Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hyperfine coupling of endohedral fullerene Sc@C82 SEUNG MI LEE, Department of Materials, University of Oxford, UK, B.J. HERBERT, J.C. GREEN, Inorganic Chemistry Laboratory, University of Oxford, UK, D. NGUYEN-MANH, UKAEA Culham Division, Culham Science Center, UK, A. ARDAVAN, Clarendon Laboratory, University of Oxford, UK, J. VAN TOL, NHMFL, Tallahassee, Florida 32310, USA, A.P. HORSFIELD, Department of Physics and Astronomy, University of London, UK, G.W. MORLEY, K. PORFYRAKIS, D.G. PETTIFOR, G.A.D. BRIGGS, Department of Materials, University of Oxford, UK — The hyperfine coupling of the endohedral metallofullerene, Sc@C_{82}, which is a candidate qubit for quantum computing, has been investigated theoretically and experimentally. Using density functional theory (DFT), we have systematically studied the molecular structures and energetics of nine isomers of $C_{82}$and Sc@C_{82} fullerenes. DFT predicts that the most stable isomer has C_{2v} symmetry with the Sc atom lying off-centre along the C_2 symmetry axis and forming partially covalent bonds with a carbon hexagonal ring of the fullerene cage. The hyperfine couplings between the unpaired electron spin and the Sc and C atoms have been calculated and compared to the electron spin resonance (ESR) spectra. The experimental isotropic hyperfine coupling constants confirm the C_{2v} symmetry predicted for the ground state isomer. Furthermore, the calculated anisotropy of the hyperfine coupling tensor is in good agreement with low temperature experimental measurements. www.nanotech.org

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Date submitted: 22 Dec 2004 Electronic form version 1.4