Electronic Supplementary Information
Soft X-ray absorption spectroscopy of Ar_2 and ArNe dimers and small Ar clusters.

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The computational packages and techniques used to calculated the data shown here are based on those described in [1–4]

References

[1] J. Wenzel, M. Wormit and A. Dreuw, *Journal of Computational Chemistry*, 2014, **35**, 1900–1915.

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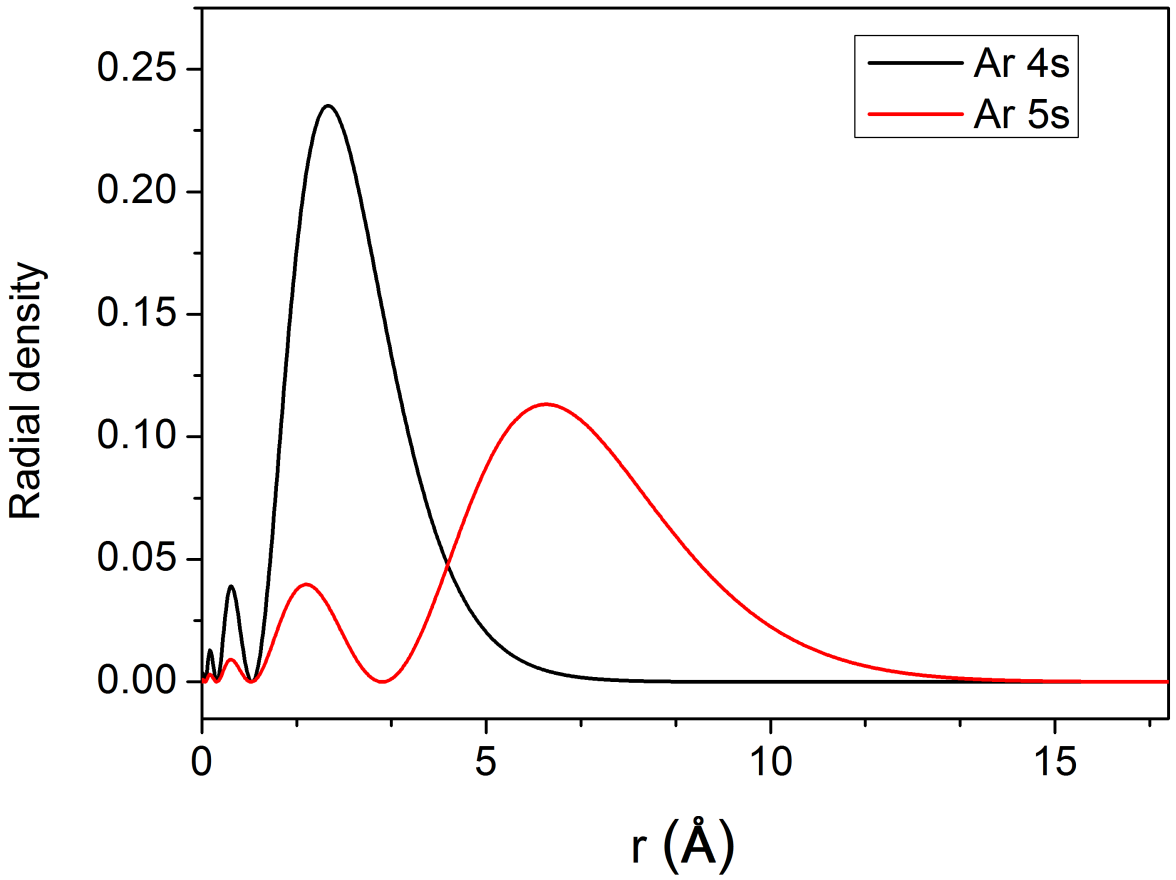

Figure S1: Radial densities of the natural atomic 4s and 5s orbitals of Ar.

