Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting information

Self-decarboxylation of trichloroacetic acid redox catalyzed by trichloroacetate ions in acetonitrile solutions

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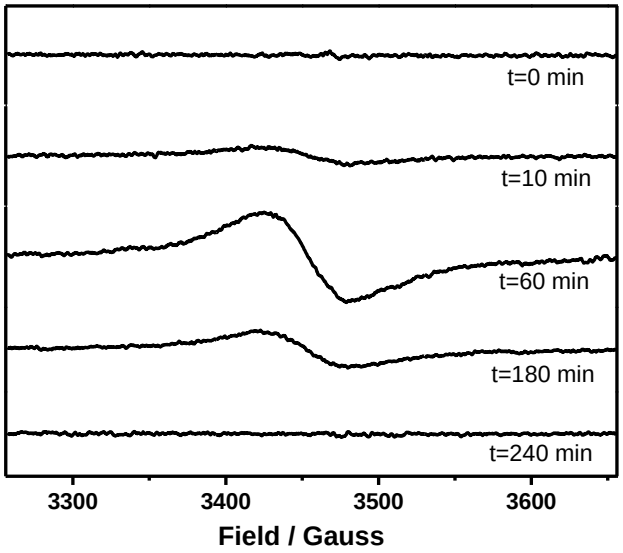

Fig. S1. Evolution with the time of the ESR spectra of a solution containing Cl_3CCOOH 30 mM + Cl_3CCOO^- 30 mM in acetonitrile. The spectra were registered in the X band (9.85 GHz), modulation amplitude 5 G, modulation frecuency 100 kHz, time constant 5.120 ms, conversion time 10 ms, averaging over 20 scan, g=2.0023, at room temperature (about 25 ^oC)

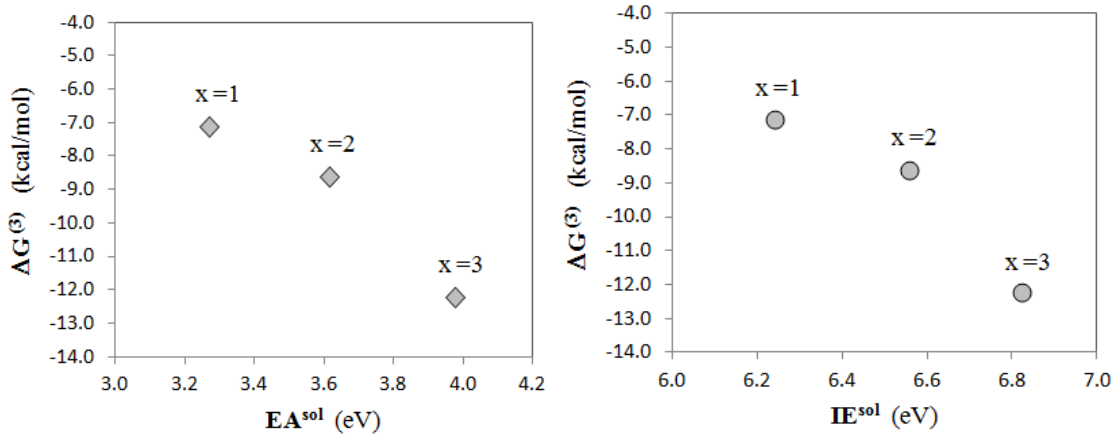

Fig. S2. Relationship of the ΔG of the self-decarboxylation processes with the electron affinity of the acid, and with the ionization energy of the acetate.

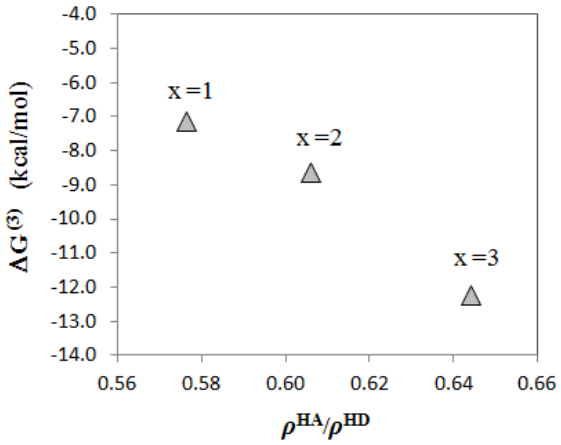

Fig. S3. Relationship of the ΔG of the self-decarboxylation processes with the relative strength of the BCP points found in the complex.