

**A New Nonlinear Optical Stilbazolium Family Crystal of (E)-1-ethyl-2-(4-nitrostyryl)
pyridin-1-ium iodide: Synthesis, Crystal Structure and its Third-Order**

Nonlinear Optical Properties

Nivetha Karuppanan^a, Sivaperuman Kalainathan^{a,*}

^{a,a,*}Centre for Crystal Growth, Vellore Institute of Technology, Vellore,

Tamil Nadu 632014, India

Corresponding author: Phone: +91-416-2202350

E-mail Id: kalainathan@yahoo.com

Supporting Figures

Figure S1. FTIR spectrum of NSPI

Figure S2. ¹H NMR spectrum of NSPI

Figure S3. ¹³C NMR spectrum of NSPI

Supporting Table

Table S1. Selected bond lengths (Å) and bond angles (°) for NSPI crystal

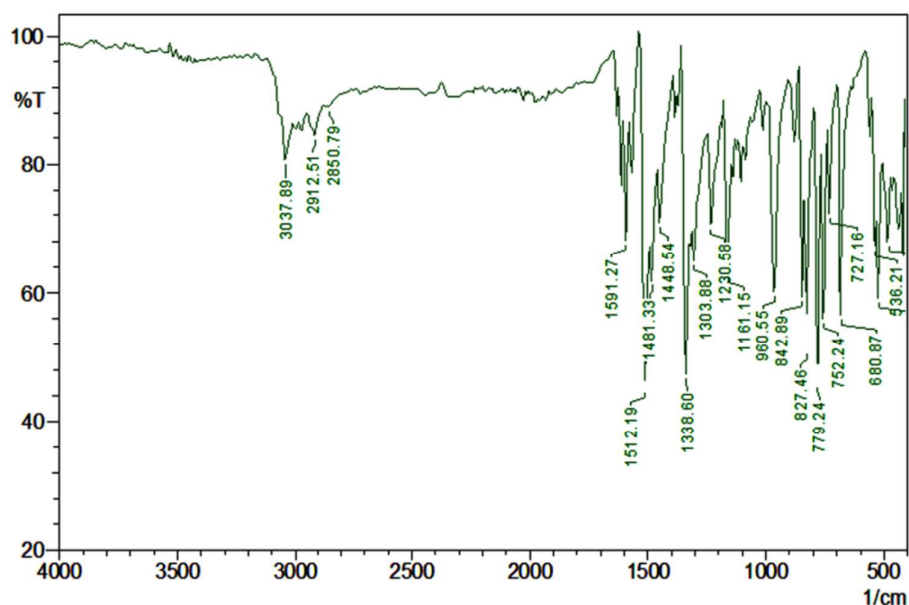


Figure S1. FTIR spectrum of NSPI

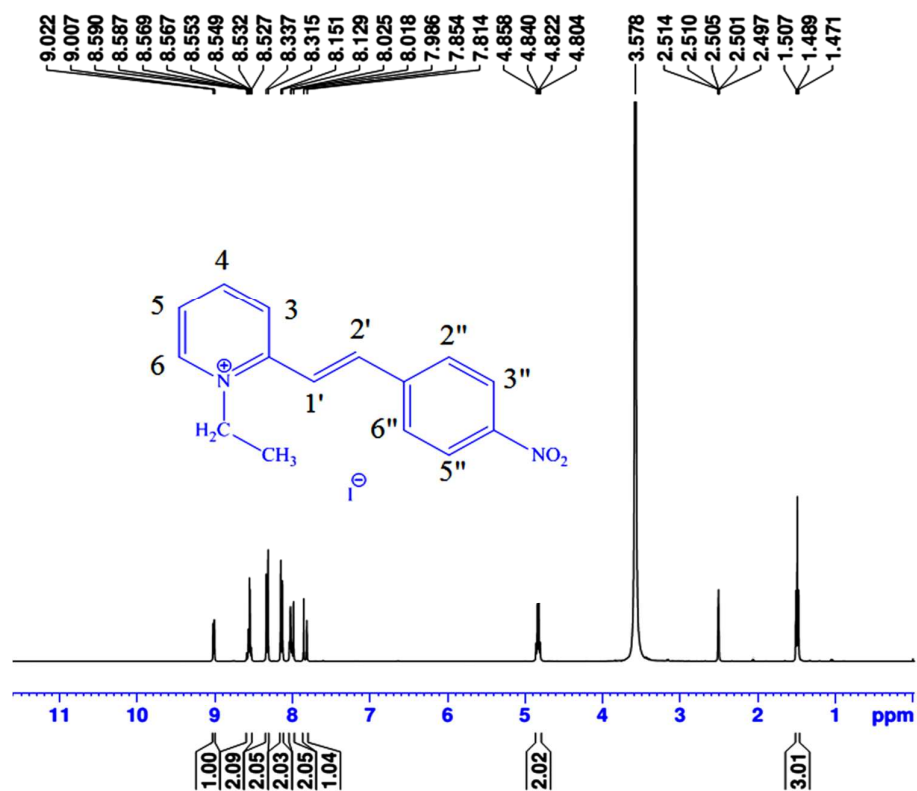


Figure S2. ¹H NMR spectrum of NSPI

