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320. CALCULATIONS OF NLO-PROPERTIES OF DONOR-ACCEPTOR DIPHENYL-SILANES
Paul F. van Hutten, George G. Malliaras, Diny Hissett, Georges Hadziioannou,
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Highly polar molecules in a polymer matrix are suitable for second harmonics
generation devices since they orient on high voltage poling above Tg. Silicon-based
donor-acceptor (DA-) compounds have potential since they are transparent in the
visible spectrum, and have large dipoles and moderate values of the first
hyperpolarizability \( \beta \). Our study (synthesis, optical characterization and calculations)
focusses on DA-diphenyl-disilanes, and their incorporation into polymer. The quantum
chemical calculations (semi-empirical and \textit{ab initio}, finite-field and sum-over-states
(SOS)), are compared mutually and with experimental results. The SOS method yields
useful predictions for \( \beta \). Acceptors containing the sulfonyl group prove to be efficient
and retain transparency for the DA-compound. Charge distributions of ground and
excited states show that the silicon chain is a charge buffer and a weak transmitter.

321. SYNTHESIS AND PROPERTIES OF 2ND-ORDER NLO-ACTIVE POLYSTYRENE AND AMYLOSE
BASED MATERIALS.
J.B.E. Hals, P.L. Ferling, M.A. Schoonderbor, A.J. Schouten
P.T.A. Klaes, TNO-Research, P.O. Box 8031, 2500 JA Delft, The Netherlands.
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Second order non-linear optical effects might lead to novel applications as integrated electro-optic devices.
Polymers functionalised with NLO-active groups seem to have good properties for these applications. We have
synthesized a polystyrene based NLO-material that can be poled by corona discharge or contact poling to give a very
good ordering (\( \theta = 0.45 \)). The \( \Delta n \) which directly after poling was 12.9 pm/V. The bleaching of the material gives
the possibility to make channel waveguides by using the material as UV-light through photoreceptors. Another way
to order macroscopic systems is the Langmuir-Blodgett (LB) technique. We have synthesized an amylase derivative
with covalently bound NLO-active groups. This material forms stable monolayers.

322. SECOND HARMONIC GENERATION FROM LB FILMS OF POLY(ISOCYANIDE).
Marcel N. Teerenstra and Arend Jan Schouten,
Univ. Groningen, Nijenborgh 4, 9747 AG Groningen (The Netherlands)

In this study poly(isocyanides) are used for Langmuir-Blodgett film formation. These rigid and helical polymers can
be obtained either racemate or optical pure. The polymers which contain aromatic-based side groups with a di-
alkylamine end group do not form stable layers. However mixing these polymers with amylase-sulfonate derivatives
resulted in stable transferrable films. Up to at least 100 layers could be deposited, \( \gamma \)-type, with constant transfer ratio.
Thicknesses and refractive indices were measured by means of ellipsometry. The monolayer thickness showed to
scale linearly with the base mole fraction poly(isocyanide) in the mixed film. Second Harmonic Generation (SHG)
from multilayers was measured and the second harmonics signal showed higher in case of the polymer obtained from
polymerization of a chiral isocyanide.

323. Silicon-Based Donor-Acceptor Compounds in a Polymer
Matrix. Diny Hisset, Henk J. Bolink, Jan-Willem Eshuis, George G. Malliaras
and Georges Hadziioannou, Department of Polymer Chemistry, University of
Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

For many applications involving nonlinear optical phenomena (e.g. frequency
doubling) transparency in the visible spectrum is a requirement. We have