



## **ASIS Analysis:**

The NMR spectrum in CDCI $_3$  is complicated by the very close chemical shift between the coupled protons H $^3$  and H $^4$  (ca 1 Hz), which leads to strong second order effects in all protons coupled to either one (H $^1$ , H $^2$ , H $^5$  and H $^6$ ). In C $_5$ D $_6$  as solvent there are some quite dramatic shifts, mostly upfield, but some also downfield. The spectrum is now complicated by a close approach of coupled protons H $^4$  and H $^6$  (ca 20 Hz). The effects on H $^3$  and H $^5$  are unusually strong because one is coupled to the H $^4$ /H $^6$  pair with a positive, and the other with a negative J. In such situations the near-degeneracy of energy levels happens when the chemical shifts are further apart than when both J are positive. H $^1$  and H $^2$  are now nearly first order since neither is coupled to the H $^4$ /H $^6$  pair.

$$\begin{array}{c|c} H^1 \\ H^2 \\ \hline O \\ O \\ \hline H^3 \\ H^4 \\ H^5 \\ H^6 \\ \end{array}$$





