Exploration of CH•••F & CF•••H Mediated Supramolecular Arrangements into Fluorinated Terphenyls and Theoretical Prediction of Their Third-order Nonlinear Optical Response

Muhammad Adeel,§*,a Muhammad Khalid,§*,b Malik Aman Ullah,a Shabbir Muhammad,c,d Muhammad Usman Khan,e,f Muhammad Nawaz Tahir,g Ilham Khan,a Muhammad Asghar Hashmi,b Khawar Shahzad Mughalb

aInstitute of Chemical Sciences, Gomal University, Dera Ismail Khan, Khyber Pukhtunkhwa, Pakistan
bDepartment of Chemistry, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan-64200, Pakistan
cDepartment of Physics, College of Science, King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia.
dResearch Center for Advanced Material Science (RCAMS), King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia.
eDepartment of Chemistry, University of Okara, Okara-56300, Pakistan
fDepartment of Applied Chemistry, Government College University, Faisalabad-38000, Pakistan
gDepartment of Physics, University of Sargodha, Sargodha, Punjab, Pakistan
hDepartment of Physics, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan-64200, Pakistan

§Both authors contributed equally to this work.

Corresponding authors, E-mail addresses: khalid@iq.usp.br, muhammad.khalid@kfueit.edu.pk (Dr. M. Khalid) & madeel@gu.edu.pk (Dr. M. Adeel).
Figure S1: The $^1$H-NMR spectra for compounds 1.
Figure S2: The $^{13}$C-NMR spectra for compounds 1.
**Figure S3**: The $^1$H-NMR spectra for compounds 2.
Figure S4: The $^{13}$C-NMR spectra for compounds 2.
**Figure S5:** The $^1$H-NMR spectra for compounds 3.
Figure S6: The $^{13}$C-NMR spectra for compounds 3.

Figure S7: The UV spectrum for compound 1.
Figure S8: The UV spectrum for compound 2.

Figure S9: The UV spectrum for compound 3.
Scheme S1: General Suzuki Miyaura mechanism for the synthesis of terphenyl using Pd⁰ catalyst