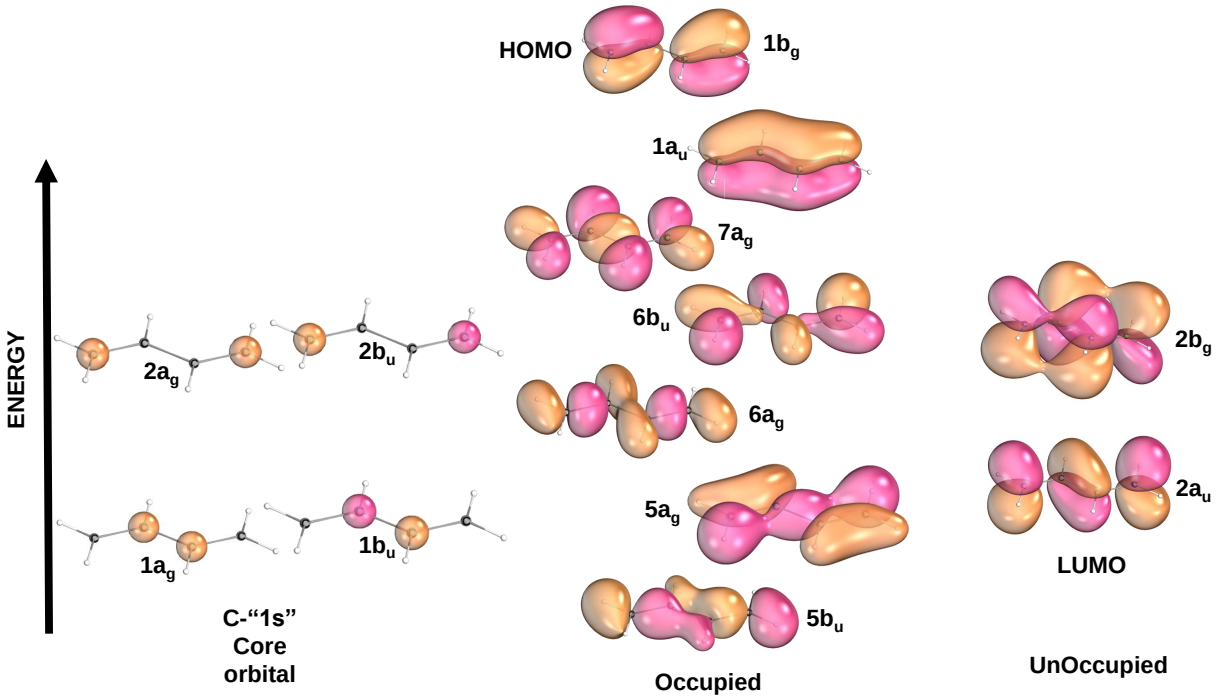

Figure S3: Kohn-Sham molecular orbitals of butadiene

Energy / eV	Oscillator Strength	Dominant Configuration
264.56	0.036	HOMO-2(1e) $\rightarrow$ 2a$_1$"1s"
264.59	0.033	HOMO-3(1e) $\rightarrow$ 1b$_2$"1s"
264.817	0.01507	HOMO-4(3b$_2$) $\rightarrow$ 1a$_1$"1s"
265.368	0.00558	HOMO-2(1e) $\rightarrow$ 1a$_1$"1s"
265.400	0.00604	HOMO-3(1e) $\rightarrow$ 1a$_1$"1s"
269.022	0.01796	HOMO-1(2e) $\rightarrow$ 1b$_2$"1s"
269.343	0.04048	HOMO(2e) $\rightarrow$ 1b$_2$"1s"
269.826	0.02350	HOMO-1(2e) $\rightarrow$ 1a$_1$"1s"

Table S2: Calculated NXES energies and oscillator strengths for allene. The energies reported in this table are uncorrected with respect to the experimental values.

