# Enhancing Your Experimental Section of Theses or Reports

#### The NMR data for this compound would normally appear thus —

 $\delta_{\rm H}(400~{\rm MHz};{\rm CDCl_3})~7.12~(2~{\rm H},{\rm td},J~8.0~{\rm and}~^4J_{\rm HF}~5.9,5-{\rm ArH}),~6.88~(2~{\rm H},{\rm tdd},^3J_{\rm HF}~8.6,J~8.6,2.5~{\rm and}~0.8,~4-{\rm ArH}),~6.79-6.73~(4~{\rm H},{\rm m},2~{\rm and}~6-{\rm ArH}),~4.27~(2~{\rm H},{\rm s},{\rm ArC}{\it H})~{\rm and}~3.27~(6~{\rm H},{\rm s},{\rm OMe});~\delta_{\rm C}(100.6~{\rm MHz};{\rm CDCl_3})~163.0^-~(^1J_{\rm HF}~204.6,3-{\rm ArC}),~140.9^-~(1-{\rm ArC}),~129.6^+~(^3J_{\rm HF}~7.8,5-{\rm ArC}),~123.7^+~(6-{\rm ArC}),~114.9^+~(^2J_{\rm HF}~21.2),~114.6^+~(^2J_{\rm HF}~21.9),~86.9^+~({\rm ArCH})~{\rm and}~57.5^+~({\rm Me});~\delta_{\rm F}(235.4~{\rm MHz};{\rm CDCl_3};~^1{\rm H}~{\rm Decoupled})~-113.9.$ 

## Enhanced format includes the FID (free induction decay) filename.

If the FID filename is 'ah1.3406' then the proton appears thus —  $\delta_{\rm H}(400~{\rm MHz};{\rm CDCl_3})\{{\rm ah1.3406}\}\ 7.12\ (2~{\rm H},{\rm td},J~8.0~{\rm and}\ ^4J_{\rm HF}~5.9,5-{\rm ArH}), 6.88\ (2~{\rm H},{\rm tdd},{}^3J_{\rm HF}~8.6,J~8.6,2.5~{\rm and}\ 0.8,4-{\rm ArH}), 6.79-6.73\ (4~{\rm H},{\rm m},2~{\rm and}\ 6-{\rm ArH}), 4.27\ (2~{\rm H},{\rm s},{\rm ArC}H)~{\rm and}\ 3.27\ (6~{\rm H},{\rm s},{\rm OMe}).$ 

The FID file must be available (with the same file name of course) on a floppy or ZIP disk. Make sure you cite the FID that you actually used for the spectral assignment.

#### More

You may include the FT (Fourier Transformed) spectrum as well as, but not instead of, the FID. If the FT filename is 'ah1.5607' then the proton appears thus -

 $\delta_{\rm H}(400~{\rm MHz};{\rm CDCl_3})\{{\rm ah1.3406~l~ah1.5607}\}\ 7.12\ (2~{\rm H,~td},\it J~8.0~{\rm and}\ ^4\it J_{\rm HF}~5.9,~5-{\rm ArH}),~6.88\ (2~{\rm H,~tdd},\ ^3\it J_{\rm HF}~8.6,\it J~8.6,~2.5~{\rm and}~0.8,~4-{\rm ArH}),~6.79-6.73\ (4~{\rm H,~m,~2~and}~6-{\rm ArH}),~4.27\ (2~{\rm H,~s,~ArC}\it H)~{\rm and}~3.27\ (6~{\rm H,~s,~OMe}).$ 

The FT file must be available if it is indicated.

### Your complete NMR data should look something like this —

 $\delta_{\rm H}(400~{\rm MHz};{\rm CDCl_3})\{{\rm ah1.3406~l~ah1.5607}\}\ 7.12\ (2~{\rm H,~td},\it J~8.0~{\rm and}\ ^4\it J_{\rm HF}~5.9,~5-{\rm ArH}),~6.88\ (2~{\rm H,~tdd},\ ^3\it J_{\rm HF}~8.6,\it J~8.6,~2.5~{\rm and}~0.8,~4-{\rm ArH}),~6.79-6.73\ (4~{\rm H,~m,~2~and}~6-{\rm ArH}),~4.27\ (2~{\rm H,~s,~ArC}\it H)~{\rm and}~3.27\ (6~{\rm H,~s,~OMe});~\delta_{\rm C}(100.6~{\rm MHz};{\rm CDCl_3})\{{\rm ah2.7205}\}\ 163.0^-\ (^1\it J_{\rm HF}~204.6,~3-{\rm ArC}),~140.9^-\ (1-{\rm ArC}),~129.6^+\ (^3\it J_{\rm HF}~7.8,~5-{\rm ArC}),~123.7^+\ (6-{\rm ArC}),~114.9^+\ (^2\it J_{\rm HF}~21.2),~114.6^+\ (^2\it J_{\rm HF}~21.9),~86.9^+\ ({\rm Ar}\it CH)~{\rm and}~57.5^+\ (Me);~\delta_{\rm F}(235.4~{\rm MHz};{\rm CDCl_3};~^1{\rm H~Decoupled})\{{\rm ah1.2209}\}\ -113.9.$ 

#### If you are daring...

The filenames can be typed in hidden text so that they can be hidden when experimental is incorporated into papers but printed **in full** in reports. They will print normally but appear like this on the screen —  $\delta_{\rm H}(400~{\rm MHz};{\rm CDCl_3})\{{\rm ah1.3406 \mid ah1.5607}\}$  7.12 (2 H, td, J 8.0 and  ${}^4J_{\rm HF}$  5.9, 5-ArH), 6.88 (2 H, tdd,  ${}^3J_{\rm HF}$  8.6, J 8.6, 2.5 and 0.8, 4-ArH), 6.79-6.73 (4 H, m, 2 and 6-ArH), 4.27 (2 H, s, ArCH) and 3.27 (6 H, s, OMe);  $\delta_{\rm C}(100.6~{\rm MHz};{\rm CDCl_3})\{{\rm ah2.7205}\}$  163.0- ( ${}^1J_{\rm HF}$  204.6, 3-ArC), 140.9- (1-ArC), 129.6+ ( ${}^3J_{\rm HF}$  7.8, 5-ArC), 123.7+ (6-ArC), 114.9+ ( ${}^2J_{\rm HF}$  21.2), 114.6+ ( ${}^2J_{\rm HF}$  21.9), 86.9+ (ArCH) and 57.5+ (Me);  $\delta_{\rm F}(235.4~{\rm MHz};{\rm CDCl_3};{}^1{\rm H}~{\rm Decoupled})\{{\rm ah1.2209}\}$  –113.9. Paul Wyatt August 1999