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320. CALCULATIONS OF NLO-PROPERTIES OF DONOR-ACCEPTOR DIPHENYLSILANES
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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)
focuses on DA-diphenyldisilanes, 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.
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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 \( r_{33} \) value directly after poling was 12.9 pm/V. The bleachability of the material gives
the possibility to make channel waveguides by exposing the material to UV-light through photomasks. Another way
to order macroscopic systems is the Langmuir-Blodgett (LB) technique. We have synthesized an amylose derivative
with covalently bound NLO-active groups. This material forms stable monolayers.

322. SECOND HARMONIC GENERATION FROM LB FILMS OF POLY(ISOCYANIDE).
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In this study poly(isocyanides) are used for Langmuir-Blodgett film formation. These rigid and helical polymers can
be obtained either racemic or optical pure. The polymers which contain arachidamino based side groups with a di-
aminostyrene end group do not form stable layers. However mixing these polymers with amylose-ester derivatives
resulted in stable transferable films. Up to at least 100 layers could be deposited, \( Y \)-type, with constant transfer ratios.
Thicknesses and refractive indices were measured by means of ellipsometry. The multilayer thickness showed to
scale linearly with the base mole fraction poly(isocyanide) in the mixed films. Second Harmonic Generation (SHG)
from multi-layers was measured and the second harmonic 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 Hissink, 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