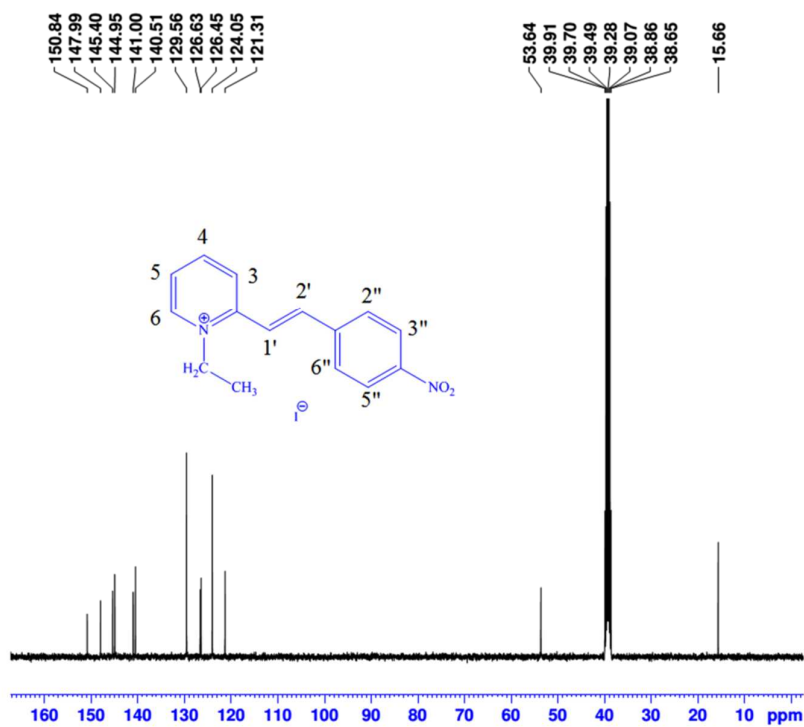


Figure S3. ¹³C NMR spectrum of NSPI

Table S1. Selected bond lengths (Å) and bond angles (°) for the NSPI crystal

Atoms	Lengths	Atoms	Angles
O1-N1	1.223(4)	O1-N1-O2	123.7(3)
N1-C1	1.472(3)	O1-N1-C1	118.0(3)
C4-C7	1.472(4)	C4-C7-C8	123.2(3)
C8-C9	1.460(4)	C7-C8-C9	124.3(3)
O2-N1	1.221(4)	N2-C9-C8	118.5(3)
C5-H3	0.950	N2-C9-C10	118.0(2)
C9-C10	1.394(4)	C7-C8-C9	124.3(3)
N2-C14	1.491(4)	C8-C9-C10	123.5(3)
C11-C12	1.386(5)	C11-C12-C13	118.7(3)
N2-C9	1.376(4)	N2-C13-C12	121.2(3)
C1-C6	1.386(4)	N2-C14-C15	112.3(2)
C12-C13	1.374(4)	C4-C7-H5	113
C7-H5	1.024	C4-C7-C8-C9	178.5(3)
C8-H6	0.834	O1-N1 -C1-C2	-169.6(3)
C14-H11A	0.990	O1-N1-C1-C6	8.1(4)
C14-H12B	0.990	O2-N1-C1-C2	9.5(4)
C15-H14B	0.980	O2-N1-C1-C6	-172.9(3)
C15-H15C	0.980	C7-C8-C9-C10	13.7(5)