# **Electronic Supplementary Information for**

# Supramolecular synthons in fluorinated benzyl nitrophenyl sulfides.

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ORTEP plots of sulfides (1) and (2)



Figure S1. ORTEP plot of 4-nitrobenzyl pentafluorophenyl sulfide 1



Figure S2. ORTEP plot of 4-nitrophenyl pentafluorobenzyl sulfide 2

### Summary of main intermolecular interactions in sulfides (1) and (2)

## 4-Nitrobenzyl 2,3,4,5,6-pentafluorophenyl sulfide (1)

#### Hydrogen bondings and similar.

(\*) One nitro oxygen atom with both one *ortho*-hydrogen atom (distance  $O \cdots H_{ortho}$  2.58 Å) and with one methylene hydrogen atom (distance  $O \cdots H$  2.76 Å).

(\*) One nitro oxygen atom with one of the phenyl meta-hydrogen (distance O···H 2.74 Å).

(\*) ortho-Hydrogen atom with one ortho-fluorine (distance F<sub>ortho</sub>····H<sub>ortho</sub> 2.51 Å).

#### **CF**...**FC** short contacts

(\*)  $CF_{ortho} \cdots F_{meta'}C$  (distance 2.82 Å;  $C_{ortho}$ - $F_{ortho}$ - $F_{meta'}$  angle = 150° e  $C_{metai}$ - $F_{meta'}$ - $F_{ortho}$  angle = 151°).

(\*)  $CF_{meta} \cdots F_{para'}$  (distance  $F_{meta} \cdots F_{para}$  2.89 Å;  $C_{para}$ - $F_{para}$ - $F_{meta'}$  angle =168°;  $C_{meta'}$ - $F_{meta'}$ - $F_{para}$  =135°).

# 4-Nitrophenyl pentafluorobenzyl sulfide (2)

#### Hydrogen bondings and similar.

(\*) One nitro oxygen atom with one methylene hydrogen atom (distance O···H 2.54 Å).

(\*) One nitro oxygen atom with one methylene hydrogen atom of a different molecule (distance  $O \cdots H 2.73 \text{ Å}$ ).

(\*) One *ortho*-hydrogen atom with one *meta*-fluorine (distance  $F_{meta}$ ···H<sub>ortho</sub> 2.65 Å).

(\*) One meta-hydrogen atom with one *para*-fluorine (distance  $F_{para}$ ... $H_{meta}$  2.50 Å).

#### $CF\cdots\pi$ short contacts

(\*) One *meta*-fluorine atom with the plane of the pentafluorophenyl group (the distance from the plane is 3.15 Å).

(\*) One *para*-fluorine atom with the plane of the nitrophenyl group (the distance from the plane is 3.18 Å).

CH…F interactions in Sulfides (1) and (2).



Figure S3. CH…F interactions in 4-nitrobenzyl pentafluorophenyl sulfide 1



Figure S4. CH $\cdots$ F interactions in 4-nitrophenyl pentafluorobenzyl sulfide 2



**Crystal Explorer Fingerprint Analysis** 

**Figure S5**. Fingerprint analysis of 4-nitrobenzyl pentafluorophenyl sulfide 1. On the left,  $O \cdots H$  contributions to the surface. On the right,  $F \cdots H$  contributions.



Figure S6. Fingerprint analysis of 4-nitrophenyl pentafluorobenzyl sulfide 2. On the left,  $O \cdots H$  contributions to the surface. On the right,  $F \cdots H$  contributions.



Figure S7.  $F \cdots F$  short contacts in 4-nitrobenzyl pentafluorophenyl sulfide 1