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Photoelectron spectroscopy as a structural probe of intermediate size clusters LEEOR KRONIK, OLGA GULIAMOV, Weizmann Institute of Science, KOBLAR A. JACKSON, Central Michigan University — We examine the utility of photoelectron spectroscopy (PES) as a structural probe of Si_n^- in the n = 20 – 26 size range by determining isomers and associated photoelectron spectra from first principles calculations. Across the entire size range, we consistently obtain good agreement between theory and experiment [Hoffmann et al., *Eur. Phys. J. D* **16**, 9 (2001)]. We find that PES can almost invariably distinguish between structurally distinct isomers at a given cluster size, but that structurally similar isomers usually cannot be reliably distinguished by PES. For many, but not all, sizes the isomer giving the best match to experiment is the lowest-energy one found theoretically. Thus, combining theory with PES experiments emerges as a useful source of structural information even for intermediate size clusters.

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