

Charge Ordering, Symmetry and Electronic Structure Issues and Wigner Crystal Structure of the Quarter-Filled Band Mott Insulators and High Pressure Metals δ -(EDT-TTF-CONMe₂)₂X, X = Br and AsF₆

**Leokadiya Zorina,^{a,b} Sergey Simonov,^{a,b} Cécile Mézière,^a Enric Canadell,^c Steve Suh,^d Stuart E. Brown,^d
Pascale Foury-Leylekian,^e Pierre Fertey,^f Jean-Paul Pouget^e and Patrick Batail^{a,*}**

^a *Laboratoire de Chimie et Ingénierie Moléculaire d'Angers, CNRS-Université d'Angers, 49045 Angers, France. E-mail: patrick.batail@univ-angers.fr*

^b *Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, MD, Russia.*

^c *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de la UAB, E-08193, Bellaterra, Spain.*

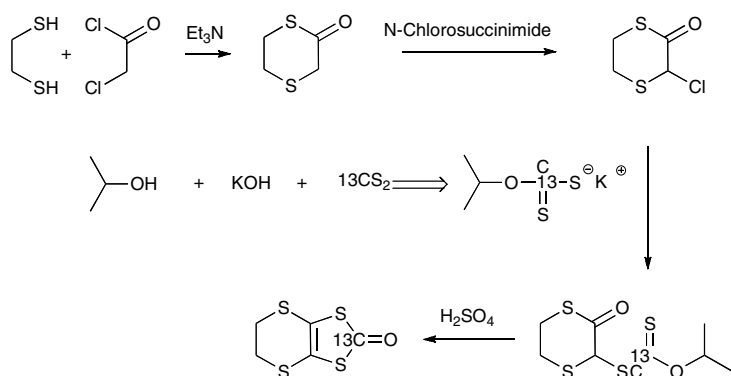
^d *Department of Physics and Astronomy, University of California, Los Angeles, USA.*

^e *Laboratoire de Physique des Solides, CNRS-Université Paris-Sud, 91405 Orsay, France.*

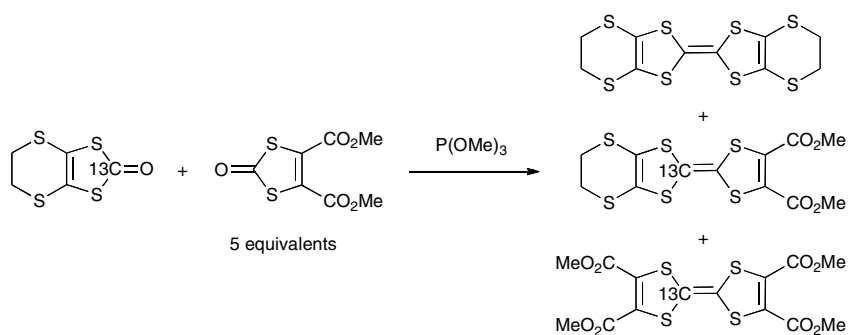
^f *Synchrotron SOLEIL, L'Orme des Merisiers - Saint Aubin, B.P. 48, 91192 Gif-sur-Yvette, France.*

† Electronic Supplementary Information (ESI) available: The Supporting Information includes Schemes S1-S3, Table S1 and the crystallographic information files (CIF). See DOI: 10.1039/b000000x/

Scheme S1. Larsen-Lenoir initial step with $^{13}\text{CS}_2$



Scheme S2. Optimized coupling procedure



Scheme S3. Acylchloride and completion of the procedure

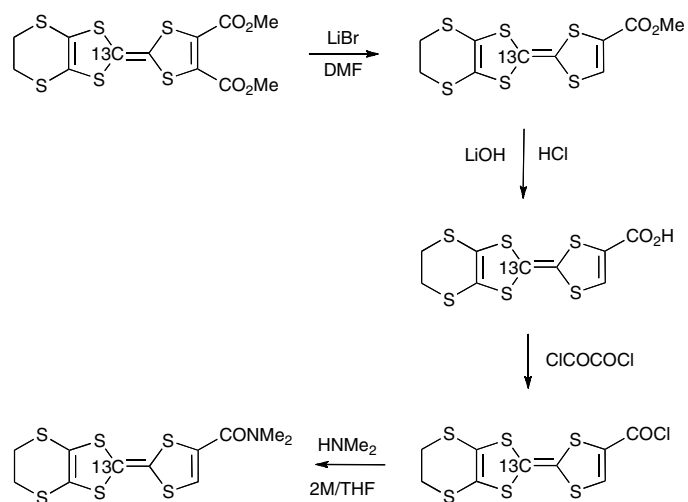


Table S1. Interstack S...S contacts ($r \leq 3.70$ Å) in the conducting layer of δ -(EDT-TTF-CONMe₂)₂Br at room temperature and 150 K

Temperature	Contact distances, Å
150 K	3.2138(7), 3.2724(8), 3.5091(8)
295 K	3.235(1), 3.313(1), 3.519(1)
293 K	3.2317(6), 3.3012(6), 3.5313(6) (interaction C in Fig. 13b)
(double cell)	3.2263(6), 3.3097(6), 3.5174(6) (interaction D in Fig. 13b)