

## Experimental and calculated Raman wavenumbers (in $\text{cm}^{-1}$ ) of OF and CF isomers

| Exptl | Calc | Assignments, <b>OF</b> isomer                                                           |
|-------|------|-----------------------------------------------------------------------------------------|
| 1614  | 1615 | Perfluorocyclopentene: $\nu(\text{C}=\text{C})$                                         |
| 1586  | 1592 | Pyridines: $\delta(\text{CHC}) + \nu(\text{C}=\text{C})$                                |
| 1517  | 1527 | Thiazole: $\nu(\text{C}=\text{N})$ ,<br>Perfluorocyclopentene: $\nu(\text{C}=\text{C})$ |
| 1500  | 1500 | Thiazole: $\nu(\text{C}=\text{C})$ , OEt: $\delta(\text{CH}_2) + \delta(\text{CH}_3)$   |
| 1471  | 1477 | Thiazole: $\nu(\text{C}=\text{C})$ , OEt: $\delta(\text{CH}_2) + \delta(\text{CH}_3)$   |
| 1438  | 1430 | Pyridines : ring vibrations, $\nu(\text{C}=\text{C}) + \nu(\text{C}-\text{C})$          |
| 1293  | 1280 | Perfluorocyclopentene: $\delta(\text{FCF})$                                             |
| 1224  | 1227 | Perfluorocyclopentene Mode                                                              |
| 994   | 980  | Pyridines: $\delta(\text{CCC})$                                                         |

| Exptl | Calc  | Assignments, <b>CF</b> isomer                                                |
|-------|-------|------------------------------------------------------------------------------|
| 1616  | 1615  | $\nu(\text{C}=\text{C}) + \delta(\text{C}=\text{N}-\text{C})$                |
| 1479  | 1488* | Thiazole: $\nu(\text{C}=\text{N}) + \nu(\text{CN}) + \nu(\text{C}=\text{C})$ |
| 1459  | 1476* | Thiazole: $\nu(\text{C}=\text{N}) + \nu(\text{CN}) + \nu(\text{C}=\text{C})$ |
| 1439  | 1428  | $\nu(\text{C}=\text{C})$ Pyridine+ $\nu(\text{C}-\text{C})$                  |
| 1174  | 1167  | $\nu(\text{C}=\text{N}) + \nu(\text{C}-\text{C}) + \nu(\text{C}-\text{F})$   |

$\nu$ : stretching vibration,  $\delta$ : in plane bending vibration

\* These values are related to two different conformers of the CF isomer.