Supplementary Information
Isomer-specific photofragmentation of $C_3H_3^+$ at the carbon K-edge

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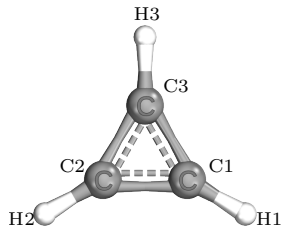
1 Geometry-optimized ground states

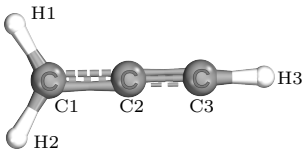
1.1 c-$C_3H_3^+$ symmetry: D_{3h}



Bond	Length [Å]
C1-C2	1.345
C2-C3	1.345
C1-C3	1.345
C1-H1	1.070
C2-H2	1.070
C3-H3	1.070

Start-Vertex-End	Angle [°]
C1-C2-C3	60.0
C2-C1-C3	60.0
C1-C3-C2	60.0
C2-C1-H1	150.0
C3-C1-H1	150.0
C1-C2-H2	150.0
C3-C2-H2	150.0
C1-C3-H3	150.0
C2-C3-H3	150.0

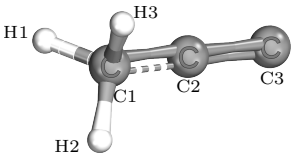
1.2 $[H_2C-C-CH]^+$ symmetry: C_{2v}



Bond	Length [Å]
C1-C2	1.339
C2-C3	1.206
C1-H1	1.078
C1-H2	1.078
C3-H3	1.065

Start-Vertex-End	Angle [°]
C1-C2-C3	180.0
C2-C3-H3	180.0
C2-C1-H1	120.4
C2-C1-H2	120.4
H1-C1-H2	119.1

1.3 $[H_3C-C-C]^+$ symmetry: C_{3v}



Bond	Length [Å]
C1-C2	1.436
C2-C3	1.332
C1-H1	1.088
C1-H2	1.088
C1-H3	1.088

Start-Vertex-End	Angle [°]
C1-C2-C3	180.0
C2-C1-H1	108.8
C2-C1-H2	108.8
C2-C1-H3	108.8
H1-C1-H2	110.2
H1-C1-H3	110.2
H2-C1-H3	110.2

