Insights into the formation of chiral second sphere coordination complexes with aromatic tris amines: combined single crystal X-ray crystallography and molecular modeling analyses

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Control over the formation of non-centrosymmetric chiral materials is highly desirable due to their potential applications in areas such as ferroelectricity, piezo- and pyroelectricity, and second harmonic generation.[1] Unfortunately, the development of a reliable approach to induce the formation of a chiral material from achiral molecules remains a great challenge in the field of molecular chemistry.[2] Furthermore, the understanding of the driving forces behind those aggregations is a prerequisite for the design and construction of chiral molecular arrays. C3-symmetrical tripodal molecules have emerged as attractive organic frameworks for the construction of chiral coordination compounds.[3] In the present contribution we report about a family of isostructural, chiral supramolecular networks obtained in the solid state by exploiting second sphere coordination interactions in the self-assembly of achiral tris amines L1 and L2 with tetrahalometallate and halide ions. Quantum-Mechanical calculations (including the usage of approaches specific for crystalline solid phases) provided important insights into the intramolecular and packing interactions which determine chirality, pointing to a direct effect of the methyl groups of the central benzene ring of the tris amines. [4]

References

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