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

Electronic Supplementary Information

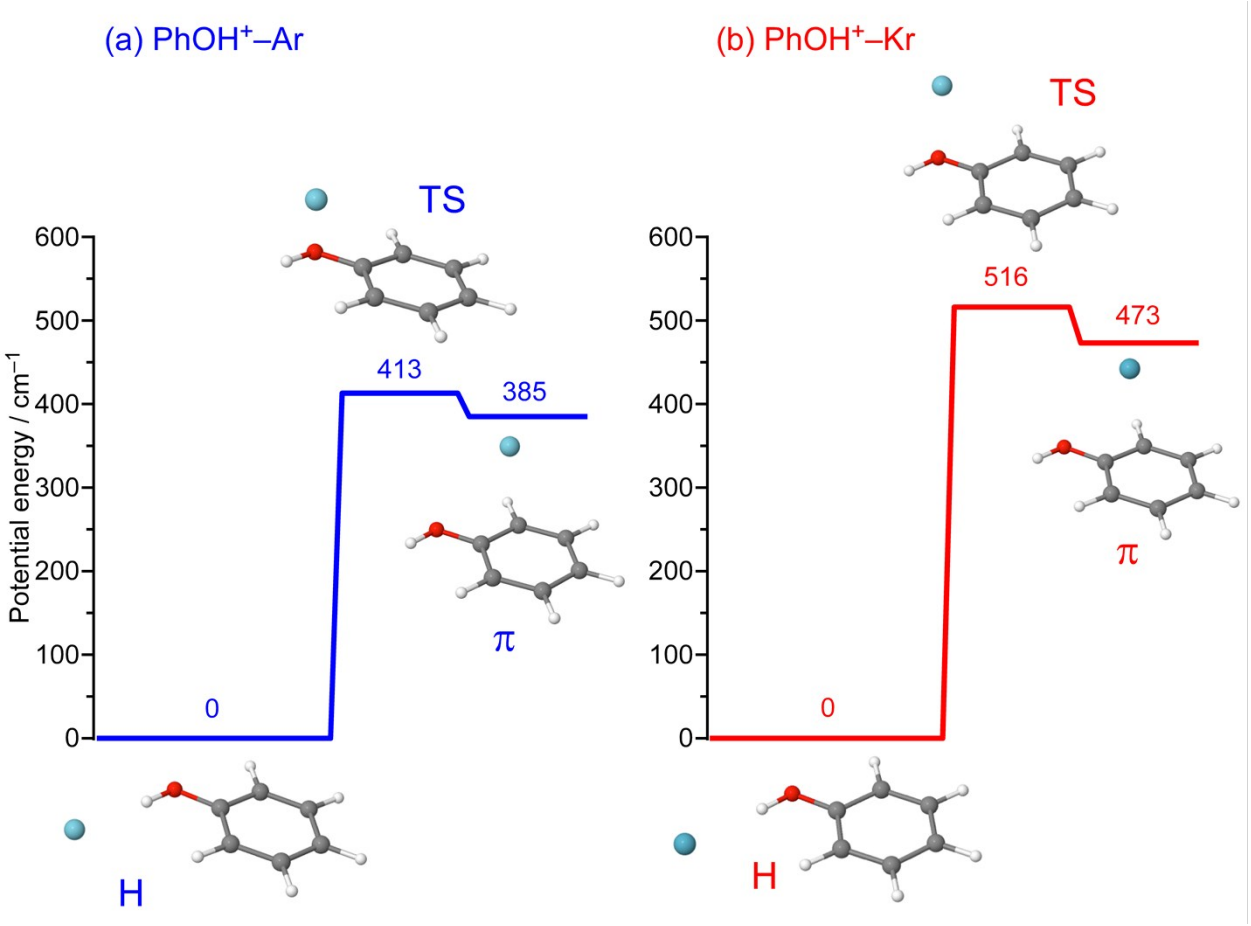

Figure S1 Potential energy diagrams of (a) $PhOH^+$–Ar and (b) $PhOH^+$–Kr calculated at the B3LYP-D3/aug-cc-pVTZ level of theory. Energies are not corrected for zero-point energies and basis set super position errors.

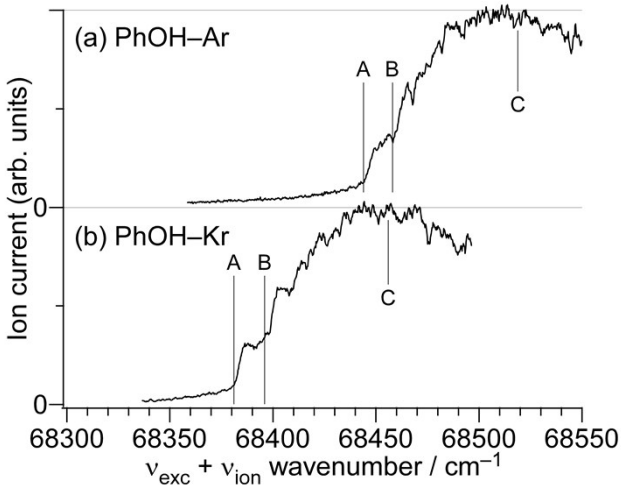

Figure S2 Photoionization efficiency curves of PhOH–Ar and PhOH–Kr clusters used for estimation of the amount of the direct ionization components measured by nanosecond lasers. Lines labeled A, B, and C show positions at which ionization efficiencies are evaluated; A: direct ionization to the H-bound isomer, B: vibrational ground level of the π-bound isomer, and C: the excess energy used in the time-resolved measurements, respectively.