Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Exciton Energy Transfer Reveals Spectral Signatures of Excited States in Clusters

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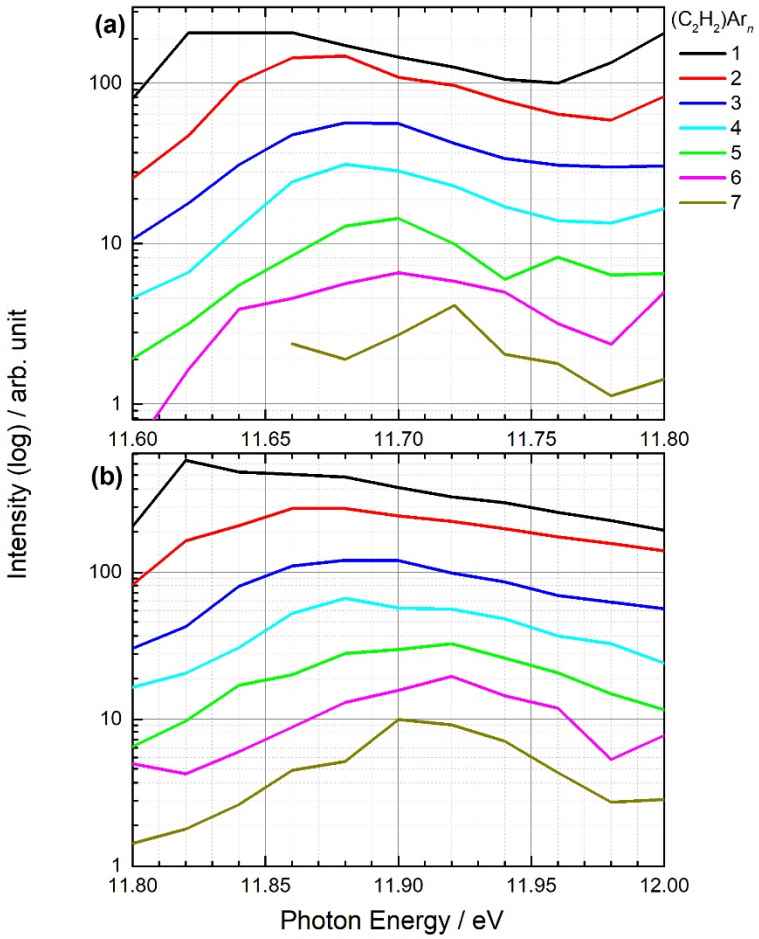

Figure S1. Expanded photoionization efficiency curves for $(C_2H_2)Ar_n$ (n = 1 – 7) depicted in Fig. 2 of main text: (a) spectra between 11.60 – 11.80 eV, and (b) spectra between 11.80 – 12.00 eV.

Coordinates of the geometries in Fig. 7:

$(C_2H_2)Ar$
C1 -2.596194 -0.468266 0.000033
H2 -3.067761 -1.420452 -0.000049
C3 -2.067401 0.602130 -0.000044
H4 -1.596807 1.554718 0.000116
Ar5 1.813674 -0.052080 0.000000

$(C_2H_2)Ar_2$
C1 0.600644 2.619164 0.057027
H2 1.658143 2.616756 0.160363
C3 -0.587807 2.620512 -0.057060
H4 -1.645305 2.620665 -0.160399
Ar5 -2.060145 -1.014501 0.012650
Ar6 2.055152 -1.023025 -0.012637

$(C_2H_2)Ar_3$
C1 -0.833965 0.415760 2.534267
H2 -1.882983 0.319255 2.396189
C3 0.345173 0.523833 2.687045
H4 1.394689 0.619798 2.821671
Ar5 2.423735 -0.542838 -0.463053
Ar6 -1.498250 -1.949199 -0.520534
Ar7 -0.735427 2.126670 -1.046731

$(C_2H_2)Ar_4$
C1 0.226808 -0.888878 2.397483
H2 0.610877 -1.877053 2.328243
C3 -0.203418 0.222262 2.472523
H4 -0.587625 1.210705 2.536843
Ar5 -0.027046 2.203708 -0.918630
Ar6 3.358335 0.041260 0.186712
Ar7 0.019574 -1.942718 -1.350765
Ar8 -3.359951 -0.043026 0.189065

$(H_2O)_3Ar$
O1 1.237562 1.519909 0.474701
H2 2.030597 2.013855 0.679077
H3 1.319657 0.676523 0.951082
O4 1.135135 -0.292275 -1.628190
H5 0.281239 -0.301536 -2.059505
H6 1.161532 0.538246 -1.122846
O7 1.331284 -1.218978 0.984125
H8 1.247366 -1.191576 0.015432
H9 2.133260 -1.709654 1.159374
Ar10 -2.100306 -0.005284 0.096239

$(H_2O)_3Ar_2$
O1 0.578920 -1.372874 -1.304660
H2 0.604361 -2.216920 -1.753602
H3 1.506403 -1.122132 -1.156371
O4 0.643877 -1.173210 1.466094
H5 0.097999 -0.459059 1.793567
H6 0.338585 -1.336842 0.557496
O7 2.924074 -0.596874 -0.014356
H8 2.306758 -0.706012 0.729366
H9 3.656440 -1.183361 0.170963
Ar10 0.457430 2.150508 -0.090348
Ar11 -2.773292 -0.363397 0.006012

$(H_2O)_3Ar_3$
O1 1.395100 2.117394 -0.550050
H2 1.817121 2.964066 -0.409719
H3 0.475140 2.315973 -0.793084
O4 0.013719 0.819747 1.483477
H5 0.106272 -0.131449 1.439017
H6 0.734602 1.176590 0.937085
O7 -1.392266 2.116228 -0.529300
H8 -1.178330 1.594256 0.263286
H9 -1.947738 2.832746 -0.225011
Ar10 0.001092 -1.104094 -1.667950
Ar11 3.315476 -0.871340 0.713682
Ar12 -3.324317 -0.867851 0.707346

$(H_2O)_3Ar_4$
O1 1.375951 -2.804620 -0.316057
H2 1.805510 -3.509518 -0.799012
H3 0.458207 -3.095343 -0.181453
O4 -0.025389 -0.788789 -1.622112
H5 0.053371 0.057499 -1.182867
H6 0.701878 -1.331755 -1.273424
O7 -1.411575 -2.822029 -0.339056
H8 -1.203647 -2.014214 -0.839857
H9 -1.957825 -3.351881 -0.918211
Ar10 -0.001292 -0.384117 2.053209
Ar11 3.292257 0.431816 -0.228981
Ar12 -3.294602 0.491989 -0.216280
Ar13 0.038671 3.047462 -0.307247