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Spin multiplicity and symmetry breaking in vanadium-benzene complexes[1] IVAN STICH, LUCIA HORVATHOVA, MATUS DUBECKY, Institute of Physics, Slovak Academy of Sciences, LUBOS MITAS, Dept. of Physics, North Carolina State University — Despite use of vanadium-benzene complexes in spintronics applications [1], reliable theoretical and experimental knowledge of energetics, dissociation energy, spin multiplicity, etc. of these systems is missing. Fixed-node DMC calculations have been done with the quest to elucidate electronic and atomic structure of vanadium-benzene half-sandwiches. At variance with DFT results which favor either low- or high-spin state, depending on the functional used [2], DMC predicts degenerate energies for spin multiplicities 2, 4, and 6, irrespective of DFT functional used to fix the nodal hypersurfaces. Ultimately, we predict high-spin ground-state, based on comparison of experimental/theory ionization energy [3]. Based again on DMC, we predict vastly different gaps for spin-up/-down electrons. The DMC results indicate that both DFT [2] as well as experimental results [4] may be biased. [1] V. V. Maslyuk *et al.*, Phys. Rev. Lett. **97**, 097201 (2006) [2] R. Pandey, B. K. Rao, P. Jena, M. A. Blanco, J. Am. Chem. Soc. **123**, 3799 (2001) [3] T. Kurikawa, *et al.*, Organomentallics **18**, 1430 (1999). [4] R. L. Hettich, T. C. Jackson, E. M. Stanko, B. S. Freiser, J. Am. Chem. Soc. **108**, 5086 (1986).

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