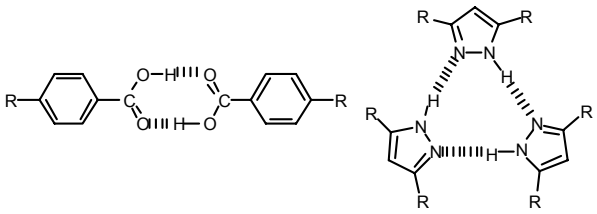
An analysis of the 'Resonance Assisted Hydrogen Bond' (RAHB) concept and its application to pyrazole clusters, José Elguero, *Instituto de Química Médica, CSIC, Juan de la Cierva 3, E-28006 Madrid, Spain*. E-mail: iqmbe17@iqm.csic.es

Keywords: RAHB; Pyrazole; Dynamic Solid-State NMR

The lecture will be divided in three parts. In the first one the curious fact that pyrazoles are one of the two classes of compounds (the other being benzoic acids) that frequently show proton transfer in the solid state (SSPT) will be summarized [1-6]. Special emphasis will be put on the necessary conditions for this phenomenon to be observed which will be discussed in relation with the number of protons transferred in the process.



In the second part, the various reasons why pyrazoles crystallize in six different patterns (catemers, dimers, trimers, tetramers, and hexamers) will be examined in order to find some regularities [7-9]. The connectivity between the centroids of the five-membered rings is a useful way to represent the catemers. Since the RAHB concept (developed for β-diketones [10]) was applied unsuccessfully to pyrazoles [11], in the last part of the lecture this concept will be analyzed theoretically for the paradigmatic case of acetylacetone using NMR (mainly coupling constants but also chemical shifts) as a tool [12].

[1] Baldy, A., Elguero, J., Faure, R., Pierrot, M., Vincent, E.-J. (1985). *J. Am. Chem. Soc*. **107,** 5290-5291.
[2] Smith, J. A. S., Wehrle, B., Aguilar-Parrilla, F., Limbach, H.-H., Foces, C., Cano, F. H., Elguero, J., A. Baldy, Pierrot, M., Khurshid, M. T. J. B. Larcombe (1989). *J. Am. Chem. Soc*. **111**, 7304-7312.
[3] Aguilar-Parrilla, F., Scherer, G. Limbach, H.-H., Foces-Foces, C., Cano, F. H., Elguero J. (1992). *J. Am. Chem. Soc*. **114**, 9657-9659.
[4] Foces-Foces, C.; Echevarría, A,; Jagerovic, N.; Alkorta, I.; Elguero, J.; Langer, U.; Klein, O.; Minguet-Bonvehí, M., Limbach,H.-H. (2001). *J. Am. Chem. Soc.* **123**, 7896-7906.
[5] de Paz, J. L. G. Elguero,J. Foces-Foces, C. Llamas-Saiz, A. L. Aguilar- Parrilla, F. O. Klein, H.-H. Limbach (1997). *J. Chem. Soc., Perkin Trans* 101-109.
[6] Limbach, H.-H., Klein, O., López del Amo, J., M. Elguero J. (2004) *Z. Phys. Chem*. **218**, 19-49.
[7] Fernández-Castaño, C., Foces-Foces, C., Jagerovic, N., J. Elguero, J. (1995). *J. Mol. Struct*., **355**, 265-271
[8] Infantes, L., Foces-Foces, J. Elguero, J. *Acta Crystallogr., Ser. B*, **55**, 411-447.
[9] Foces-Foces, C., Alkorta, I., Elguero, J. *Acta Crystallogr*., *Ser. B* (2000). **B56**, 1018-1028.
[10] Gilli, G.; Bellucci, F.; Ferretti, V.; Bertolasi, V. (1989). *J. Am. Chem. Soc*. **111**, 1023-1028.
[11] Bertolasi, V.; Gilli, P.; Ferretti, V.; Gilli, G.; Fernández-Castaño, C. (1999). *Acta Crystallogr., Sect. B*, **B55**, 985-993.
[12] Alkorta, I., Elguero, J., Mó, O., Yáñez, M., Del Bene, J. E. paper in preparation.