Appendix A – N@PCBM

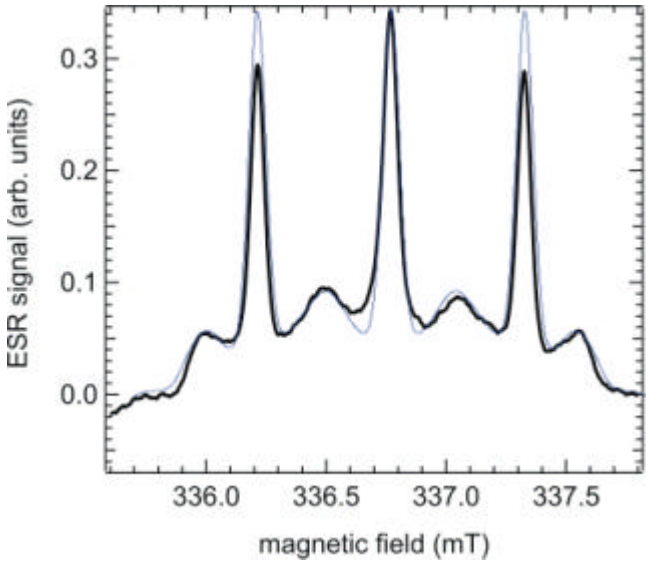

Fig. A.1: The N@PCBM spectrum (black) is compared to a simulated powder pattern (blue) using an axial deformation and a smaller non axial term.

The powder spectrum of the [5,6] derivate of N@PCBM is shown in Fig. A.1 (black line). The synthesis of the material has been done by J.C. Hummelen (University of Groningen). It has been measured with a Miniscope 100 (Magnettech) with microwave power of P = 3.5 mW and modulation amplitude of 20 µT. The simulation (blue line) reveals an axial deformation of the fullerene cage D = 260 µT with a much smaller non–axial contribution E = 20 µT. As expected, this is in the same order of magnitude as for the other known mono–adduct (D = 215 µT, E = 15 µT).

In some organic solar cells PCBM is used as electron acceptor. However, it also limits the electron transport properties of the solar cell. As this has an influence on the efficiency of the cell one would like to monitor the charge propagation. Our aim is to use N@PCBM as tracer molecule for the electron transport.

If a charge is located on an endohedral fullerene, the nitrogen signal vanishes completely due to the strong interaction [1]. Some more information, e.g. how many electrons reside on the fullerene, can be gained, if the spectrum of the spin on the outside of the fullerene is monitored. However, in solar cells the [6,6] PCBM derivate is used and it remains to be shown that this exists as endohedral fullerene.

[1] P. Jakes, B. Goedde, M. Waiblinger, N. Weiden, K.-P. Dinse, A. Weidinger, *Electronic Properties of Novel Materials – Progress in Molecular Nanostructures*, eds. H. Kuzmany, J. Fink, M. Mehring, S. Roth, *AIP Conf. Proc.* **544**, 174 (2000)