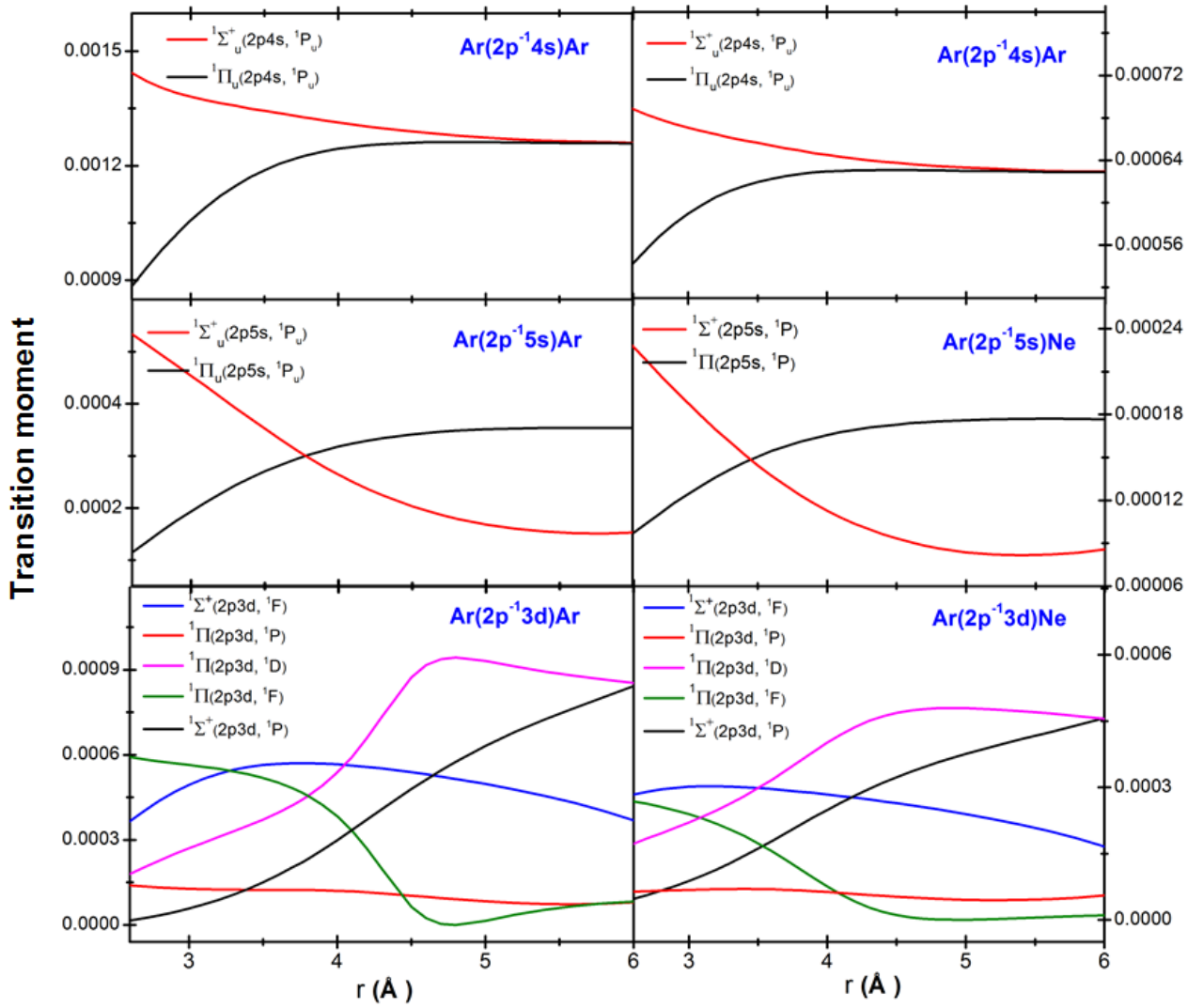

Figure S2: The transition moments as a function of the internuclear distance for transition from the ground state to the core excited states shown in Figure 5 of the main text.