Chirale Erkennung bei Tris(diimin)-Metallkomplexen, 10 [1]. Vergleich der intermolekularen Wechselwirkungs- und Packungsmuster in der Reihe $[Cr(bpy)_3]^{n+}(PF_6)_n$ ($n = 0-3$)

Chiral Recognition among Tris(diimine)-metal Complexes, 10 [1]. Comparison of Intermolecular Interactions and Packing Patterns in the Series $[Cr(bpy)_3]^{n+}(PF_6)_n$ (n = 0 – 3)

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Due to their conformational rigidity, the corrugated, chiral molecular structure, and the variability in the central metal and its oxidation state, $[M(bpy)_3]^{n+}$ complexes are particularly well suited to study chiral recognition and to identify intermolecular interaction patterns in the crystalline state. For $[Cr(bpy)_3]^{n+}(PF_6)_n$ ($n = 0-3$) four oxidation states are readily accessible which allows to investigate the influence of the cation/anion ratio on the observed packing patterns.

The crystal structures of all four oxidation states are governed by so-called 'π–π-interactions'. Apparently, in molecular salts the Madelung energy is less important as compared to classical inorganic salts.

Interestingly, $[Cr(bpy)_3](PF_6)$ and $[Cr(bpy)_3](PF_6)_2$ comprise the same homochiral layers. However, while the former crystallises as true racemate, the latter spontaneously resolves into a conglomerate. This two-dimensional building block of homochiral layers is the most popular structural motif in this class of compounds which has been observed in a great variety of racemic and homochiral stackings.

Key words: Chiral Recognition, Conglomerate Crystallisation, Molecular Recognition, Polymorphism