Magnetic molecules are candidates for solid-state spin qubits from which quantum devices can in principle be constructed, and indeed compared with other candidates they present potential advantages in terms of tunability and scalability. One major obstacle towards this aspiration is the uncontrolled magnetic interactions of such molecules, either with each other or with other sources of magnetic noise in the environment. This typically lead to the loss of quantum information, also known as decoherence, and it needs to be avoided if we want to advance towards quantum technologies. Decoherence can be minimized if the magnetic molecules are well separated from each other and from other environmental spins, yet it can be argued that this limits the ability of the qubits to process quantum information together. Moreover, the implementation of practical devices is challenging, as it is, so the more we can ease the requirements, the better.

Some of us recently demonstrated a way out of this dilemma: we found that certain polyoxometalate [HoW10O42]n- presents an electronic structure which energetically protects their spin dynamics against the decoherence-inducing interactions that normally plague such systems. This polyoxometalates can then be packed at unusually high concentrations while retaining desirable long coherence times, a step towards useful devices in which a large number of qubits can exist in close proximity. The effect exploited is termed Atomic Clock Transitions (ACTs), and consists in systems where the first derivative of the transition frequency versus the magnetic field vanishes, thus minimizing the effect of small magnetic noise (see Figure 1).

Since this seminal contribution, a number of other works have employed the same kind of transitions. [Freedman] [others?] [other, previous uses of molecular ACTs??] Indeed, ACTs appear for every avoided crossing, which is to say in magnetic molecules presenting extradiagonal elements in their spin Hamiltonians, whether these arise from the crystal field or from the hyperfine coupling. If the form of the spin Hamiltonian is known, the magnetic field of the ACTs is a trivial question, and so is their energy: both can be expressed in terms of the crystal field parameters and/or the hyperfine coupling. The non-trivial problem is the detailed form of the ACT. Whereas a vanishing first derivative is what defines an ACT, the best behavior will be obtained if the second derivative is as small as possible. In other words, it would be useful to obtain a recipe for designing magnetic molecules with ACTs that are as shallow as possible.

In this work we search for the parameter region where the most shallow ACTs are found, that is, where a qubit can be best protected.  In particular we will aim to minimize the energy difference Delta\_E0.01=|E\_ACT-E\_0.01| where E\_ACT is the energy of the transition happening at the ACT field B\_ACT and E\_0.01 is the energy of the transition at a slightly larger field B\_0.01=B\_ACT\*1.01 (see Figure 1). We work this in three phases. First we focus on the crystal field, and study, analytically, the advantages and disadvantages of ACTs arising from anticrossings of different kinds of Mj doublets. Next, we move on to hyperfine crossings and study the dependence of ACT shallowness with the ratio between parallel and perpendicular hf coupling. Again, this can also be done analytically.  Finally, we study off-anticrossing ACTs, which can occur when a third magnetic level is near an anticrossing, and demonstrate that these are in principle advantageous to regular ACTs.