Supplementary Material (ESI) for Chemical Communications

Cyclopentathiadiazines, new heterocyclic materials from cyclic enaminonitriles.

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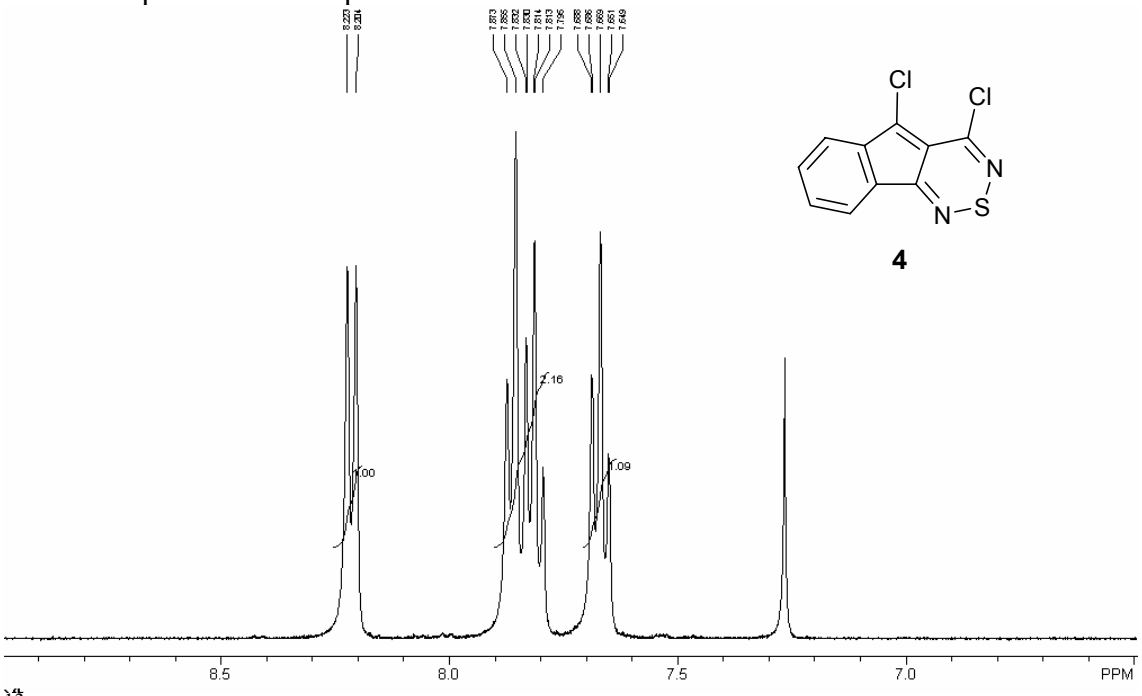
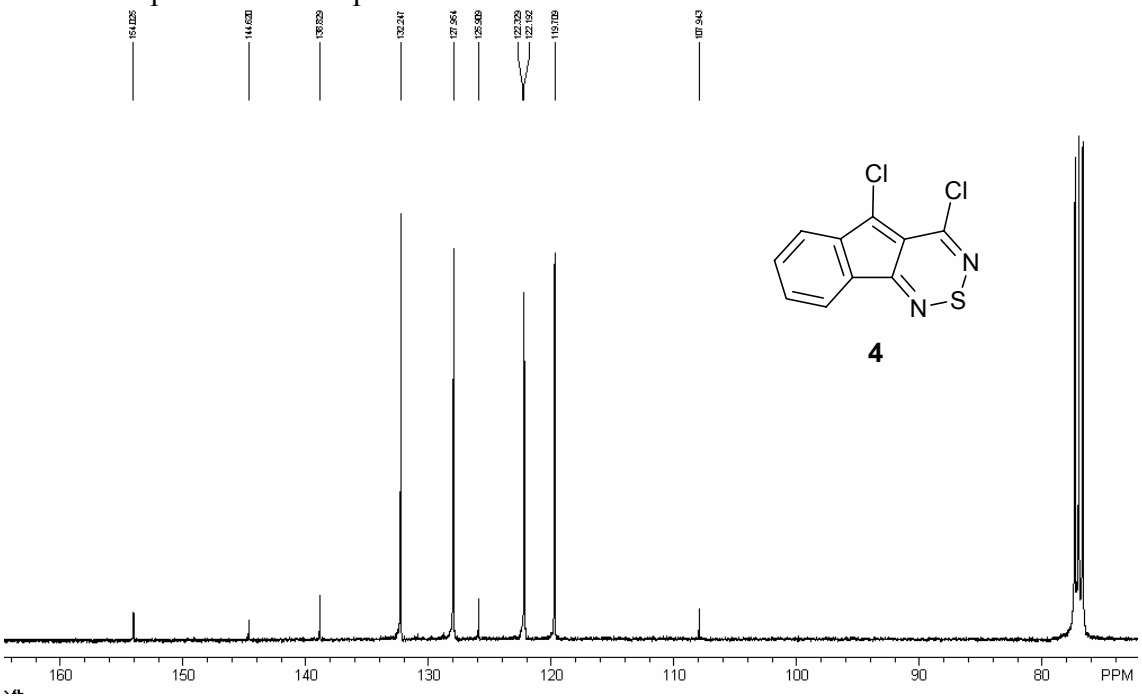
^{1}H- and ^{13}C-NMR spectra of compounds **4** and **6**.