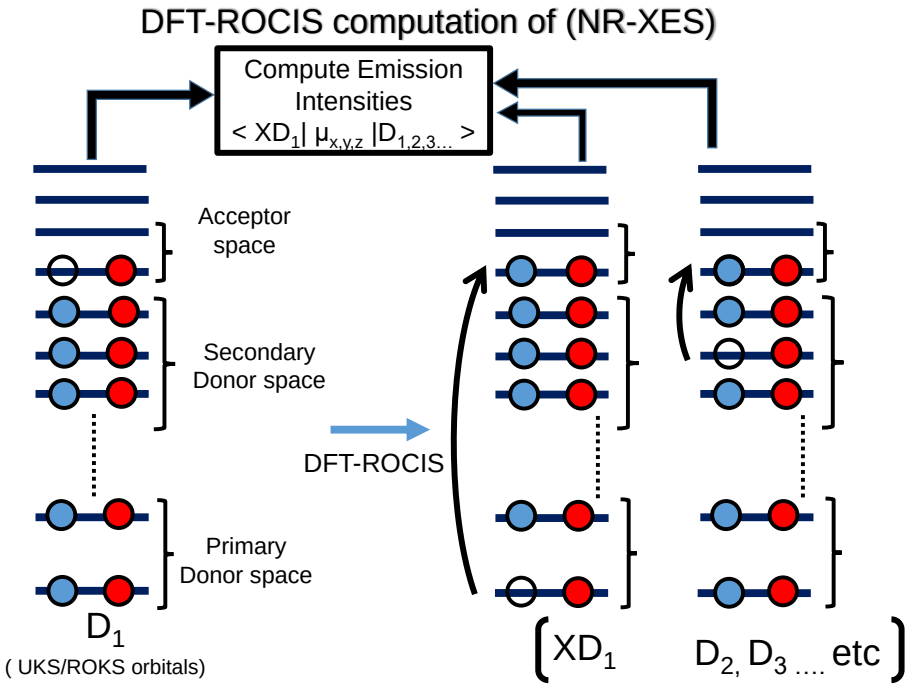

Figure S4: Computation of NXES spectra using ROCIS in ORCA.

Energy / eV	Oscillator Strength	Dominant Configuration
262.938	0.02437	HOMO-6($5b_u$)→$1a_g$"$1s$"(0.7)+HOMO-6($5b_u$)→$2a_g$"$1s$"(0.1)
264.648	0.03340	HOMO-4($6a_g$)→$2b_u$"$1s$"(0.6)+HOMO-4($6a_g$)→$1b_u$"$1s$"(0.2)
265.158	0.02106	HOMO-3($6b_u$)→$2a_g$"$1s$"(0.7)+HOMO-3($6b_u$)→$1a_g$"$1s$"(0.1)
265.848	0.03007	HOMO-4($6a_g$)→$1b_u$"$1s$"(0.7)+HOMO-4($6a_g$)→ $2b_u$"$1s$"(0.2)
266.209	0.00813	HOMO-1($1a_u$)→$2b_u$"$1s$"(0.6)+ HOMO-1($1a_u$)→$1b_u$"$1s$"(0.2)
266.319	0.00612	HOMO-3($6b_u$)→$1a_g$"$1s$"(0.8)+ HOMO-3($6b_u$)→$2a_g$"$1s$"(0.1)
267.371	0.01632	HOMO-1($1a_u$)→$1a_g$"$1s$"(0.8) + HOMO-1($1a_u$)→$1a_g$"$1s$"(0.1)
267.407	0.02185	HOMO-2($7a_g$)→$1b_u$"$1s$"(0.7) + HOMO($1b_g$)→$2b_u$"$1s$"(0.2)
268.327	0.04155	HOMO($1b_g$)→$2b_u$"$1s$"(0.6)+HOMO($1b_g$)→$1b_u$"$1s$"(0.2)
269.527	0.01675	HOMO($1b_g$)→$1b_u$"$1s$"(0.7)+HOMO($1b_g$)→$2b_u$"$1s$"(0.2)

Table S3: Calculated NXES energies and oscillator strengths for butadiene. The energies reported in this table are uncorrected with respect to the experimental values.

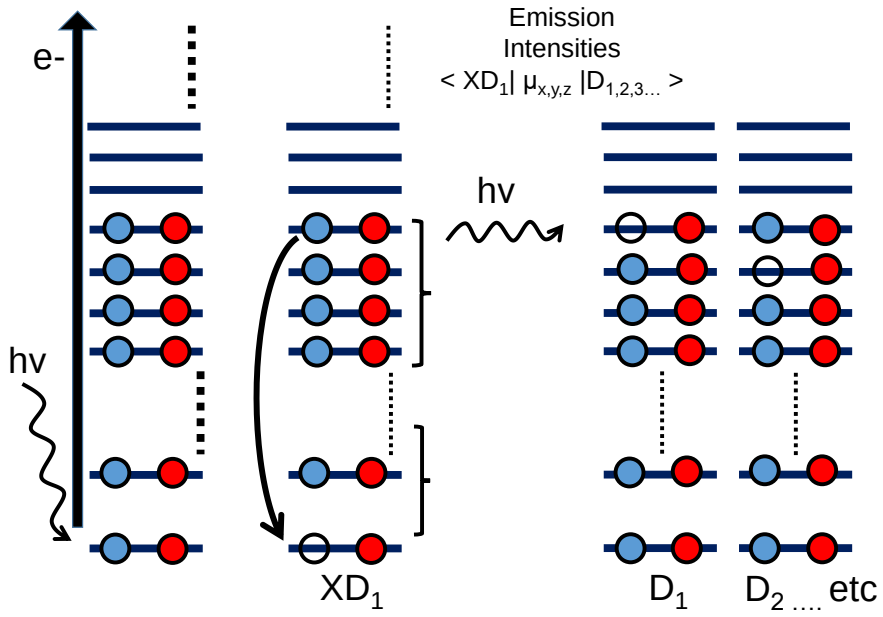

Figure S5: Electronic states involved in NXES process and the corresponding emission intensities underlying the NXES spectra.XD_1 signifies the core-ionized doublet state and D_i are valence-ionized doublet states. D_1 is the reference state in the ROCIS calculations.