An *ab initio* Hartree-Fock Investigation of Endohedral Sc@C_{82}

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Z. Naturforsch. **53 a,** 801–805 (1998); received June 12, 1998

The electronic structure of endohedral Sc@C_{82} with a C_{82} cage of C_{2v} symmetry has been studied by *ab initio* Hartree-Fock (HF) calculations. The optimized position of Sc in the configuration of minimum energy is predicted to be on the two-fold axis of the fullerene cage. In the corresponding configuration Sc is above the center of a hexagon of site symmetry C_2. This structure of C_{2v} symmetry is nearly degenerate with C_s and C_1 structures with Sc slightly displaced from the center of the coordinated hexagon. The binding energy of the endohedral complex is larger than 3.55 eV. The *ab initio* HF data of the C_{2v} topoisomer of the fullerene unit are compared with new experimental findings and HF results derived for the 3(C_2) topoisomer of the C_{82} cage.

Key words: Endohedral Fullerenes; Electronic Structure; *ab initio* Calculations.

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