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On the nature of the oligoacene ground state JOHANNES HACHMANN, JONATHAN DORANDO, Cornell University, MICHAEL AVILES, Arcadia University, GARNET KIN-LIC CHAN, Cornell University — The nature of the oligoacene ground state - its spin, singlet-triplet gap, and diradical character as a function of chain-length - is a question of ongoing theoretical and experimental interest with notable technological implications. Previous computational studies have given inconclusive answers to this challenging electronic structure problem (see e.g. [1]). In the present study we exploit the capabilities of the local *ab initio* Density Matrix Renormalization Group (DMRG) [2], which allows the numerically exact (FCI) solution of the Schrödinger equation in a chosen 1-particle basis and active space for quasi-one-dimensional systems. We compute the singlet-triplet gap from first principles as a function of system length ranging from naphthalene to tetradecacene, correlating the full π -space (i.e. up to 58 electrons in 58 orbitals) and converging the results to a few μE_h accuracy [3]. In order to study the diradical nature of the oligoacene ground state we calculate expectation values over different diradical occupation and pair-correlation operators. Furthermore we study the natural orbitals and their occupation. [1] Bendikov, Duong, Starkey, Houk, Carter, Wudl, *JACS* 126 (2004), 7416. [2] Hachmann, Cardoen, Chan, *JCP* 125 (2006), 144101. [3] Hachmann, Dorando, Avilés, Chan, *in preparation*.

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