



Experiment title: High-resolution powder diffraction of a homologous series of mono-acid odd-numbered triacylglycerols.

Experiment number:  
CH-617

Beamline: BM16	Date of experiment: from: 11 April 1999 7:00 to: 13 April 1999 7:00	Date of report: 18 August 1999
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### Report:

In this session a series of  $\beta$ -C<sub>n</sub>C<sub>n</sub>C<sub>n</sub> (n = odd) triacylglycerols was measured for determination of cell parameters only (see proposal). Again, the expected cell parameters of these long-chain compounds were based upon crystallographic data of other triacylglycerols. A combination of one long (ranging from ? to ? Å) and one short cell axis (~5.5 Å) was expected and huge cell volumes. The powder diffraction patterns of C<sub>13</sub>C<sub>13</sub>C<sub>13</sub>, C<sub>15</sub>C<sub>15</sub>C<sub>15</sub>, C<sub>17</sub>C<sub>17</sub>C<sub>17</sub> and C<sub>19</sub>C<sub>19</sub>C<sub>19</sub> were measured. From these patterns the cell parameters could be determined. From C<sub>13</sub>C<sub>13</sub>C<sub>13</sub> it was possible to solve the structure, but refinement is still not completed. With this data obtained at ESRF it must be possible to make a predictive structural model for all series members.

Since the sample of  $\beta$ -LOL (melting point ~15° C) was molten in the last session we decided to try it again in this session. Now, we succeeded in measuring the  $\beta$  polymorph of LOL and determined the cell parameters.

For structure determination three undoped poly(phenylene vinylene) compounds were measured. The patterns of these long-chain organic molecules were indexed, but no structures are solved yet.