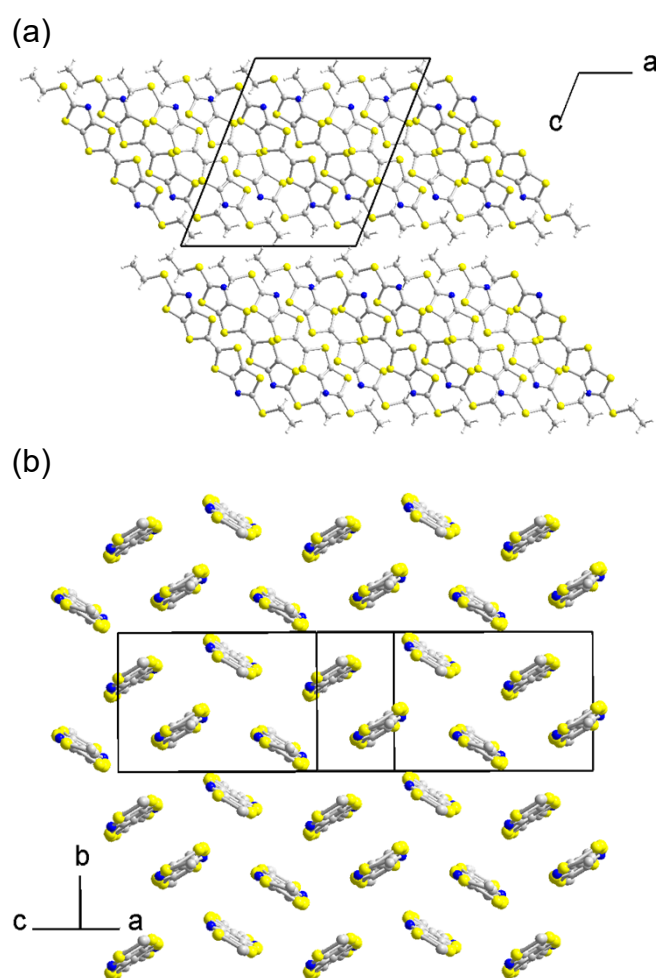


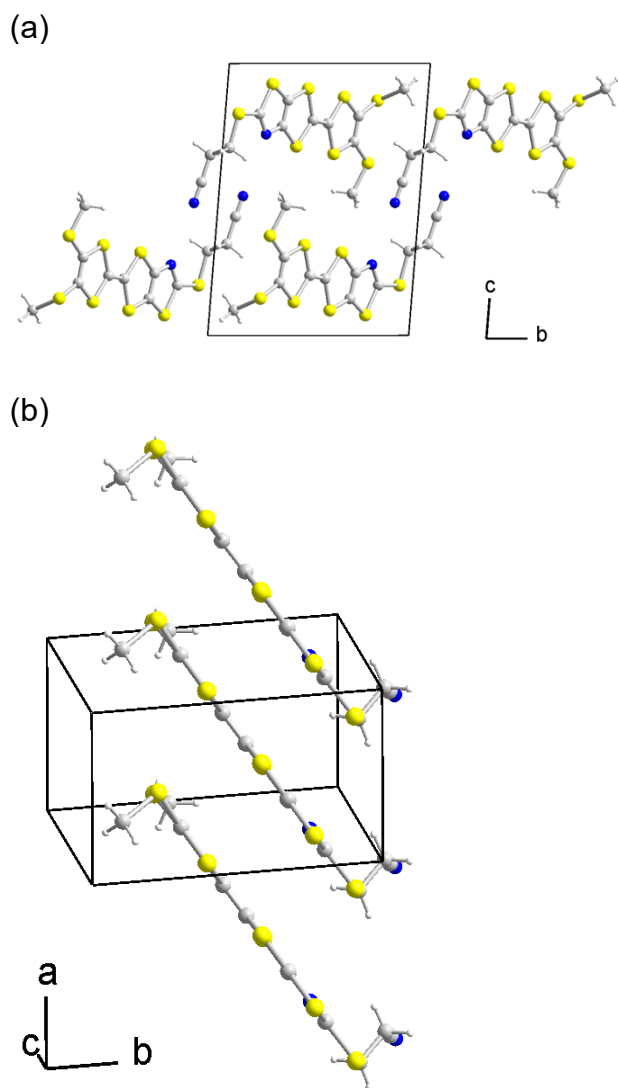
## Non-covalent interactions in neutral and oxidized tetrathiafulvalenes

Haia Kharraz, Hadi Hachem, Yann Le Gal, Thierry Roisnel, Olivier Jeannin, Frédéric Barrière, Thierry Guizouarn, Dominique Lorcy\*

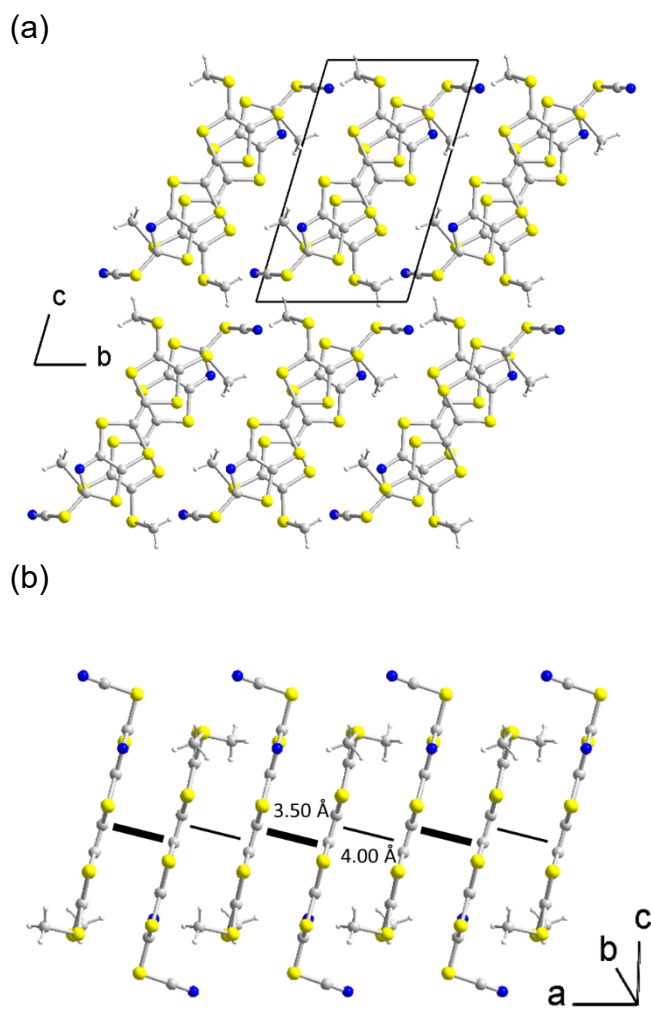
*Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France*



**Fig S1.** Details of the structure of **3d** (Only the major component of the molecule exhibiting a disorder with 89:11 distribution is shown) with, (a) projection view along the *b* axis showing the layered structure, (b) detail of one layer viewed along the long molecular axis, showing the  $\kappa$ -type arrangement (Hydrogen atoms were omitted for clarity).



**Fig. S2** Details of the structure of **4a** with (a) projection view of the unit cell along the  $a$  axis, (b) detail of the uniform stacks.



**Fig S3.** Details of the structure of **4e** (a) a projection view of the structure along the stacking *a* axis showing the layered organization, (b) detail of the strongly dimerized stacks running along the *a* axis.