2 Calculated spectra using the BLYP and PBE functionals

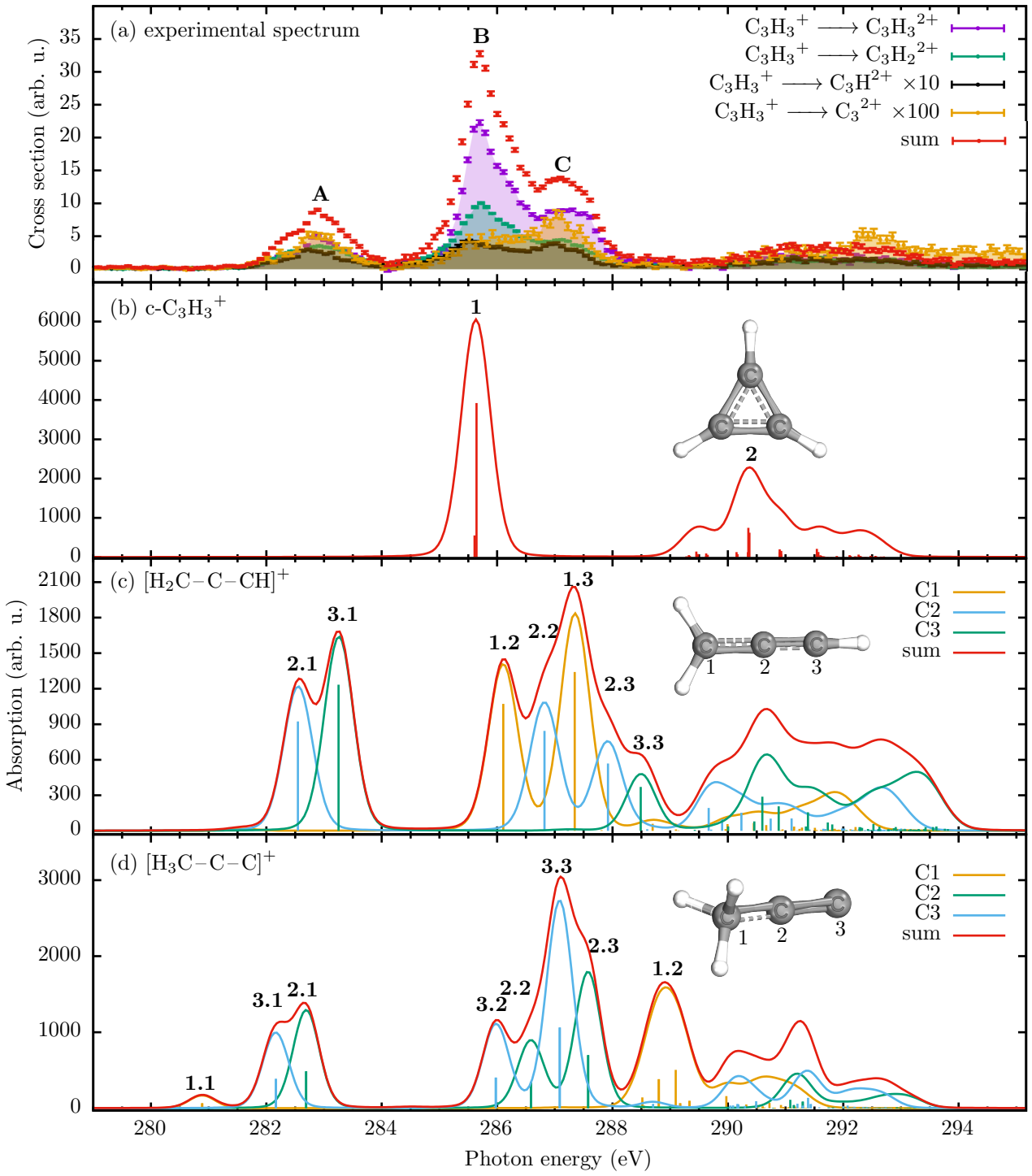


Figure 1: The effect of a particular functional on the calculated spectra is illustrated by a new calculation with BLYP. The differences in the spectra caused by the various functionals are only small.

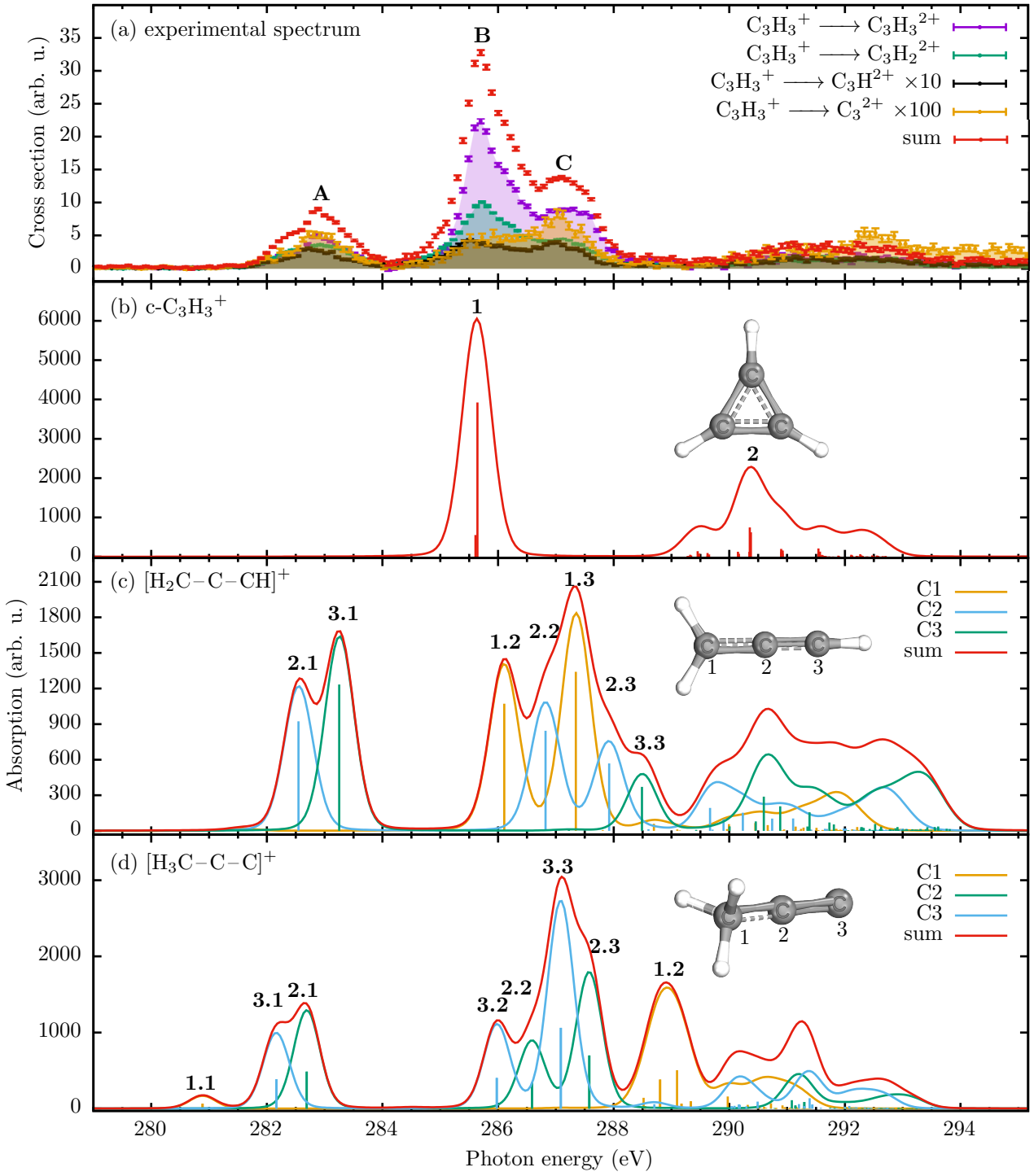


Figure 2: The calculated spectra using the PBE functional. As already mentioned in the caption of the Fig. 1, the differences are only small.