MS32-2-1 Octahedral distortion through the CSD to reveal structure-properties relationship in spin crossover complexes
#MS32-2-1

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Abstract
Spin crossover (SCO) compounds are molecules, mainly based on transition metal complexes in an octahedral geometry, that can adopt two electronic states depending of their surrounding environment. SCO compounds can thus switch from a Low Spin (LS) state to a High Spin (HS) state upon an external stimulus like temperature pressure, light, or many others, what lead to a great interest from the scientific community due to their potential applications as captors, actuators, memories, smart pigments and many others. One of the key point, nevertheless, is to synthesize the right complex with optimal and controlled properties. From this point of view, the very high versatility of molecular materials is an evident advantage to obtain several complexes with very different switching properties such as large range of transition temperatures, smooth to very abrupt transitions or the apparition of large hysteresis loops… This high versatility can however turn into a drawback to properly identify the key structural parameters that will guide the chemist to design the right material with the expected properties as the implied structural parameters are numerous and subtle.
For decades, researchers of the SCO community have explored the structure-properties relationships of several families of SCO compounds, and some trends are now well established[1]. The role of octahedral distortion, for example, has been identified as a key parameter to obtain long lifetimes in photo-induced systems and is also linked to the thermal transition temperature[2]. Several distortion parameters have then been proposed: from the simplest analysis of metal to ligand bond lengths (d_{M-L}) to more sophisticated ones such as Θ, that measures the trigonal distortion of an octahedral geometry and require more complicated calculations. In order to make the evaluation of the octahedral geometry distortion accessible to a large scale of exploration, it appeared mandatory to unify its calculation as it was not straightforward. Also, we recently proposed a new program called OctaDist (Octahedral Distortion calculator) leading to an universally agreed method that allows to make comparisons across the increasingly diverse structural SCO databases[3]. This program has been then used to explore the huge CSD database to extract a clear chemical meaning related to the distortion parameters using, in our example, more than 6000 iron complexes (figure 1).
This new approach clearly opens the way to use such a program, conjointly with Artificial Intelligence (AI), to go beyond the limited number of complexes generally used within the different families to find structure-properties relationships. It should lead to new wider correlations combining, for example, several parameters or even new totally not envisaged ones, by deep learning methods.

References
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Mean Fe-N distance vs Θ for 6546 Fe complexes