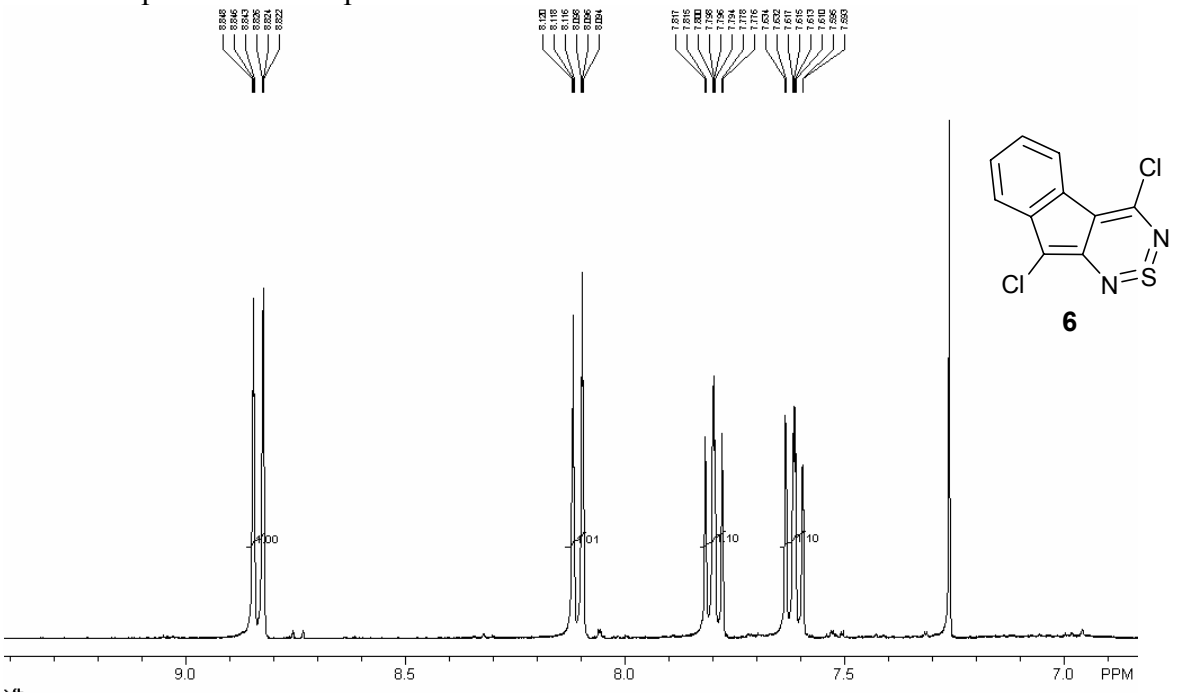
^{1}H-NMR spectrum of compound **4**:



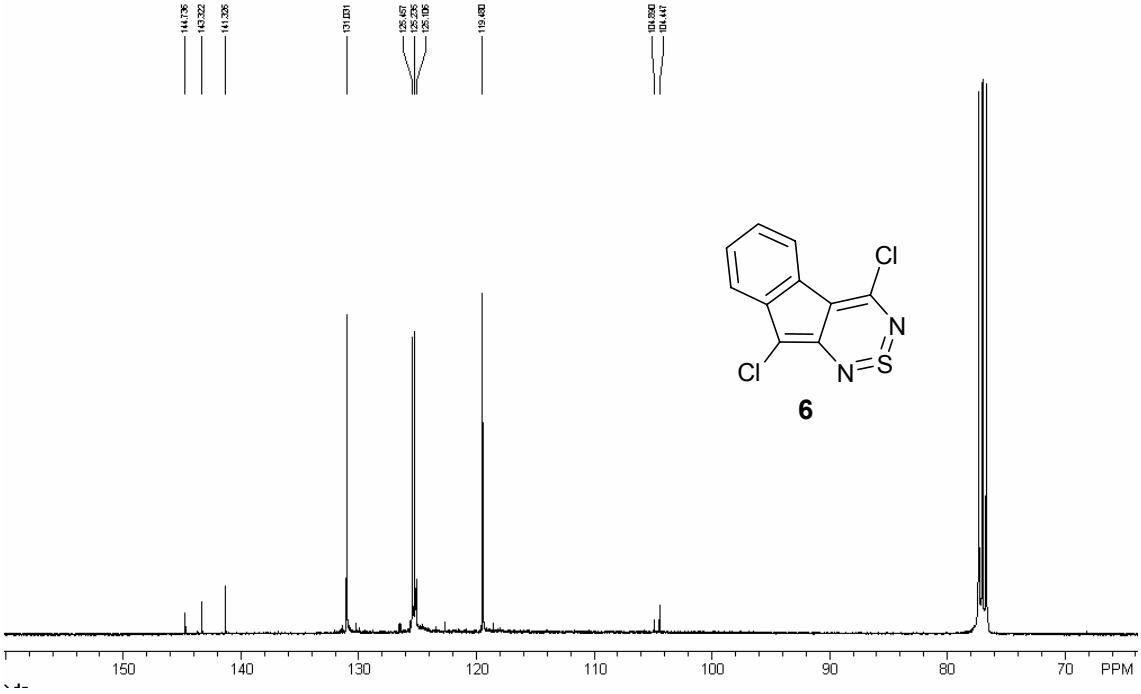
^{13}C-NMR spectrum of compound **4**:



^{1}H-NMR spectrum of compound **6**:



^{13}C-NMR spectrum of compound **6**:



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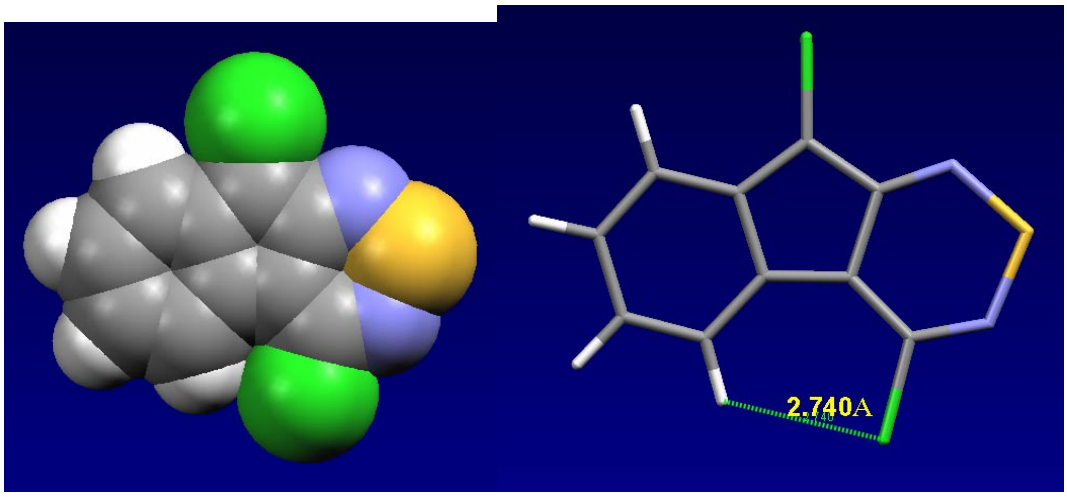
In the ^{1}H-NMR spectrum of compound **6**, one proton appears in a very low field. To explain this behavior we have performed *ab-initio* calculations (Unrestricted Hartree-Fock, 6-31G*) to get insight into the most plausible geometry of structure **6**. The structure found showed that the distance between the chlorine atom in position 8 and the next hydrogen atom in position 7 is 2.740 Å. The van der Waals spheres of both atoms interpenetrate themselves in the spacefill representation of structure **6**. It is therefore expected that the hydrogen atom should appear in the ^{1}H-NMR spectrum at a lower field than the rest of hydrogen atoms in the molecule, in fact this hydrogen signal appears at δ 8.8. This feature constitutes a confirmation of the proposed structure of **6**.



Spacefill and stick representations of the calculated structure of compound **6** showing the closest distance between a chlorine atom and a near hydrogen atom.