## Appendices

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APPENDIX A

Instrumentation for Characterization of New Materials

Melting temperatures of solids were determined using capillary melting point apparatus (Superfit, India); values reported are uncorrected. Infra red spectra were recorded on a Jasco5300 FTIR spectrometer. All the spectra were calibrated against polystyrene absorption at 1601 cm$^{-1}$. Solid samples were recorded as KBr pellets. Electronic absorption (UV-Vis) spectra were recorded on a Shimadzu UV 3101 PC spectrophotometer. Specular reflectance (8° incidence) or diffuse reflectance spectra of solid pellets were recorded on the same spectrometer using the integrating sphere (ISR 3100) attachment. Circular dichroism spectra were recorded on a Jasco Spectropolarimeter Model J-810. $^1$H and $^{13}$C NMR spectra were recorded on Bruker AC200 NMR spectrometer. $^1$H NMR (200 MHz) spectra were measured with TMS ($\delta = 0$) as internal standard. $^{13}$C NMR (50 MHz) spectra were recorded using the solvent peaks as the internal standard. Elemental analysis was carried out on a Perkin Elmer Model - 2400 CHNS/O, AD2B or 240 CHN analyzer. Sartorius BP211D balance was used for high precision weighing.

Morphology of films coated on glass/aluminum foil substrates using a photoresist spinner was examined using a Philips XL 30 ESEM Scanning Electron Microscope. Gold coating was provided on the films prior to examination. X-ray photoelectron spectroscopy was carried out on a Kratos Axis 165 Spectrometer with a Mg K$_\alpha$ x-ray source (1253.6 eV). The x-ray power supply was run at 15 kV and 5 mA. The pressure in the analysis chamber during the scans was $\sim 10^{-9}$ Torr. The peak positions are based on calibration with respect to the C1s peak at 284.6 eV.
APPENDIX B

X-ray Crystallography

X-ray diffraction data were collected on an Enraf-Nonius MACH3 diffractometer. MoKα radiation (λ = 0.71073 Å) with a graphite crystal monochromator in the incident beam. Standard CAD4 centering, indexing and data collection programs were used. The general routine used for the data collection is as follows; minor variations in settings were done in specific cases. The unit cell dimensions were obtained by a least square fit of 24 centered reflections in the neighborhood of θ = 10°. Intensity data were collected using the ω scan method at a scan speed of 4.12°/min to a maximum 20 of 50°. The scan width A0, for each reflection was 0.80 + 0.35 tanθ. During data collection the intensities of three standard reflections were monitored every 1.5 hour of x-ray exposure. In all the cases we have studied, no decay was observed. In addition three orientation standards were monitored every 250 reflections to check the effects of crystal movement. Data was reduced using Xtal 3.4; Lorentz and polarization corrections were included. All non-hydrogen atoms were found using the direct method analysis in SHELX-97 and after several cycles of refinement the positions of the hydrogen atoms were calculated and added to the refinement process. Empirical absorption correction was applied in the relevant cases, using ψ scan data. Refinement proceeded to convergence by minimizing the function \( \sum w (F_o^2 - F_c^2) \). A final difference Fourier synthesis map showed the largest difference peak and hole to be acceptably small. The R indices were calculated as \( R = \frac{\sum |(F_o - |F_c|)|}{\sum |F_o|} \) and \( wR^2 = \left[ \frac{\sum w (F_o^2 - F_c^2)^2}{\sum (F_o^2)^2} \right]^{1/2} \). Graphics were handled using ORTEX6a and Platon.4

Table B.1 lists the space groups and REFCODE (Cambridge Crystallographic Database) or deposition number from Cambridge Crystallographic Data Centre for the new crystal structures presented in this thesis. The fractional atomic coordinates (x 104) and isotropic displacement parameters, \( U_{eq} (A^2 \times 10^{3}) \) are provided in Tables B.2-B.11. \( U_{eq} \) is defined as one third of the trace of the orthogonal \( U_{ij} \) tensor. Estimated standard deviations (e.s.d) are given in paranthesis.
Appendix

References


Table B.1  Space groups and the REFCODE / deposition number from CSD and the reference in the thesis.

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| H(6)  | $-2755$ | $4127$ | $3466$ | $45$ |
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**Compound 19 H₂O**
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Appendix
APPENDIX C

Powder Second Harmonic Generation Measurement

We have measured the second harmonic generation from microcrystalline powders of compounds 11(TPA) (Sec. 3.2) and 19.H₂O (Sec. 3.3) using the Kurtz and Perry¹ method with minor modifications of the original layout. Particle sizes were graded using standard sieves; sizes ranging from 50 - 420 um were studied. Samples were loaded in glass capillaries having an inner diameter of 600 um. Fundamental beam (1064 nm) of a Q-switched ns-pulsed (6 ns, 10 pps) Nd:YAG laser (Spectra Physics, Model INDI 40) was used. The beam was split and approximately 10% was passed through a 200 um thick powder sample of N-4-nitrophenyl-(S)-prolinol, NPP (average particle size ~ 175 µm) to monitor pulse to pulse fluctuation of the beam. The main beam was split further into two halves and focused onto the sample from opposite directions. The scattered SHG signal was collected using a concave mirror and lens combination with a 45° disposition to the incident beams (Fig. C.1). The second harmonic signal from reference and the sample were collected using appropriate optics and detected using a monochromator (Jobin-Yvon Model HRS–2), PMT (Hamamatsu, Model C956-06/131) and oscilloscope (Tektronix, Model TDS 210, 60MHz). Calibrated neutral density filters were used when needed, so that the signal measured on the oscilloscope was in the same range for all samples and the reference; this ensures that readings are taken in a linear region of the PMT. Microcrystalline urea having particle sizes 150 - 350 um was used as the reference in all SHG measurements. The measured SHG signal from the sample is first corrected for the background noise and the fluctuation in reference before comparing with similarly corrected signal of the standard, urea. Measurements for the sample and the standard were carried out for different particle sizes. Our setup is calibrated by measurements on urea and NPP. The SHG measured for NPP is 138 U (1U = SHG of urea) at saturation. The errors in the measurements are ~ 10 - 15 %.

The compounds we have studied showed good stability under laser irradiation and no sign of decomposition was detected, even on continuous irradiation with a laser power of 1GW cm⁻². Each measurement was repeated at least three times over a period of time and the value of SHG reported is the average of such measurements. In all cases we have
studied, the SHG saturated at higher particle sizes, indicating phase matchable behavior of the materials.

Figure C.1 Setup for measurements of SHG from microcrystalline powders.

Reference

APPENDIX D

Powder and Thin Film Conductivity Measurements

The 2-probe powder conductivity measurements on PANI-PSS (Sec. 4.2) as well as the polyanion salts of TTF (Sec. 4.3) were carried out using the pressed pellet technique in a home-built stainless steel cell’ based on a modification of the apparatus described by Wudl and Bryce.\textsuperscript{2} 4-probe measurements of the PANI-PSS films (Sec 4.2) were carried out on 15-layer films coated on glass. Samples were mounted on a Perspex platform; electrical connections were made either through equally spaced thin wire press contacts or sublimed aluminum strips. In the case of the (TTF)\textsubscript{3}(PMC)\textsubscript{2} single crystals, contacts were established by attaching thin wires with conducting silver paint. All conductivity measurements were carried out at room temperature. A Keithly Model 224 Constant Current Source and Keithly Model 175 Multimeter were used. Typically, currents in the range 1 - 4 mA were employed where Ohmic behavior was observed.

References